

# A stochastic method for solving Smoluchowski's coagulation equation

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\*Research partially supported by grant INTAS-RFBR No. 95-IN-RU-726.  
This article was partially written while the first two authors were visiting the WIAS in Berlin

**Abstract.** – This paper studies a stochastic particle method for the numerical treatment of Smoluchowski equation governing the coagulation of particles in a host gas. Convergence in probability is established for the Monte Carlo estimators, when the number of particles tends to infinity. The deterministic limit is characterized as the solution of a discrete in time version of the Smoluchowski equation. Under some restrictions it is shown that this stochastic finite difference scheme is convergent to the solution of the original Smoluchowski equation. Extensions on a nonhomogeneous Smoluchowski equation are given, and in particular, a coagulation process in an isotropic fully developed turbulent flow is studied.

## 1 Introduction

The coagulation processes of aerosol particles or clusters in a spatially homogeneous flow are governed by the Smoluchowski equation (e.g., see, [22], [23]):

$$\frac{\partial n_l}{\partial t} = \frac{1}{2} \sum_{i+j=l} K_{ij} n_i n_j - n_l \sum_{i=1}^{\infty} K_{li} n_i + F_l(t) \quad (1.1)$$

with the initial conditions  $n_l(0) = n_l^{(0)}$ ,  $l = 1, 2, \dots$ .

We use the notation:  $\{l\}$ -cluster, for a cluster containing  $l$  monomers (or structural units);  $n_i$ , for the number density of the  $\{i\}$ -cluster;  $K_{ij}$ , for the coagulation coefficient characterizing the collision frequencies between an  $\{i\}$ - and a  $\{j\}$ -clusters; and  $F_l(t)$ , for the intensity of the source of  $\{l\}$ -clusters. We will use also the symbol  $\delta(t)$  for the Dirac delta-function, and  $\delta_{i,j}$  for the Kronecker's function.

Under rather general assumptions about the coagulation coefficients  $K_{ij}$  there are known the existence and uniqueness results for the solution to the equation (1.1) (e.g., see [2]).

The structure of  $K_{ij}$  for different collision regimes is presented, e.g., in [25], [19]. In the case of isotropic turbulent mixing of the host gas, which is the situation we are interested in, the coefficients  $K_{ij}$  were derived in [21]

$$K_{ij} = \left( \frac{\pi^2 \bar{\varepsilon}}{120\nu} \right)^{1/2} V_1 (i^{1/3} + j^{1/3})^3, \quad (1.2)$$

where  $\bar{\varepsilon}$  is the mean rate of dissipation of kinetic energy per unit mass,  $\nu$  is the kinematic viscosity of the fluid, and  $V_1$  is the volume of the monomer. This seems to describe satisfactorily the evolution of the size spectrum of particles mixed by a fully developed turbulence without taking into account the intermittency. A strong assumption however was made by the authors [21] that the colliding particles do not much differ in their sizes.

In the intermittent turbulence,  $\varepsilon$  is considered as a random process with lognormal distribution [4]. Thus mathematically, we have the Smoluchowski equation whose coefficients are random processes. As concerning the deterministic numerical methods for solving the deterministic Smoluchowski equation, see, e.g., [11], [8].

Generally, even linear PDE's with stochastic coefficients are very difficult to be solved by conventional numerical methods. To evaluate statistical characteristics of solutions of this kind of random equations by Monte Carlo methods, the double randomization method is an efficient technique (e.g., see [17]). In nonlinear case the situation is more complicated. However it is also possible to develop the double randomization technique (see [18]).

It should be noted that stochastic models of the coagulation process were considered first by physicists (e.g., see [3], [5], [12], [13]). In [16], [17] we suggested a series of stochastic algorithms for solving the Smoluchowski equation and gave in [19] a convergence justification under the *molecular chaos hypothesis*. In [7] the authors gave the convergence proof of the Nanbu type algorithm without the *molecular chaos hypothesis*; namely it was shown that the Nanbu type algorithm converges in probability to the solution of a finite difference analog of the Smoluchowski equation.

Note that the stochastic algorithm we present is analogous to Nanbu's method for the Boltzmann equation [15]. The relevant convergence justifications in the case of Boltzmann equation are given in [24] and [1].

In this paper we extend the Nanbu type algorithm for solving the homogeneous Smoluchowski equation presented in [7] and [18] to the inhomogeneous case, and of our special interest is the case when  $v(t, x)$ , the velocity of the host gas, is a random field taken in the form of a randomized spectral representation of the stationary isotropic high-Reynolds number velocity field with the Kolmogorov energy spectrum [17], [10].

The Smoluchowski equation in the inhomogeneous case governing the coagulation of particles dispersed by this velocity field  $v(t, x)$  reads

$$\frac{\partial n_l(t, x)}{\partial t} + v(t, x) \cdot \nabla_x n_l(t, x) = \frac{1}{2} \sum_{i+j=l} K_{ij} n_i n_j - n_l \sum_{i=1}^{\infty} K_{il} n_i + F_l(t, x), \quad (1.3)$$

with the initial conditions  $n_l(0, x) = n_l^{(0)}(x)$ ,  $l = 1, 2, \dots$ . Here  $n_l$  is the concentration of particles of size  $l$ ,  $l = 1, 2, \dots$  at a point  $x$  at time  $t$ ;  $v$  is the velocity of the host gas,  $K_{ij}$  is the coagulation coefficient,  $F_l(t)$  is the intensity of  $l$ -cluster generation source.

## 2 The spatially homogeneous case

### 2.1 Description of the algorithm

Here we describe the stochastic algorithm for the spatially homogeneous Smoluchowski equation

$$\frac{\partial}{\partial t} n_l(t) = \frac{1}{2} \sum_{i+j=l} K_{ij} n_i(t) n_j(t) - n_l(t) \sum_{i=1}^{\infty} K_{il} n_i(t), \quad l = 1, 2, \dots, \quad (2.1)$$

with the initial condition

$$n_l(0) = n_l^{(0)}, \quad l = 1, 2, \dots. \quad (2.2)$$

Concerning the **initial value**, we assume that

$$n_l^{(0)} \geq 0, \quad l = 1, 2, \dots, \quad (2.3)$$

$$n_l^{(0)} = 0, \quad l > L_0, \quad (2.4)$$

and

$$\max_l n_l^{(0)} > 0. \quad (2.5)$$

Concerning the **coagulation kernel**  $K$ , we assume that

$$\inf_{i,j \geq 1} K_{ij} > 0 \quad (2.6)$$

and

$$K_{ij} = K_{ji}, \quad i, j = 1, 2, \dots \quad (2.7)$$

Let us consider a stochastic particle system, where each particle is characterized by its size  $l = 1, 2, \dots$ . The **state of the system** is determined by the sequence

$$N_1(t), N_2(t), \dots, \quad (2.8)$$

where  $N_l(t)$  is the number of particles of size  $l$  at time  $t \geq 0$ . The system depends on a parameter  $N = 1, 2, \dots$ , and its state is defined at discrete moments

$$t_k^{(N)}, \quad k = 0, 1, \dots, \quad t_0^{(N)} = 0,$$

according to the rules following below. Between these points the system does not change.

**Initial state:** At time zero the system consists of  $N$  particles approximating the initial value in condition (2.2). More precisely, let

$$N = \sum_{l \geq 1} N_l(0) \quad (2.9)$$

and

$$\frac{N_l(0)}{c_0^{(N)}} \rightarrow n_l^{(0)} \quad \text{in probability as } N \rightarrow \infty, \quad l = 1, 2, \dots, \quad (2.10)$$

for some appropriate **normalizing sequence**  $c_0^{(N)}$ . In correspondence with (2.4), we assume that

$$N_l(0) = 0, \quad l > L_0. \quad (2.11)$$

**Time evolution:** Given the state of the system (2.8) at time  $t_k^{(N)}$ , for some  $k = 0, 1, \dots$ , and a normalizing sequence  $c_k^{(N)}$ , the state at time  $t_{k+1}^{(N)}$  is constructed in several steps.

1. Choose the **time increment**

$$\Delta_k^{(N)} = \frac{\alpha}{\max_{1 \leq i \leq 2^k L_0} \left\{ \sum_{j \geq 1} \frac{N_j(t_k^{(N)})}{c_k^{(N)}} K_{ij} \right\}}, \quad (2.12)$$

where

$$0 < \alpha \leq 1 \quad (2.13)$$

is a **discretization parameter**, and define

$$t_{k+1}^{(N)} = t_k^{(N)} + \Delta_k^{(N)}. \quad (2.14)$$

2. Denote

$$N'_1 = N'_1(t_{k+1}^{(N)}) := N_1(t_k^{(N)}), \quad N'_2 = N'_2(t_{k+1}^{(N)}) := N_2(t_k^{(N)}), \quad \dots \quad (2.15)$$

3. For each particle of size  $l$ , where  $l = 1, 2, \dots$ , examine with the **reaction probability**

$$P_l^{(N)} := \frac{1}{2} \Delta_k^{(N)} \sum_{j \geq 1} \frac{N_j(t_k^{(N)})}{c_k^{(N)}} K_{lj}, \quad (2.16)$$

whether it interacts with any other particle.

3.1 If yes, then find the random size  $m$  of the reaction partner according to the **size distribution**

$$p_{l,m}^{(N)} := \frac{N_m(t_k^{(N)}) K_{lm}}{\sum_{j \geq 1} N_j(t_k^{(N)}) K_{lj}}, \quad m = 1, 2, \dots, \quad (2.17)$$

and change

$$N'_l := N'_l - 1, \quad N'_m := N'_m - 1, \quad N'_{l+m} := N'_{l+m} + 1. \quad (2.18)$$

Note that the probabilities (2.16), (2.17) are the same for all particles of the same size.

3.2 If no, then do not change anything.

4. To keep all components non-negative **truncate** the system if necessary, i.e., we define

$$\tilde{N}_l(t_{k+1}^{(N)}) := \max(0, N'_l(t_{k+1}^{(N)})), \quad l = 1, 2, \dots \quad (2.19)$$

5. Check whether the number of particles satisfies

$$\sum_{l \geq 1} \tilde{N}_l(t_{k+1}^{(N)}) \leq \frac{N}{2}. \quad (2.20)$$

5.1 If yes, then **double** the system, i.e., we define

$$N_l(t_{k+1}^{(N)}) := 2 \tilde{N}_l(t_{k+1}^{(N)}), \quad c_{k+1}^{(N)} := 2 c_k^{(N)}. \quad (2.21)$$

5.2 If no, then do not change anything, i.e., define

$$N_l(t_{k+1}^{(N)}) := \tilde{N}_l(t_{k+1}^{(N)}), \quad c_{k+1}^{(N)} := c_k^{(N)}. \quad (2.22)$$

An appropriate choice of the initial normalizing sequence is

$$c_0^{(N)} = \frac{N}{\sum_{l \geq 1} n_l^{(0)}} \quad (2.23)$$

thus depending on the normalization of (2.1)-(2.2). In the case  $\sum_{l \geq 1} n_l^{(0)} = 1$  one simply obtains

$$c_0^{(N)} = N. \quad (2.24)$$

The other normalizing sequences satisfy  $c_k^{(N)} = 2^{\beta_k^{(N)}} c_0^{(N)}$ , where  $\beta_k^{(N)}$  is the (random) number of those time steps up to  $t_k^{(N)}$  at which the doubling procedure (2.21) took place. Thus, one obtains

$$c_0^{(N)} \leq c_k^{(N)} \leq 2^k c_0^{(N)}, \quad k = 0, 1, \dots \quad (2.25)$$

During one time step, the largest non-zero component of the sequence  $(N_l)$  may increase at most by a factor 2 (cf. (2.18)). Thus, according to (2.11), one obtains

$$N_l(t_k^{(N)}) = 0, \quad l > 2^k L_0, \quad k = 0, 1, \dots \quad (2.26)$$

Consequently, the infinite sums in (2.12), (2.16) and (2.17) are actually finite.

## 2.2 Convergence results

We consider a **discrete approximation** to Eq. (2.1), namely

$$\hat{n}_l(t_{k+1}) = \hat{n}_l(t_k) + \Delta_k \left( \frac{1}{2} \sum_{i+j=l} K_{ij} \hat{n}_i(t_k) \hat{n}_j(t_k) - \hat{n}_l(t_k) \sum_{i \geq 1} K_{il} \hat{n}_i(t_k) \right), \quad (2.27)$$

$$l = 1, 2, \dots, \quad k = 0, 1, \dots,$$

with the initial condition

$$\hat{n}_l(0) = n_l^{(0)}, \quad l = 1, 2, \dots \quad (2.28)$$

The time steps are defined as

$$\Delta_k = \frac{\alpha}{\max_{1 \leq i \leq 2^k L_0} \left\{ \sum_{j \geq 1} \hat{n}_j(t_k) K_{ij} \right\}}, \quad (2.29)$$

where  $\alpha$  is the parameter from (2.12), (2.13), and

$$t_{k+1} = t_k + \Delta_k, \quad k = 0, 1, \dots, \quad t_0 = 0. \quad (2.30)$$

The following result is proved in [7].

**Theorem 2.1.** *Let the assumptions (2.9)-(2.11) be fulfilled. Then*

$$\frac{N_l(t_k^{(N)})}{c_k^{(N)}} \rightarrow \hat{n}_l(t_k) \text{ in probability as } N \rightarrow \infty, \quad l = 1, 2, \dots; k = 0, 1, \dots, \quad (2.31)$$

where  $\hat{n}_l$  is the solution of (2.27) and  $N_l(t_k^{(N)})$ ,  $c_k^{(N)}$  were defined previously.

It is convenient to work with the normalized equation

$$\frac{\partial}{\partial t} f_l(t) = \frac{1}{2} \sum_{i+j=l} k_{ij} f_i(t) f_j(t) - f_l(t) \sum_{i=1}^{\infty} k_{il} f_i(t), \quad l = 1, 2, \dots, \quad (2.32)$$

with initial conditions  $f_l(0) = n_l^{(0)}/n$ , and  $k_{ij} = K_{ij}/K_{11}$ . Then the obvious relation is true:

$$n_l(t) = n f_l(n K_{11} t), \quad \text{where } n = \sum_{i=1}^{\infty} n_i^{(0)}. \quad (2.33)$$

Let us denote by  $\hat{f}_l(t_k)$  the finite difference approximation to  $f_l(t)$  constructed according to (2.27). The following convergence result and estimations are given in [18]:

**Theorem 2.2.** *Assume that there exists a solution  $f_l(t)$ ,  $l = 1, \dots$  to (2.32) with initial conditions  $n_1^{(0)} = n$ ,  $n_l^{(0)} = 0$  for  $l \geq 2$ , continuous on the interval  $[0, T]$ , and there exist  $K_{\max}$ , such that  $K_{\max} = \max_{ij} k_{ij}$  and  $K_{\min}$ , such that  $0 < K_{\min} = \min_{ij} k_{ij}$ .*

For each  $\alpha \in (0, 1)$  and  $k \geq 0$

$$1. \quad \alpha D_1 \leq \Delta(t_k) \leq \alpha D_2; \quad D_1 = \frac{1}{K_{\max}}, \quad D_2 = \frac{e^{TK_{\max}/2}}{K_{\min}}. \quad (2.34)$$

$$2. \quad \max_l |f_l(t_k) - \hat{f}_l(t_k)| \leq C_1 \alpha, \quad C_1 = e^{TK_{\max} h_2} \left( h_1 + \frac{h_3}{h_2} \right), \quad (2.35)$$

where

$$h_1 = \frac{9}{4} K_{\max}^2 D_2^2; \quad h_2 = 2K_{\max} D_2;$$

$$h_3 = \frac{9}{4} K_{\max}^2 D_2^2 e^{TK_{\max} D_2} (K_{\max} D_2 + 1) + \frac{9}{4} K_{\max}^2 D_2^2.$$

$$3. \quad \sum_{l=2^{k+1}+1}^{\infty} |f_l(t_k) - \hat{f}_l(t_k)| \leq C_2 \alpha^2; \quad C_2 = e^{TK_{\max} h_2} \left( h_1 + \frac{h_3}{h_2} \right); \quad (2.36)$$

where

$$h_1 = \frac{3}{4} K_{\max}^2 D_2^2 + \frac{27}{8} K_{\max}^3 D_2^3; \quad h_2 = \frac{5}{2} K_{\max} D_2 + \frac{7}{2} K_{\max}^2 D_2^2;$$

$$h_3 = \frac{3}{4} K_{\max}^2 D_2^2 F + \frac{27}{24} K_{\max}^3 D_2^3; \quad F = C_1 + \frac{3}{2} K_{\max} + \frac{9}{4} K_{\max}^2 D_2^2,$$

Note that these results can be generalized to the case when the Smoluchowski equation (1.1) has a constant source:  $F_l(t) = \text{const}$ ; the main idea is described in [18].

### 3 Nonhomogeneous case

Let us rewrite the equation (1.3) in the vector form and introduce the superscript  $E$  to indicate that we are in an Eulerian coordinate system:

$$\frac{\partial n^E(t, x)}{\partial t} + v(t, x) \cdot \nabla_x n^E(t, x) = K(n^E(t, x)) + F(t, x); \quad (3.1)$$

$$n^E(0, x) = n^{(0)}(x); \quad x \in R^3; \quad t \in [0, T].$$

Here

$$n^E(t, x) = \{n_i^E(t, x)\}_{i=1}^{\infty}; \quad n^{(0)}(x) = \{n_i^{(0)}(x)\}_{i=1}^{\infty}; \quad F(t, x) = \{F_i(t, x)\}_{i=1}^{\infty};$$

$$K(n^E(t, x)) = \left\{ \frac{1}{2} \sum_{i+j=l} K_{ij} n_i^E(t, x) n_j^E(t, x) - n_l^E(t, x) \sum_{i=1}^{\infty} K_{il} n_i^E(t, x) \right\}_{l=1}^{\infty}.$$

We denote by  $X(t, x_0)$  the Lagrangian trajectory defined as the solution to the Cauchy problem:

$$\frac{\partial X(t, x_0)}{\partial t} = v(t, X(t, x_0)), \quad t \in [0, T]; \quad X(0, x_0) = x_0. \quad (3.2)$$

We assume that the velocity field  $v(t, x)$  is incompressible, which implies that for each  $x_0$  and  $t \in [0, T]$  there exists a unique solution  $X(t, x_0)$  to (3.2) and conversely, for each  $x$  and  $t \in [0, T]$  there exists a unique  $x_0$ , such that  $X(t, x_0) = x$ . Thus the following one-to-one-correspondent transformation is defined:

$$X_t : x_0 \rightarrow x; \quad X_t(x_0) = X(t, x_0).$$

From incompressibility it follows that the Jacobian of this transformation is equal to 1:  $\frac{DX_t(x_0)}{Dx_0} = 1$  for each  $x_0$  and  $t \in [0, T]$ . In what follows, we use the change of variables from the Eulerian  $(x, t)$  to the Lagrangian coordinates  $(x_0, t)$  where  $x_0 = X_t^{-1}(x)$ .

The solution to the nonhomogeneous equation (3.1) is then expressed through

$$n^E(t, x) = n^L(t, X^*(t, x)), \quad (3.3)$$

where  $n^L$  solves the problem

$$\frac{\partial n^L(t, x_0)}{\partial t} = K(n^L(t, x_0) + F(t, X(t, x_0))), \quad (3.4)$$

$$n^L(0, x_0) = n^{(0)}(x_0), \quad x_0 \in \mathbb{R}^3, \quad t \in [0, T], \quad (3.5)$$

and the trajectory  $X^*$  is defined by

$$\frac{\partial X^*(\tau, x)}{\partial \tau} = -v(t - \tau, X^*(\tau, x)), \quad X^*(0, x) = x. \quad (3.6)$$

Let us introduce a function  $\Phi = \{\Phi_i(S; t)\}_{i=1}^\infty$  which is defined as a solution of the following homogeneous problem:

$$\frac{\partial \Phi(S; t)}{\partial t} = K(\Phi(S; t)) + F(t), \quad \Phi(S; 0) = S, \quad (3.7)$$

where  $S$  is a given vector  $S = \{S_i\}_{i=1}^\infty$ .

### 3.1 The point source

Let us consider the case of a point source situated at a point  $x_*$ . In this case the equation (3.1) reads

$$\begin{aligned} \frac{\partial n^E(t, x)}{\partial t} + v(t, x) \cdot \nabla_x n^E(t, x) &= K(n^E(t, x)); \\ n^E(0, x) &= 0; \quad x \neq x_*, \quad x \in \mathbb{R}^3; \quad t \in [0, T]. \\ n^E(t, x_*) &= S^P(t). \end{aligned} \quad (3.8)$$

In Lagrangian coordinates this takes the form

$$\frac{\partial n^L(t, x_0)}{\partial t} = K(n^L(t, x_0)); \quad n^L(0, x_0) = 0, \quad x_0 \neq x_*; \quad (3.9)$$

$$n^L(t, X_t^{-1}(x_*)) = S^P(t). \quad (3.10)$$



We assume here first for simplicity that the velocity  $v$  depends only on  $x$ . Let us take a point  $x_{0T} = X_T^{-1}(x_*)$  and consider the set of points of the trajectory  $X(t, x_{0T})$  which arrives at  $x_*$  at the time  $T$ . We denote this set by  $G_0$ :

$$G_0 = \{x_0 \in R^3 : x_0 = X(t, x_{0T}), \text{ where } X(T, x_{0T}) = x_*\}_{t \in [0, T]} .$$

Now we can define on the set  $G_0$  a transformation  $\tau_{x_*}$  which relates each  $x_0 \in G_0$  with the time  $t$  at which a trajectory started at  $x_0$  arrives at the point  $x_*$ , i.e., it is defined by  $X(\tau_{x_*}(x_0), x_0) = x_*$ .

Then we can write for each  $t$  that  $n^L(t, X_t^{-1}(x_*)) = S^P(t)$  is equivalent that for each  $x_0 \in G_0$   $n^L(\tau_{x_*}(x_0), x_0) = S^P(\tau_{x_*}(x_0))$ .

After this remark we conclude that the equation (3.9)-(3.10) implies that

$$\frac{\partial n^L(t, x_0)}{\partial t} = K(n^L(t, x_0)); \quad n^L(0, x_0) = 0, \quad x_0 \in R^3 \setminus G_0.$$

which means that in  $x_0 \in R^3 \setminus G_0$ , the function  $n^L(t, x_0)$  is zero, and in  $G_0$ , it is defined by

$$\begin{aligned} \frac{\partial n^L(t, x_0)}{\partial t} &= K(n^L(t, x_0)); \quad n^L(0, x_0) = 0, \\ n^L(\tau_{x_*}(x_0), x_0) &= S^P(\tau_{x_*}(x_0)) . \end{aligned}$$

Thus let us consider the problem

$$\begin{aligned} \frac{\partial n^L(t, x_0)}{\partial t} &= K(n^L(t, x_0)); \quad n^L(0, x_0) = 0, \\ n^L(\tau_{x_*}(x_0), x_0) &= S^P(\tau_{x_*}(x_0)) , \quad x_0 \in G_0. \end{aligned} \tag{3.11}$$

We fix  $x_0$  and the corresponding  $\tau = \tau_{x_*}(x_0)$ . Then obviously the solution to (3.11) is zero in the interval  $0 \leq t \leq \tau$ , while in the interval  $\tau \leq t \leq T$ , it is defined from

$$\frac{\partial n^L(t, x_0)}{\partial t} = K(n^L(t, x_0)); \quad n^L(\tau, x_0) = S(\tau).$$

Using the shift  $t' = t - \tau$  we find that

$$\frac{\partial n^L(t', x_0)}{\partial t'} = K(n^L(t', x_0)); \quad n^L(0, x_0) = S^P(\tau) \quad \text{for } 0 \leq t' \leq T - \tau.$$

Thus,

$$n^L(t, x_0) = \Phi(S^P(\tau); t - \tau), \quad \tau \leq t \leq T, \quad x_0 \in G_0$$

while  $n^L(t, x_0) \equiv 0$  if  $0 \leq t \leq \tau$ ,  $x_0 \in G_0$ , or  $x_0 \notin G_0$ . Here  $\Phi(S; t)$  is the function defined in (3.7) with  $F(t) \equiv 0$ . From this, we find the solution in Eulerian coordinates for all  $x \in \{X(t, x_*)\}_{t \in [0, T]}$

$$n^E(T, x) = \Phi(S^P(\tau); T - \tau); \quad x = X(\tau, x_*), \quad \tau = \tau_{x_*}(X_T^{-1}(x)), \tag{3.12}$$

and  $n^E(T, x) = 0$  if  $x \notin \{X(t, x_*)\}_{t \in [0, T]}$ .

## 3.2 Instantaneous source

Let us consider the case  $F(x, t) = 0$ , and let  $D = \text{supp } S^I(x)$ ,  $S^I(x)$  being a given initial distribution.

Thus we solve the problem

$$\begin{aligned} \frac{\partial n^E(t, x)}{\partial t} + v(t, x) \cdot \nabla_x n^E(t, x) &= K(n^E(t, x)); \\ n^E(0, x) &= S^I(x); \quad x \in R^3; t \in [0, T]. \end{aligned} \quad (3.13)$$

and let us first consider the case when  $v$  is a deterministic velocity field.

### Proposition 3.1.

The following relation is true for all  $t \in [0, T]$ :

$$\int_{\Omega} n^E(t, x) dx = \int_D \Phi(S^I(x_0); t) \chi(X(t, x_0) \in \Omega) dx_0, \quad (3.14)$$

$\Phi$  is defined by (3.7) with  $F(t) \equiv 0$ ,  $X(t, x_0)$  is the Lagrangian trajectory defined in (3.2), and  $\chi$  is the indicator function:  $\chi = 1$  if  $X(t, x_0) \in \Omega$ , and  $\chi = 0$  otherwise.

**Proof.** Let us denote  $D_t = \{x \in R^3 : x = X(t, x_0); x_0 \in D\}$ . Then from (3.3) we get

$$\int_{\Omega} n^E(t, x) dx = \int_{\Omega \cap D_t} n^E(t, x) dx = \int_{D_t} n^E(t, x) \chi(x \in \Omega) dx.$$

Since the Jacobian is equal to 1, we get from (3.14) and (3.7)

$$\begin{aligned} \int_{D_t} n^E(t, x) \chi(x \in \Omega) dx &= \int_{D_t} n^E(t, X(t, x_0)) \chi(X(t, x_0) \in \Omega) dX(t, x_0) \\ &= \int_D \Phi(S^I(x_0); t) \chi(X(t, x_0) \in \Omega) \frac{DX(t, x_0)}{DX_0} dx_0 = \int_D \Phi(S^I(x_0); t) \chi(X(t, x_0) \in \Omega) dx_0. \end{aligned}$$

□

Note that from (3.14) it follows that

$$\int_{R^3} n^E(t, x) dx = \int_D \Phi(S^I(x_0); t) dx_0$$

does not depend on the velocity  $v$ .

Let us now consider the equation (3.8), where  $v(t, x)$  is a random velocity field with the probability density function (pdf)  $p_E(v; t, x)$ . We define the Lagrangian pdf through

$$p_L(t, x | x_0) = \langle \delta(X(t, x_0) - x) \rangle. \quad (3.15)$$

**Proposition 3.2.** For each  $x$  and  $t \in [0, T]$  the expectation of  $n^E$  can be represented as follows

$$\langle n^E(t, x) \rangle = \int_D \Phi(S^I(x_0); t) p_L(t, x | x_0) dx_0, \quad (3.16)$$

where  $\Phi(S^I(x_0); t)$  is defined in (3.7).

**Proof.** Note, that

$$\begin{aligned} \langle n^E(t, x) \rangle &= \int n^E(t, x) p_E(v; t, x) dv = \\ &= \int \int_{\mathbb{R}^3} n^E(t, X(t, x_0)) \delta(X(t, x_0) - x) p_E(v; t, X(t, x_0)) dX(t, x_0) dv. \end{aligned}$$

By Proposition 3.1 and from the incompressibility we find

$$\begin{aligned} \langle n^E(t, x) \rangle &= \int \int_D \Phi(S^I(x_0); t) \delta(X(t, x_0) - x) p_E(v; t, X(t, x_0)) dx_0 dv = \\ &= \int_D \Phi(S^I(x_0); t) \left( \int \delta(X(t, x_0) - x) p_E(v; t, X(t, x_0)) dv \right) dx_0. \end{aligned}$$

Hence from the formal relation

$$\int \delta(X(t, x_0) - x) p_E(v; t, X(t, x_0)) dv = \langle \delta(X(t, x_0) - x) \rangle$$

we conclude with (3.16). □

## 4 Algorithm description in inhomogeneous case

Here we describe the simulation algorithms which follow from the representation of the solution in Lagrangian coordinates. Indeed, the solution to (3.1) is calculated from (3.3) where the trajectory  $X^*(t, x)$  is obtained by solving the equation (3.6).

Note that in particular case when  $F(t, x) = F(t)$ , the algorithms is simpler since the solution in this case can be expressed through the solution to the homogeneous equation (3.7):  $n^E(t, x) = \Phi(S(X^*(t, x)); t)$ . We consider also the next two important cases.

### 4.1 Point source

We first formulate the algorithm of calculation of the solution  $n^E(t, x)$  to the inhomogeneous problem (3.8) at a time instant  $t = T$  and for a set of points  $x_i$  which we specify below. For simplicity, we take the source  $S^P$  in the form:  $(S_1^P, 0, \dots, 0)$ .

- First we choose a mesh in the interval  $[0, \sup_{t \in [0, T]} S_1^P(t) K_{11} T]$ :

$$0 = t_0 \leq t_1 \leq \dots \leq t_{M_1} = \sup_{t \in [0, T]} S_1^P(t) K_{11} T$$

and calculate the solution to (2.32) with the initial conditions  $f_1(0) = 1, f_l(0) = 0$  for  $l \geq 2$  for all the mesh points by the algorithms constructed for the homogeneous case.

- Take a subdivision of  $[0, T]$ :  $0 = \tau_0 \leq \tau_1 \leq \dots \leq \tau_M = T$  and find  $x_i = X(\tau_i, x_*)$ ,  $i = 1, \dots, M$  (say, using the Euler scheme) from

$$\frac{\partial X(t, x_*)}{\partial t} = v(X(t, x_*)); \quad X(0, x_*) = x_*. \quad (4.1)$$

- For each  $x_i$  we approximate the solution  $n^E$  using the representation (3.12) and (2.32):

$$n_l^E(T, x_i) \approx S_1^P(T - \tau_i) f_l \left( \min\{t_j : t_j \geq S_1^P(T - \tau_i) K_{11} \tau_i\} \right).$$

Note that this algorithm gives the solution only at the points  $x_i$  which belong to the trajectory defined by (4.1).

## 4.2 Instantaneous source

We first describe the algorithm for calculating the solution to (3.13) in a point  $x$  at a time  $t$ . In this case, to use the direct Lagrangian trajectories is not a proper choice. It is quite natural to use the backward trajectories which start in the point  $x$  at the time  $t$ . It is especially efficient if the domain  $D$  is sufficiently large. Thus let us describe the technique based on the backward Lagrangian trajectories.

### Adjoint algorithm.

The backward Lagrangian trajectory starting in the point  $x$  is defined as the solution  $X^*(t, x)$ ,  $0 \leq t \leq T$  to

$$\frac{\partial X^*(t, x)}{\partial t} = -v(X^*(t, x)); \quad X^*(0, x) = x. \quad (4.2)$$

By (3.3) we find from (2.33) that the solution is then represented as

$$n^E(t, x) = \Phi(S^I(X^*(t, x); t)). \quad (4.3)$$

Note that in the case considered we assume  $S_l^I(x) = 0$ ,  $l \geq 2$ , then

$$n^E(t, x) = S_1^I(X^*(t, x)) f(S_1^I(X^*(t, x)) K_{11} t). \quad (4.4)$$

From this follows that it is possible to calculate the solution  $n^E(t, x)$  for all desired phase points  $(x, t)$  by solving the equation (2.32) only once. Indeed, in the implementation of the algorithm, one first precalculates once the solution to (2.32), and then use it for all points  $X^*(t, x)$ .

Thus the relation (4.3) defines the adjoint algorithm: one constructs the backward trajectory from (4.2) and calculates the solution from (4.3).

The adjoint algorithm is also convenient to apply to the evaluation of the integral of  $n^E(t, x)$  over a domain  $\Omega$ . This algorithms follows from the relation

$$\int_{\Omega} n^E(t, x) dx = \mathbf{E}_p \frac{n^E(t, \xi)}{p(\xi)},$$

where the expectation is taken over the random points  $\xi$  distributed in  $\Omega$  with a density  $p(x)$ . For instance,  $p(x)$  can be chosen as a uniform distribution. This relation shows that to evaluate the integral, one first choose a random point  $x_1$  in  $\Omega$  with respect to the density  $p(x)$ , then constructs the trajectory which starts in  $x_1$  and calculate  $n^E(t, x) = S_1^I(X^*(t, x_1)) f(S_1^I(X^*(t, x_1)) K_{11} t)$ . Then the final result is obtained by averaging over a sufficient number of such trajectories.

**Remark 4.1.** It is clear that the adjoint algorithm is efficient if the size of the domain  $D$  is considerably larger than that of  $\Omega$ . Otherwise, it is recommended to use the direct trajectories which start in  $D$  and apply the relation (3.14).

#### Calculation of the expectations in the case of random velocity

The adjoint algorithm is used also when we calculate the expectation  $\langle n^E(t, x) \rangle$ . Indeed, by averaging (4.3) over the random velocities we get

$$\langle n^E(t, x) \rangle = \langle S_1^I(X^*(t, x))f(S_1^I(X^*(t, x))K_{11}t) \rangle. \quad (4.5)$$

Thus the algorithm reads as follows: first construct a sample of the random velocity field  $v(t, x)$ , then calculate the solution  $n^E(t, x)$  by the adjoint algorithm; the final result is obtained by averaging over a large number of samples of the velocity field.

## 5 Coagulation in a fully developed turbulence

There are many different mechanisms that bring two particles to each others: Brownian diffusion, gravitational sedimentation, free molecule collisions, turbulent motion of the host gas, acoustic waves, the density, concentration and temperature gradients, particle electric charges, etc. We will deal here mainly with the case of coagulation of particles in a fully developed turbulence whose small scale statistical structure is specified by  $\bar{\epsilon}$ , the kinetic energy dissipation rate, and  $\nu$ , the kinematic viscosity. We assume that  $\bar{\epsilon}$  specifies the flow in average small scales, and suppose that the fluctuations are caused only by the large scale velocity fluctuations. It means that we assume that the coagulation coefficient (5.2) is deterministic, and the velocity  $v$  is random. The model for  $v$  is described in details in Sect.5.2. We refer to this as to a stochastic case. The deterministic case is governed by the solution to Smoluchowski equation with the average velocity. Since we deal with the case  $\langle v \rangle = 0$ , this means that the deterministic case is governed by the standard homogeneous Smoluchowski equation.

The main problem is to study the difference between the stochastic and deterministic cases. In this section we present this comparison for a series of examples. Of special interest is a situation, when a so-called *coagulation homogenisation* happens, i.e., a case when the stochastic solution approaches to the deterministic solution of the Smoluchowski equation with the average velocity field. On the other hand, the cases when there is a big difference between the stochastic and deterministic cases is also of much practical interest.

### 5.1 Formulation of the problem

Let us now study the influence of the velocity fluctuations to the coagulation process, governed by the equation

$$\begin{aligned} \frac{\partial n^E(t, x)}{\partial t} + v(t, x) \cdot \nabla_x n^E(t, x) &= K(n^E(t, x)); \\ n_1^E(0, x) &= S^I(x), \text{ supp } S^I(x) = D; \quad n_l^E(0, x) = 0, \quad l \geq 2 \\ t &\in [0, T] \end{aligned} \quad (5.1)$$

with turbulent coagulation coefficient (1.2):

$$K_{ij} = \left( \frac{\pi^2 \bar{\epsilon}}{120\nu} \right)^{1/2} V_1 \left( i^{1/3} + j^{1/3} \right)^3 \quad (5.2)$$

and random velocity field  $v(t, x)$  with Kolmogorov's energy spectrum. A randomized model for simulation such a field is described in the next section.

It is interesting to consider it in the comparison with the process governed by the same equation but with  $\langle v(t, x) \rangle$  instead of  $v(t, x)$ :

$$\begin{aligned} \frac{\partial \bar{n}(t, x)}{\partial t} &= K(\bar{n}(t, x)); \\ \bar{n}_1(0, x) &= S^I(x), \text{ supp } S^I(x) = D; \quad \bar{n}_l(0, x) = 0, \quad l \geq 2; \\ t &\in [0, T]. \end{aligned} \tag{5.3}$$

For the simplicity we suppose that  $D$  is a sphere of radius  $R$ , and consider the cases

$$\begin{aligned} (1) \quad S^I(x) &= S; \\ (2) \quad S^I(x) &= \left(1 - \frac{|x|}{R}\right) S. \end{aligned} \tag{5.4}$$

As we will see later, these two cases lead to essentially different results since they present spatially uniform and non-uniform initial distribution in the domain  $D$  which in turn, according to the representation (3.14), (4.4) give different contributions to the solution.

The following notations will be used

$\Omega_r$  is a sphere of radius  $r$ ,

$In_l(r, t)$  is the number of particles of size  $l$  in  $\Omega_r$  at a time  $t$

$$In_l(r, t) = \int_{\Omega_r} n_l^E(t, x) dx; \tag{5.5}$$

$In(r, t)$  is the number of all particles in  $\Omega_r$  at the time  $t$

$$In(r, t) = \int_{\Omega_r} \sum_i n_i^E(t, x) dx; \tag{5.6}$$

$Ms(r, t)$  for the mean size of the particle in  $\Omega_r$  at the time  $t$

$$Ms(r, t) = \frac{\int_{\Omega_r} \sum_i i n_i^E(t, x) dx}{\int_{\Omega_r} \sum_i n_i^E(t, x) dx}; \tag{5.7}$$

and  $Sp(r, t, l)$  is the relative number of clusters of size  $l$  in  $\Omega_r$  at the time  $t$

$$Sp(r, t, l) = \frac{\int_{\Omega_r} n_l^E(t, x) dx}{\int_{\Omega_r} \sum_i n_i^E(t, x) dx}. \tag{5.8}$$

To specify the same functionals in the case of (5.3) we use the bars.

In calculations, it is convenient to deal with dimensionless functions of dimensionless arguments. We choose the following normalization: for each  $l$

$$\frac{n_l(t, x)}{S} = g_l(t', x'; R', L', \beta), \tag{5.9}$$

$$\frac{\bar{n}_l(t, x)}{S} = g_2(t', x'; R', \beta). \quad (5.10)$$

Here

$$t' = \frac{t}{\tau_\eta}, \quad x' = \frac{x}{\eta}, \quad R' = \frac{R}{\eta}, \quad L' = \frac{L}{\eta},$$

where  $\eta$  and  $\tau_\eta$  are the inner spatial and temporal Kolmogorov scales,  $L$  is the integral spatial scale of the velocity field. The argument  $\beta$  in the dimensionless functions  $g_1$  and  $g_2$  is defined as  $\beta = V_1 S$  which is the total volume occupied by monomers in a unit volume. In this problem  $\beta$  determines the coagulation rate relative to the rate of velocity fluctuations; indeed,  $T_c = \tau_\eta/\beta$  is a characteristic coagulation time. We have taken  $\beta = 0.0039$  which can be considered as a low coagulation rate which corresponds to the situation that during the time when the initial volume is enlarged 8 times via the transport by the velocity flow  $v$ , the total number of clusters is decreased 10 times.

The parameters were chosen as  $L' = 1000$ ,  $R' = 100$ . We compare the functionals (5.6) for the problems (5.1) and (5.3) in the following way. We study the behaviour of the expectations of the total number of clusters in  $\Omega_r$  (5.6) as a function of  $r' = r/\eta$ , for a fixed time  $t'$ . The same is done for the mean cluster size (5.7). In addition, the expectation of the size spectrum (5.8) is calculated.

## 5.2 Randomized model of the classical pseudo-turbulence

Let us assume that the Eulerian pseudo-turbulent velocity field  $v(x) = \mathbf{U}_E(x)$  has the following partial spatial-temporal spectral tensor (e.g., see [14]):

$$\Psi_{jl}(\mathbf{k}) = \frac{E(k)}{4\pi k^2} \left( \delta_{jl} - \frac{k_j k_l}{k^2} \right), \quad j, l = 1, 2, 3, \quad (5.11)$$

where  $E(k)$  is the energy spectrum, and  $k = |\mathbf{k}|$ .

The energy spectrum is defined by

$$E(k) = \begin{cases} C_1 \bar{\varepsilon}^{2/3} k^{-5/3}, & k_0 \leq k \leq k_{\max}, \\ 0, & \text{otherwise} \end{cases} \quad (5.12)$$

with the normalization

$$\int_0^\infty E(k) dk = \frac{3}{2} u_0^2, \quad (5.13)$$

where  $C_1 \simeq 1.4$  is the universal constant in the Kolmogorov-Obukhov five thirds law,  $3u_0^2 = \langle |\mathbf{U}_E|^2 \rangle$  is the energy of turbulence.

In the model, the following input parameters are involved:  $\bar{\varepsilon}$  is the mean rate of dissipation of kinetic energy,  $k_0$ ,  $k_{\max}$  are the minimal and maximal wave numbers, respectively. The inner and external spatial scales of our model are  $\eta = 2\pi/k_{\max}$ , and  $L = 2\pi/k_0$ , respectively. Therefore, since the Reynolds number is expressed by (e.g., see [14], [4])  $Re \sim (\frac{L}{\eta})^{4/3}$ , it is naturally in our case to define the model Reynolds number as  $\hat{Re} = (\frac{k_{\max}}{k_0})^{4/3}$ .

The general simulation formula of the pseudo-turbulent velocity field with the tensor (5.11) is [17]:

$$\mathbf{U}_E(\mathbf{x}, t) = \sum_{j=1}^n \sqrt{E_j} \left\{ (\boldsymbol{\xi}_j \times \boldsymbol{\Omega}_j) \cos(\theta_j) + (\boldsymbol{\eta}_j \times \boldsymbol{\Omega}_j) \sin(\theta_j) \right\}, \quad (5.14)$$

where  $\theta_j = k_j(\boldsymbol{\Omega}_j, \mathbf{x})$ , and  $\boldsymbol{\Omega}_j = (\Omega_j^{(1)}, \Omega_j^{(2)}, \Omega_j^{(3)})$ ,  $j = 1, \dots, n$  are independent three-dimensional random isotropic unit vectors;  $\boldsymbol{\xi}_j = (\xi_j^{(1)}, \xi_j^{(2)}, \xi_j^{(3)})$  and  $\boldsymbol{\eta}_j = (\eta_j^{(1)}, \eta_j^{(2)}, \eta_j^{(3)})$  are mutually independent standard Gaussian random vectors;  $k_j, j = 1, \dots, n$  are random variables with the densities

$$p_j(k) = \begin{cases} \frac{1}{E_j} E(k), & k \in \Delta_j, \\ 0, & \text{otherwise} \end{cases}$$

with

$$E_j = \int_{\Delta_j} E(k) dk, \quad j = 1, \dots, n$$

and  $\Delta_j, j = 1, \dots, n$  are nonoverlapping intervals which compose a partition of  $\Delta = (k_0, k_{\max})$ , the support of the spectrum.

In [20], we have chosen the partition of the spectrum support

$$\Delta = \bigcup_{j=1}^n \Delta_j, \quad \Delta_j \cap \Delta_l = \emptyset, \quad j \neq l,$$

where  $\Delta_j = [\tilde{k}_j, \tilde{k}_{j+1})$ ,  $j = 1, \dots, n$ ,  $\tilde{k}_1 = k_0$ ,  $\tilde{k}_{n+1} = k_{\max}$ , so that

$$\int_{\Delta_j} E(k) dk = \frac{1}{n} \int_{\Delta} E(k) dk. \quad (5.15)$$

From this,

$$\tilde{k}_{j+1} = \left[ k_0^{-2/3} \left( 1 - \frac{j}{n} \right) + \frac{j}{n} k_{\max}^{-2/3} \right]^{-3/2}, \quad j = 1, \dots, n.$$

The random numbers  $k_j$  are simulated by

$$k_j = \left[ \tilde{k}_j^{-2/3} - \frac{u_0^2}{nC_1 \bar{\varepsilon}^{2/3} \gamma_j} \right]^{-3/2}, \quad j = 1, \dots, n. \quad (5.16)$$

In the above formulae,  $\gamma_j$ , ( $j = 1, \dots, n$ ) are mutually independent random numbers uniformly distributed in  $[0, 1]$ .

Note that in [10] we have suggested a different version of the simulation formula. First, we divide the interval  $[k_0, k_{\max})$  into  $n_0$  parts  $[\hat{k}_i, \hat{k}_{i+1})$ , ( $i = 0, \dots, n_0 - 1$ ) uniformly in logarithmic scale:  $\hat{k}_i = k_0 Q^i$ ,  $i = 0, \dots, n_0$ , where  $Q$  is chosen so that  $\hat{k}_{n_0} = k_{\max}$ . Then in each subinterval  $[\hat{k}_i, \hat{k}_{i+1})$  we apply the same subdivision (energy uniformly) as in the formula (5.15). This algorithm provides better statistics in all parts of the energy spectrum. The number of simulated harmonics in this model equals  $n_0 n$  and is proportional to  $\ln(\hat{R}e)$ .

### 5.3 Uniform initial conditions

Let us first consider the initial condition in the case (1), see (5.4).



From (3.2) we can write out the functionals  $\langle In(r', t') \rangle$  and  $\overline{In}(r', t')$  as follows:

$$\frac{\langle In(r', t') \rangle}{S} = \sum_i f_i(\beta t') \int_{\Omega_{r'}} \int_D p_L(t', x|x_0) dx_0 dx, \quad (5.17)$$

$$\frac{\overline{In}(r', t')}{S} = \begin{cases} \sum_i f_i(\beta t') \cdot \frac{4}{3}\pi r'^3 & \text{if } r' \leq R' \\ \sum_i f_i(\beta t') \cdot \frac{4}{3}\pi R'^3 & \text{if } r' > R'. \end{cases} \quad (5.18)$$

Analogously, for each  $l$

$$\frac{\langle In_l(r', t') \rangle}{S} = f_l(\beta t') \int_{\Omega_{r'}} \int_D p_L(t', x|x_0) dx_0 dx, \quad (5.19)$$

$$\frac{\overline{In}_l(r', t')}{S} = \begin{cases} f_l(\beta t') \cdot \frac{4}{3}\pi r'^3 & \text{if } r' \leq R' \\ f_l(\beta t') \cdot \frac{4}{3}\pi R'^3 & \text{if } r' > R'. \end{cases} \quad (5.20)$$

In this case the velocity fluctuations do not affect the size spectrum and the mean cluster size, since

$$\langle M_s(r', t') \rangle = \frac{\sum_i i f_i(\beta t')}{\sum_i f_i(\beta t')} = \overline{M}_s(r', t');$$

$$\langle Sp(r', t', l) \rangle = \frac{f_l(\beta t')}{\sum_i f_i(\beta t')} = \overline{Sp}(r', t', l).$$

Note that these functions do not depend on the velocity  $v$  in this particular case.

The turbulent dispersion causes the difference in the distribution of particles over the domains  $\Omega_r$  for different values of  $r$ .

In Figs.1 and 2 we present the total number of clusters in  $\Omega_{r'}$  as a function of  $r'$ , for stochastic and deterministic cases at the time instants  $t' = 1.25$  and  $t' = 55$ , respectively. Here  $\frac{\langle In(r', t') \rangle}{S}$  corresponds to the stochastic case (dashed), and  $\frac{\overline{In}(r', t')}{S}$  is the deterministic case (solid).

From Fig.1 it is clearly seen that the stochastic and deterministic cases are very close if the time  $t \sim \tau_\eta$ . The reason of it is that the main part of particles remains still in  $D$ , the domain where the monomers were generated. However for larger times ( $50\tau_\eta$ ) the turbulent dispersion affects the total number of clusters in the domains  $\Omega_{r'}$  (Fig.2.) since after this time, the clusters are dispersed over a larger domain  $\Omega_{r', r'} \sim 700$ , while the number of clusters in the domain  $D$  becomes 50 times smaller.

The same picture remains true for the functions  $In_l(r', t')$  and  $\overline{In}_l(r', t')$ . Indeed, the relations (5.17)-(5.20) yield

$$\langle In_l(r', t') \rangle = C(t') \langle In(r', t') \rangle; \quad \overline{In}_l(r', t') = C(t') \overline{In}(r', t'). \quad (5.21)$$

where  $C(t')$  is a constant not depending on  $r'$ .

## 5.4 Linear initial conditions

We consider here the problems (5.1) and (5.3) with the initial conditions  $S^I(x) = (1 - \frac{|x|}{R})S$ . Then we find from (2.33) by a change of integration variable

$$\overline{In}_l(\Omega_{r'}, t')/S = \left(\frac{4}{3}\pi R'^3\right) \cdot \frac{3}{\beta t'} \int_{\beta(1-\frac{r'}{R'})t'}^{\beta t'} \frac{u}{\beta t'} \left(1 - \frac{u}{\beta t'}\right)^2 f_l(u) du; \quad (5.22)$$

$$\overline{In}(\Omega_{r'}, t')/S = \left(\frac{4}{3}\pi R'^3\right) \cdot \frac{3}{\beta t'} \int_{\beta(1-\frac{r'}{R'})t'}^{\beta t'} \frac{u}{\beta t'} \left(1 - \frac{u}{\beta t'}\right)^2 \left(\sum_i f_i(u)\right) du; \quad (5.23)$$

$$\overline{Ms}(\Omega_{r'}, t') = \frac{\left(\frac{r'}{R'}\right)^3 \cdot \left(1 - 0.75 \frac{r'}{R'}\right)}{\frac{3}{\beta t'} \int_{\beta(1-\frac{r'}{R'})t'}^{\beta t'} \frac{u}{\beta t'} \left(1 - \frac{u}{\beta t'}\right)^2 \sum_i f_i(u) du} \quad (5.24)$$

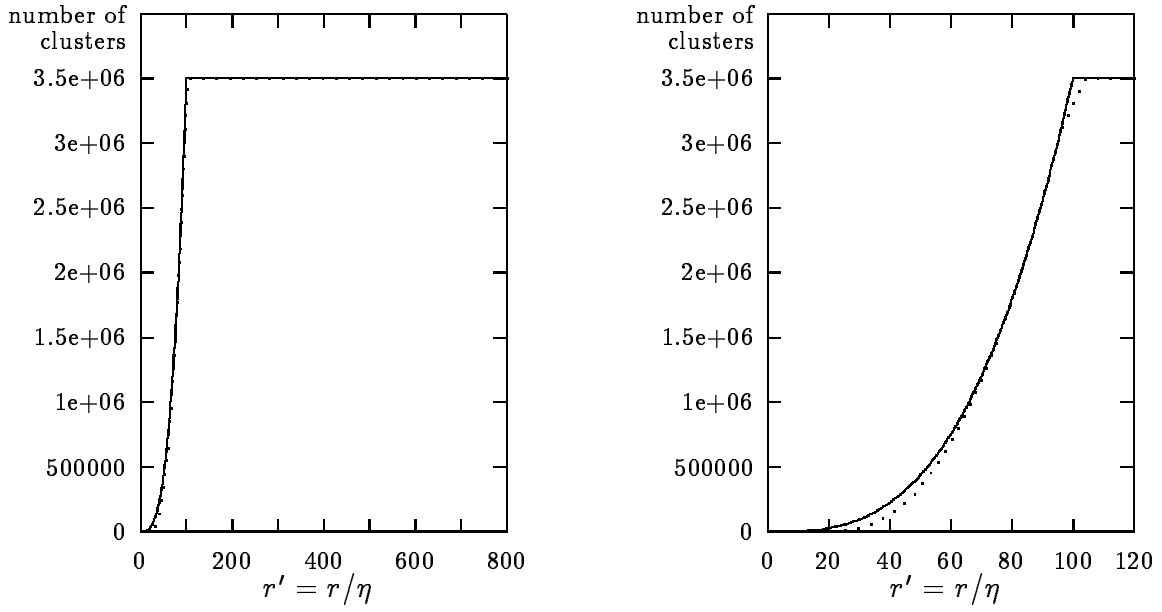
and

$$\overline{Sp}(\Omega_{r'}, t', l) = \frac{\int_{\beta(1-\frac{r'}{R'})t'}^{\beta t'} \frac{u}{\beta t'} \left(1 - \frac{u}{\beta t'}\right)^2 f_l(u) du}{\int_{\beta(1-\frac{r'}{R'})t'}^{\beta t'} \frac{u}{\beta t'} \left(1 - \frac{u}{\beta t'}\right)^2 \sum_i f_i(u) du}. \quad (5.25)$$

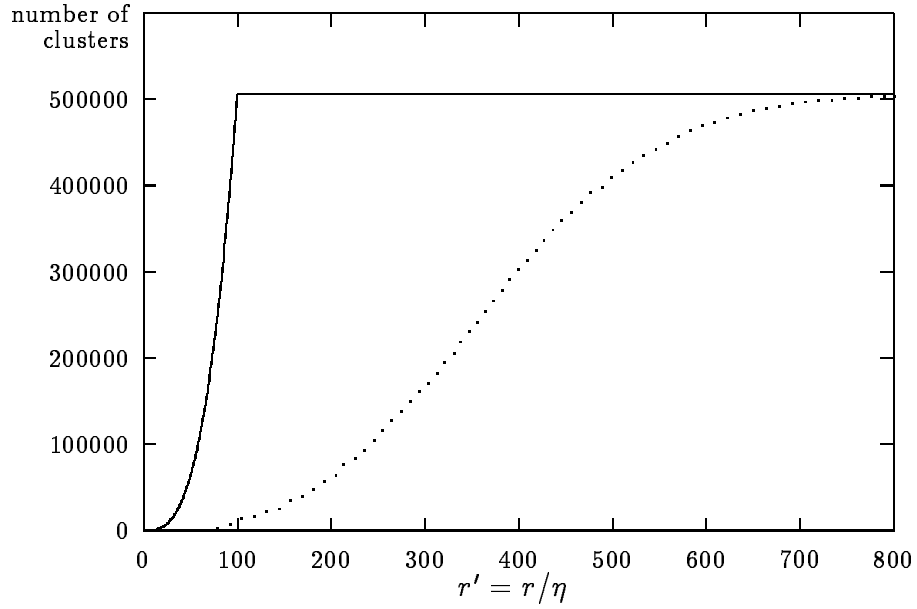
In this case the velocity fluctuations influence the formation of particle size spectrum. In Fig.3 and Fig.4 we plot  $\langle Sp(r', t', l) \rangle$  (dashed lines show the confidence interval) and  $\overline{Sp}(r', t', l)$  at time instants  $t' = 1.25$  and  $t' = 55$ , respectively, for  $r' = 0.1R'$  in both cases. The difference between the stochastic and deterministic cases is seen for  $l$ -mers,  $l > 4$  at the time  $t \sim \tau_\eta$ , and  $l > 10$  at  $t \sim 50\tau_\eta$ . This difference decreases with the growth of  $r'$ . Note that at  $r' = R'$  this difference is already not seen in Figs.5,6 where we plot the same curves as in Figs.3,4, but for  $r' = R'$ . This can be explained by the following arguments: for larger domains  $\Omega_{r'}$ , the averaging is carried out over trajectories which have therefore longer living times. The averaging is then similar to the case of uniform initial conditions where the difference between the stochastic and deterministic cases is small.

Thus the size spectra in stochastic and deterministic cases are different, namely the number of large clusters in stochastic case is smaller than that in the deterministic case. Therefore, the expectation of the mean cluster size is less than the mean cluster size in the deterministic case. This is clearly seen from Figs.7 and 8. Note that this effect is more pronounced for small  $r'$  ( $r' \sim 0.5R' = 50$  at time  $t' = 1.25$ ). With the growth of time, the average of the mean cluster size approaches a constant value slowly dependent on  $r'$  (see Fig.8).

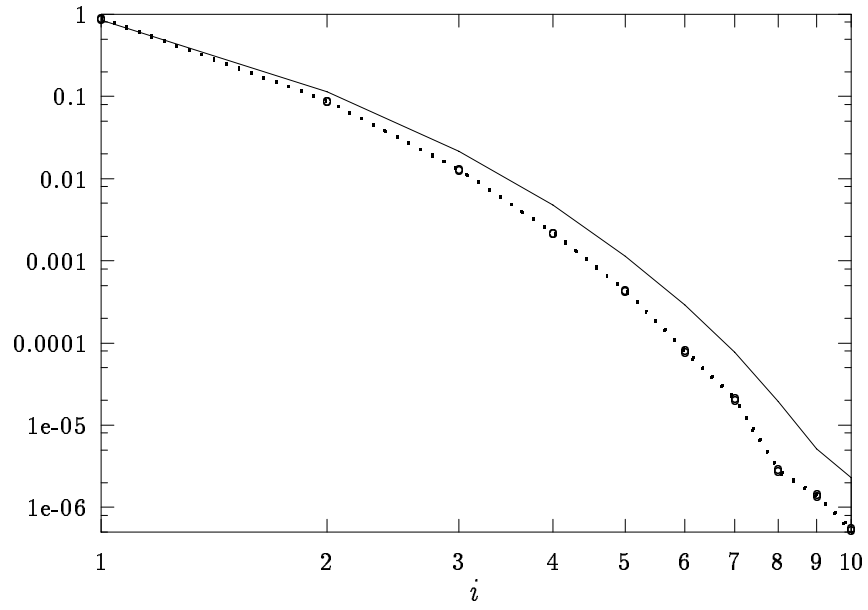
**Remark 5.1.** Note, that in both solutions to (5.1) and to (5.3) we use one and the same solution  $f_l(t)$  to the homogeneous coagulation equation. Thus the confidential interval is calculated with respect to the random velocity field  $v(t, x)$ , taking fixed solution  $f_l(t)$ .



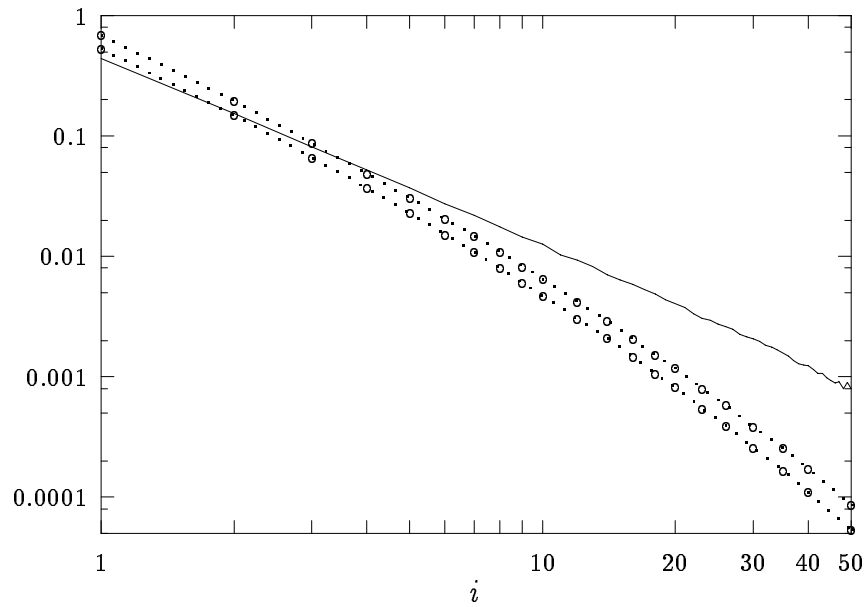
**Fig. 1.** Uniform initial conditions. The mean number of clusters  $\langle In(\Omega_{r'}, t) \rangle / S$  (dashed line) in the domain  $\Omega_{r'}$  at a time instant  $t/\tau_\eta = 1.25$  compared against  $\bar{In}(\Omega_{r'}, t) / S$  (solid line). We show both the whole picture (left) and a zoom (right).



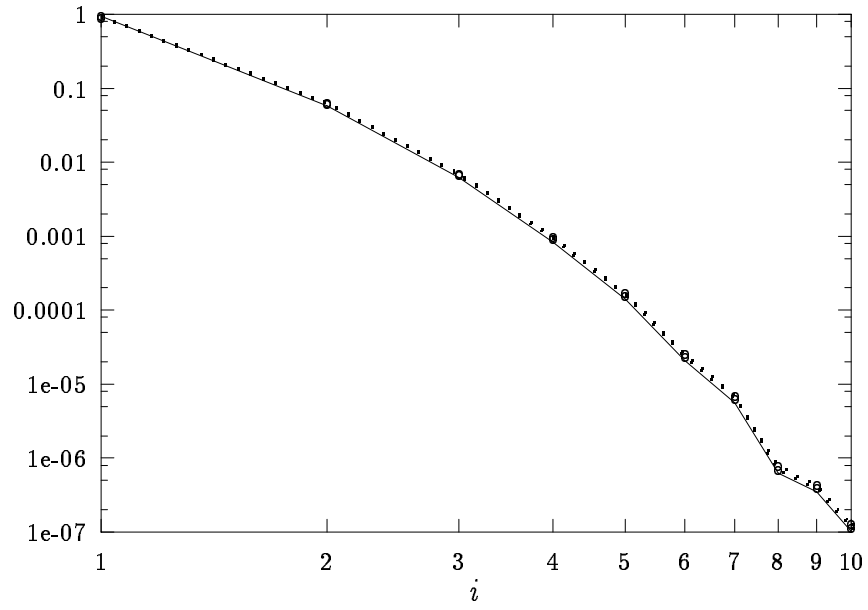
**Fig. 2.** The same, as in Fig.1, but for  $t/\tau_\eta = 55$ .



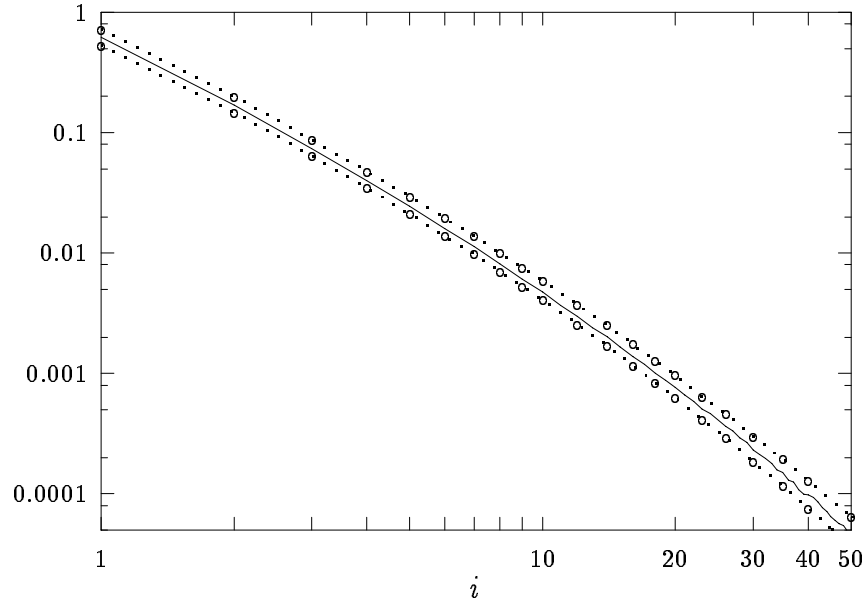
**Fig.3** Linear initial conditions. The size distribution  $\langle Sp(r', t, i) \rangle$  (dashed lines show the confidential interval) in the domain  $\Omega_{r'}$ ,  $r' = 0.1R'$ , at a time instant  $t/\tau_\eta = 1.25$ .



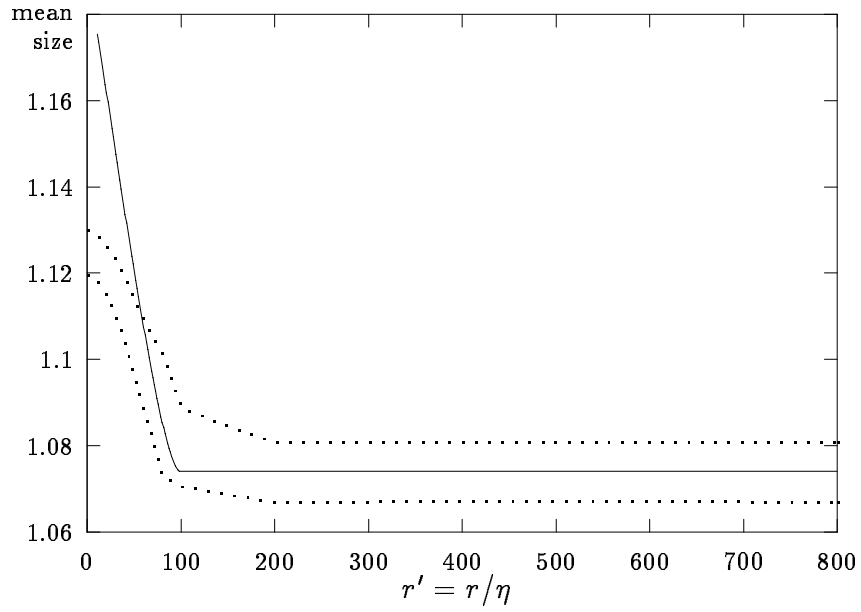
**Fig.4** The same, as in Fig.3, but for  $t/\tau_\eta = 55$ .



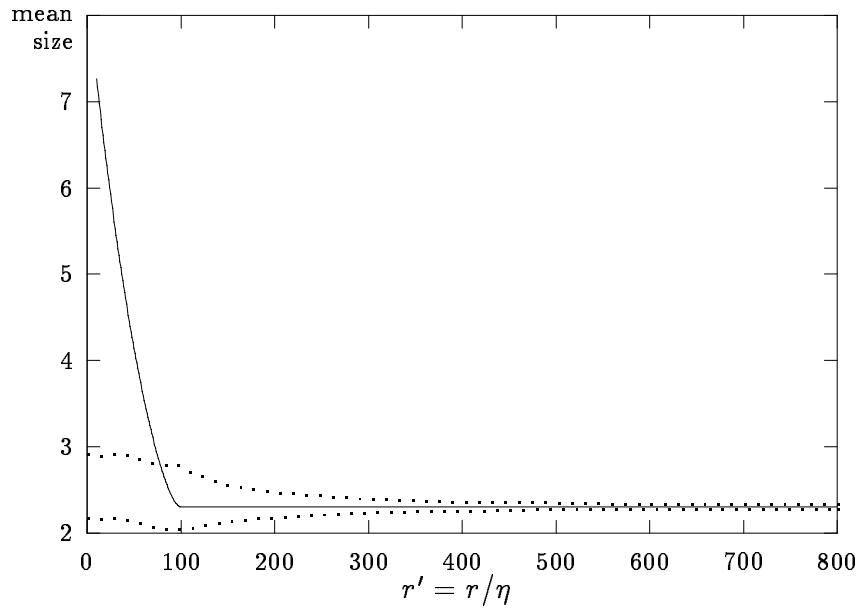
**Fig.5** The same, as in Fig.3, but for  $r' = R'$ .



**Fig.6** The same, as in Fig.5, but for  $t/\tau_\eta = 55$ .



**Fig.7.** Linear initial conditions. The mean size of particle  $\langle Ms(r', t) \rangle$  (dashed lines show the confidential interval) in the domain  $\Omega_{r'}$  at a time instant  $t/\tau_\eta = 1.25$  in the comparison with  $\bar{M}s(r', t)$  (solid line).



**Fig.8.** Linear initial conditions. The same, as in Fig.7, but for  $t/\tau_\eta = 55$ .

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