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Stochastic Lagrangian model for spatially inhomogeneous Smoluchowski equation governing coagulating and diffusing particles

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Abstract

The following generally unsolved yet problem is studied: construct the solution of a spatially inhomogeneous Smoluchowski equation governing coagulating and diffusing particles in a host gas, on the basis of solutions to homogeneous Smoluchowski equation. In [3] we solved this problem in the case when there is no diffusion. The non-zero diffusion term drastically complicates the situation. Under some general assumptions we give the interrelations between the homogeneous and inhomogeneous cases. This provides an effective numerical scheme especially when the host gas is incompressible. New Lagrangian scheme leads to a new model governing by a Smoluchowski type equation with an additional effective source. We give a numerical comparison of these two models.

The computer time of the new algorithm is so dramatically decreased, compared to the conventional deterministic algorithm (tens of hours drop down to several minutes) that many practical problems like the formation of soot particles in flames or chemical reactions coupled to formation of a new phase can be solved in a reasonable computer time. However this method works only if the diffusion coefficient of all particles is the same which can be a reasonable approximation only for special systems. The problem of generalisation of the method presented to the case when the diffusion coefficient depends on the particle's size is open.

1 Introduction

The coagulation processes of aerosol particles or clusters in a spatially homogeneous flow when the diffusion can be neglected are governed by the Smoluchowski equation (e.g., see, [14]):

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

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

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 the $\{i\}$- and $\{j\}$-*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.

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) (e.g., see [1]). To assure that these assumptions are satisfied, we assume for simplicity that

$$K_{ij} \leq \mathrm{const} \cdot i\, j \ . \tag{2}$$

The phenomenon of coagulation is crucial in a wide range of applications, e.g., in the aerosol science (formation and growth of particles), chemistry and meteorology, formation of soot particles in the combustion processes, physics of polymers, etc. (e.g., see [14]). Finite difference and finite element methods (e.g., [6]) are usually applied in spatially homogeneous case, provided the range of particle sizes is not too large.

The structure of the coagulation kernel K_{ij} for different collision regimes is presented, e.g., in [14], [9]. In the case of isotropic turbulent transport of the host gas, which is the situation we are interested in, the coefficients K_{ij} were derived in [13]

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

where $\bar{\varepsilon}$ is the mean rate of dissipation of kinetic energy per unit mass, ν 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 [13] that the colliding particles do not much differ in their sizes.

In the intermittent turbulence, ε is considered as a random process with lognormal distribution [2]. Thus mathematically, we have the Smoluchowski equation whose coefficients are random processes. The most interesting question which arises here is how much may the mean solution differ from the solution given by Saffman and Turner in their paper [13]. We solved this problem in [11].

As concerning the deterministic numerical methods for solving the deterministic Smoluchowski equation, see, e.g., [6], [4].

Generally, even linear PDE's with stochastic coefficients are very difficult for solving 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 [7]). In nonlinear case the situation is more complicated. However it is also possible to apply the double randomization technique (see [8]).

In this presentation we extend our considerations of inhomogeneous coagulation alowing the particles to be not only involved in the turbulent mixing, but also in the molecular diffusion of a parcel of flow carrying these particles.

Stochastic particle systems play an important role in the numerical analysis of the coagulation equation. The standard stochastic model related to the coagulation equation is a Markov jump process, which in the rarefied gas dynamics is known as the Bird method (see [9]). Some stochastic algorithms involve an additional approximation parameter, the time step, thus providing solutions to time discretized approximations of the coagulation equation e.g., like in the Nanbu algorithm (e.g., see [9], [3]). In the last paper we have considered the spatially inhomogeneous case where the coagulating particles are transported by the velocity field $v(t,x)$

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

with the initial conditions $n_l(0,x) = n_l^{(0)}(x)$, $l = 1,2,\ldots$. In the vector form it reads

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

$$n^E(0,x) = n^{(0)}(x); \quad x \in R^3;\ t \in [0,T]. \tag{4}$$

Here the following notations are used:

$$n^E(t,x) = \left\{n_i^E(t,x)\right\}_{i=1}^{\infty};\ n^{(0)}(x) = \left\{n_i^{(0)}(x)\right\}_{i=1}^{\infty};\ F(t,x) = \{F_i(t,x)\}_{i=1}^{\infty};$$
$$K(n^E(t,x)) = \left\{\frac{1}{2}\sum_{i+j=l} K_{ij} n_i^E(t,x) n_j^E(t,x) - n_l^E(t,x)\sum_{i=1}^{\infty} K_{il} n_i^E(t,x)\right\}_{l=1}^{\infty}.$$

The superscrip ^{E} stands to show that the equation is considered in fixed Eulerian coordinates.

In applied problems, inhomogeneous Smoluchowski equation has to be solved. For instance, even in the case of homogeneous isotropic turbulence, one needs to handle the inhomogeneous Smoluchowski equation (e.g., see [13],[10],[11]).

The idea how to solve the inhomogeneous equation through the homogeneous ones is based on the transformation from Eulerian to Lagrangian coordinates, with the integration over Lagrangian trajectories defined as the solutions to the Cauchy problem:

$$\frac{\partial X(t,x_0)}{\partial t} = v\left(t, X(t,x_0)\right),\ t \in [0,T]; \quad X(0,x_0) = x_0. \tag{5}$$

We will see that in the case of non-zero diffusion the Lagrangian trajectories are governed by stochastic differential equations.

2 Formulation of the problem

Let us assume that in addition to the coagulation, all the particles do diffuse with a parcel of flow, the diffusion coefficient being a constant D. The coagulation equation (4) is then generalized to (for simplicity we omit the source):

$$\begin{aligned} &\frac{\partial n^E(t,x)}{\partial t} + v(t,x)\cdot\nabla_x n^E(t,x) = D\Delta_x\, n^E(t,x) + K(n^E(t,x)); \\ &n^E(0,x) = n^{(0)}(x); \quad x \in G = R^3;\ t \in [0,T], \end{aligned} \tag{6}$$

where Δ_x is the Laplace operator acting in the spatial coordinates x. Note that for simplicity we assume that the solution is defined in the whole space $G = R^3$ so that there is no need to consider the boundary conditions.

These equations may be considered as a conventional description of the balance of particles which are moving in the host gas with the mean velocity $v(t,x)$, coagulating according to the kernel K, and diffusing all with the diffusion coefficient D not depending on the particle size.

Now, the problem can be formulated as follows. Find a probabilistic representation of the solution to (6) as an expectation of solutions of a stochastic differential equation governing the Lagrangian trajectories of the parcel of flow which moves according to the mean velocity field v and undergoes a diffusion with the constant D.

3 Stochastic Lagrangian model

Let us denote through $\Phi(t, \Phi^{(0)})$ the solution of the following spatially homogeneous coagulation equation:

$$\frac{\partial}{\partial t}\Phi(t) = K(\Phi) \tag{7}$$

with the initial conditions $\Phi(0) = \Phi^{(0)}$.

Let us introduce the following system of stochastic differential equations:

$$\begin{aligned} dX(t) &= v(t, X(t))\,dt + \sqrt{2D}\,dW(t), \\ X(0) &= x_0. \end{aligned} \tag{8}$$

We denote by $p(x, t; x_0)$ the transition density function of the process $X(t)$ defined in (8), and introduce the functional:

$$n^L(t,x) = \int\limits_G \Phi(t, n^{(0)}(x_0))p(x,t;x_0)dx_0 \ . \tag{9}$$

In what follows we present a theorem, establishing the connection between $n^L(t,x)$ and $n^E(t,x)$, the solution to the problem (6).

Let us consider the system of stochastic differential equations

$$\begin{aligned} dX(t) &= v(t, X(t))\,dt + \sqrt{2D}\,dW(t), \\ d\Phi(t) &= K(\Phi)\,dt, \\ X(0) &= x_0, \quad \Phi(0) = n^E(0, x_0) = n^{(0)}(x_0). \end{aligned}$$

Denote by $p_{X,\Phi}(x, \phi, t; x_0)$ the probability density function of the process $(X(t), \Phi(t))$, then

$$p_{X,\Phi}(x, \phi, t; x_0) = p_\Phi(\phi, t; x_0)\,p(x, t; x_0) = \delta(\phi - \Phi(t, n(0, x_0))p(x, t; x_0) \tag{10}$$

which makes the functions X and Φ dependent.

The following statement presents the main result.

Theorem 1. *The function $n^L(t,x)$ solves the equation*

$$\frac{\partial}{\partial t} n^L(t,x) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\Big(v_i(t,x)n^L(t,x)\Big) = D\Delta_x\, n^L(t,x) + K(n^L) + \alpha(t,x),$$

where

$$\alpha(t,x) = K\left(\int\limits_G \Phi\, p(x,t;x_0)dx_0\right) - \int\limits_G K(\Phi)\, p(x,t;x_0)\,dx_0$$

with the following property:

$$\frac{1}{2}F(t,x) \le \|\alpha(t,x)\|_0 \le \frac{3}{2}F(t,x), \tag{11}$$

$$F(t,x) = \sum_{i\ge1}\sum_{j\ge1} K_{ij} \left| \int\limits_G \Phi_i p(x,t;x_0)dx_0 \int\limits_G \Phi_j p(x,t;x_0)dx_0 - \int\limits_G \Phi_i\Phi_j p(x,t;x_0)dx_0 \right| .$$

In the case of incompressible flow ($div\, v = 0$) the equation for n^L differs from (6) only by the term $\alpha(t,x)$:

$$\frac{\partial}{\partial t} n^L(t,x) + v(t,x)\cdot\nabla_x n^L(t,x) = D\Delta_x\, n^L(t,x) + K(n^L) + \alpha(t,x)\ .$$

Proof. To prove this statement, we evaluate the integral (9). By definition, from (9) and (10) we find that

$$n_l^L(t,x) = \int_G\int \phi_l\, p_{X,\Phi}(x,\phi,t;x_0)\, dx_0\, d\phi.$$

The pdf $p_{X,\Phi}(x,\phi,t;x_0)$ satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t} p_{X,\Phi} + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\Big(v_i(t,x)p_{X,\Phi}\Big) = D\,\Delta_x p_{X,\Phi} - \sum_{i\geq 1}\frac{\partial}{\partial \phi_i}\Big(K_i(\phi)p_{X,\Phi}\Big) \tag{12}$$

with the initial condition

$$p_{X,\Phi}(x,\phi,0;x_0) = \delta(\phi - n^{(0)}(x_0))\delta(x-x_0).$$

Multiplying (12) by ϕ_l and integrating over ϕ and x_0 we get

$$\begin{aligned}\frac{\partial}{\partial t}\int_G\int \phi_l p_{X,\Phi}\, d\phi\, dx_0 + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[v_i(t,x)\int_G\int \phi_l p_{X,\Phi}\, d\phi\, dx_0\right] \qquad (13)\\ = D\,\Delta_x\int_G\int \phi_l p_{X,\Phi}\, d\phi\, dx_0 - \sum_{i\geq 1}\int_G\int \phi_l\frac{\partial}{\partial\phi_i}(K_i(\phi)p_{X,\Phi})d\phi\, dx_0\ .\end{aligned}$$

Let us now evaluate the integral

$$I = \sum_{i\geq 1}\int_G\int \phi_l\frac{\partial}{\partial\phi_i}(K_i(\phi)p_{X,\Phi})d\phi\, dx_0\ .$$

Note, that

$$I = \sum_{i\neq l}\int_G\int \frac{\partial}{\partial\phi_i}\left(\phi_l K_i(\phi)p_{X,\Phi}\right)\, d\phi\, dx_0 + \int_G\int \phi_l\frac{\partial}{\partial\phi_l}\left(K_l(\phi)p_{X,\Phi}\right)\, d\phi\, dx_0 = I_1 + I_2,$$

where

$$\begin{aligned}I_1 &= \sum_{i\neq l}\int_G\int\left(\int\frac{\partial}{\partial\phi_i}\phi_l K_i(\phi)p_{X,\phi}\, d\phi_i\right)\, d\phi_1\ \ldots\ d\phi_i\ \ldots\ dx_0\\ &= \sum_{i\neq l}\int_G\int\left(\phi_l K_i(\phi)p_{X,\Phi}\Big|_{\phi_i=0}^{1}\right)\, d\phi_1\ \ldots\ d\hat{\phi}_i\ \ldots\ dx_0 = 0.\end{aligned}$$

(here the hat over $d\phi_i$ means that this multiplier should be omitted), and

$$I_2 = \int_G\int\frac{\partial}{\partial\phi_l}\phi_l K_l(\phi)p_{X,\Phi}\, d\phi\, dx_0 - \int_G\int K_l(\phi)p_{X,\Phi}\, d\phi\, dx_0.$$

The first term in the last relation is equal to zero due to the same arguments, as used in the case of I_1. Thus,

$$I_2 = -\int_G \int K_l(\phi) p_{X,\Phi}\, d\phi\, dx_0$$

and the equation (13) reads

$$\frac{\partial}{\partial t} n_l^L(t,x) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(v_i(t,x) n_l^L(t,x)) = D\,\Delta_x\; n_l^L(t,x) + \int_G \int K_l(\phi) p_{X,\Phi} d\phi\, dx_0\ .$$

We rewrite it in the form

$$\frac{\partial}{\partial t} \int_G n_l^L(t,x) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(v_i(t,x) n_l^L(t,x)) = D\Delta_x n_l^L(t,x) + K_l(n^L) + \alpha_l(t,x),$$

where

$$\alpha_l(t,x) = K_l\left(\int_G \int \phi\, p_{X,\Phi} d\phi\, dx_0\right) - \int_G \int K_l(\phi)\, p_{X,\Phi} d\phi\, dx_0\ .$$

Note that

$$\int_G \left(\int \phi\, p_{X,\Phi} d\phi\right)\, dx_0 = \int_G \Phi(t, n^{(0)}(x_0)) p(x,t;x_0)\, dx_0.$$

Therefore,

$$\alpha_l(t,x) = \frac{1}{2}\sum_{i+j=l} K_{ij}\left(\int_G \Phi_i p_{X,\Phi}\, dx_0 \int_G \Phi_j p_{X,\Phi}\, dx_0 - \int_G \Phi_i \Phi_j p_{X,\Phi}\, dx_0\right)$$
$$- \sum_{i\geq 1} K_{il}\left(\int_G \Phi_i p_{X,\Phi}\, dx_0 \int_G \Phi_l p_{X,\Phi}\, dx_0 - \int_G \Phi_i \Phi_l p_{X,\Phi}\, dx_0\right).$$

From this we get the inequality (11), and the theorem is proved.

In conclusion we note that we expect that for many practical kernels K_{ij} the term α is small enough. In these cases the Theorem ensures that $n^E(x,t) \approx n^L(x,t)$. This implies that using (9) one can solve the inhomogeneous Smoluchowski equation by integration over solutions to homogeneous Smoluchowski equation. Let us describe this in more details.

4 Stochastic Lagrangian Algorithm

In this section we consider the problem of evaluation of the integral

$$I_h(\Omega,t) = \int_\Omega n^L(t,x)\cdot h(x) dx.$$

Here Ω is the domain in R^3, $h(x) = \{h_l(x)\}_{l\geq 1}$ is an arbitrary function defined in Ω. In what follows we assume that the initial conditions have the following form:

$$n^{(0)}(x) = 0, \quad x \notin \Omega_0. \tag{14}$$

We present the algorithms based on the construction of the forward and backward stochastic Lagrangian trajectories.

Direct estimator

Using the representation (9) and the condition (14), we can represent the integral $I_h(\Omega,t)$ as follows:

$$I_h(\Omega,t) = \mathbb{E}\left[\frac{h\left(X(t,\xi)\right)}{r(\xi)}\Phi\left(t, n^{(0)}(\xi)\right)\chi\left(X(t,\xi)\in\Omega\right)\right] . \tag{15}$$

Here ξ is a random value, distributed in Ω_0 with a density $r(x)$ chosen arbitrarily, according to some physical arguments; $X(t,\xi)$ is the Lagrangian trajectory, starting at the point ξ and governing by (8); Φ is the solution to the homogemeous equation (7) and χ is the indicator function. Standard Monte Carlo calculation of $I_h(\Omega,t)$ is then carried out as follows

$$I_h(\Omega,t) \approx \frac{1}{N}\sum_{i=1}^{N}\theta^{(i)}; \quad \theta^{(i)} = \frac{h\left(X^{(i)}(t,\xi^{(i)})\right)}{r(\xi^{(i)})}\Phi\left(t, n^{(0)}(\xi^{(i)})\right)\chi\left(X^{(i)}(t,\xi^{(i)})\in\Omega\right).$$

The superscript (i) shows that i independent samples of the random variable ξ and the random process X are taken.

Then, the algorithm of the calculation of $\theta^{(i)}$ can be formulated as follows.

Direct algorithm

1. Choose the random point ξ in Ω_0 with the density $r(x)$.

2. Construct the stochastic trajectory $X(\tau,\xi)$, $\tau\in[0,t]$, as the solution to (8) with the initial conditions $X(0,\xi)=\xi$; let

$$x := X(t,\xi).$$

3. Check, wether $x\in\Omega$.

3.1. If not, let $\theta^{(i)} := 0$.

3.2. If yes, then construct the solution $\Phi\left(t, n^{(0)}(\xi)\right)$ to the problem (7) and calculate

$$\theta^{(i)} := \frac{h(x)}{r(\xi)}\Phi\left(t, n^{(0)}(\xi)\right).$$

Adjoint estimator

The direct algorithm cannot be applied if $h(x)$ is the delta-function, or is defined on a small support domain. In this case the adjoint algorithm, based on the construction of the backward Lagrangian trajectories can be used.

Let us consider the random trajectory $X_t^*(\tau,x)$, backward in time, governing by the stochastic differential equation

$$dX_t^*(\tau) = v^*\left(\tau, X_t^*(\tau)\right)d\tau + \sqrt{2D}\ \overleftarrow{d}\ W,\ \tau\in[0,t]; \quad X_t^*(t) = x. \tag{16}$$

Here, the differential $\overleftarrow{d}\, W$ means that the backward Ito integral is taken[1].

We will denote by $p^*(x_0; t, x)$ the transition density function of the solution to (16).

In [12] there has been shown, that if one takes

$$v^*(t,x) = v(t,x) - \frac{2D}{\rho(t,x)} \mathrm{div}\, \rho(t,x) \ ,$$

where $\rho(t, x)$ is a positive solution to the equation

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(v_i \rho) = D \Delta \rho,$$

then there exists the following connection between $p(x, t; x_0)$ and $p^*(x_0; t, x)$:

$$p(x,t;x_0) = \frac{\rho(t,x)}{\rho(0,x_0)} p^*(x_0;t,x). \tag{17}$$

Substituting (17) into (9), we can analagously to the direct case represent the integral $I_h(\Omega, t)$ as follows:

$$I_h(\Omega,t) = \mathbb{E}\left[\frac{h(\xi)}{s(\xi)} \frac{\rho(t,\xi)}{\rho\left(0, X_t^*(0,\xi)\right)} \Phi\left(t, n^{(0)}\left(X_t^*(0,\xi)\right)\right) \chi\left(X_t^*(0,\xi) \in \Omega_0\right)\right] .$$

Here ξ is a sample point, chosen in Ω with a density $s(x)$; $X_t^*(\tau, \xi)$ is the backward Lagrangian trajectory, starting at the point ξ and governing by (16); Φ is the solution to the homogeneous equation (7) and χ is the indicator function.

Using this representation, the following estimator for $I_h(\Omega, t)$ can be constructed:

$$I_h(\Omega,t) \approx \frac{1}{N} \sum_{i=1}^{N} \theta^{*(i)};$$

$$\theta^{*(i)} = \frac{h(\xi^{(i)})}{s(\xi^{(i)})} \frac{\rho(t,\xi^{(i)})}{\rho(0, X_t^{*(i)}(0,\xi^{(i)}))} \Phi\left(t, n^{(0)}\left(X_t^{*(i)}(0,\xi^{(i)})\right)\right) \chi\left(X_t^{*(i)}(0,\xi^{(i)}) \in \Omega_0\right).$$

The superscript (i) denotes, that the i-th realization of the random variable ξ and the random process X_t^* are taken.

So, we have the following algorithm of the calculation of $\theta^{*(i)}$.

[1] The backward Ito integral is defined by

$$\int_s^t \xi(\tau)\, \overleftarrow{d} W(\tau) := \int_{T-t}^{T-s} \xi(T-\tau)\, dW_T(\tau),$$

$s \le t \le T$, $W_T(\tau) := W(T) - W(T-\tau)$ is a standard Wiener process. This integral does not depend on the choice of T. For details see, e.g., [5].

Adjoint algorithm

1. Choose the random point ξ in Ω with the density $s(x)$.
2. Construct the backward stochastic trajectory $X_t^*(\tau, \xi)$, $\tau \in [0, t]$, as the solution to (16) with $X_t^*(t, \xi) = \xi$; let
$$x_0 := X_t^*(0, \xi).$$
3. Check, wether $x_0 \in \Omega_0$.

3.1. If not, let $\theta^{*(i)} := 0$.

3.2. If yes, then construct the solution $\Phi\left(t, n^{(0)}(x_0)\right)$ to the problem (7) and calculate
$$\theta^{(i)} := \frac{h(\xi)}{r(\xi)} \frac{\rho(t, \xi)}{\rho(0, x_0)} \Phi\left(t, n^{(0)}(x_0)\right).$$

The algorithms presented above are especially efficient in the case of monodisperse initial conditions
$$n_l^{(0)}(x) = \delta_{1l} f(x).$$
In this case the function $\Phi(t, n^{(0)}(x))$ for each x can be expressed through the solution $u(t)$ to the normalized homogeneous coagulation equation
$$\frac{\partial u(t)}{\partial t} = K(u); \quad u_l(0) = \delta_{1l},\ l \geq 1. \tag{18}$$
Namely, we have
$$\Phi(t, n^{(0)}(x)) = f(x) u(f(x)t).$$
Hence it is not necessary to solve the homogeneous problem along all the Lagrangian trajectories. It is sufficient to solve once the problem (18) in the time interval $[0; \sup_{x \in \Omega_0} f(x)t]$.

5 Estimation of $\alpha(t, x)$

For simplicity let us consider the case
$$v(t, x) = 0.$$

In this case the system (10) reads:
$$\begin{aligned} dX(t) &= \sqrt{2D}\, dW(t), \\ d\Phi(t) &= K(\Phi)\, dt, \\ X(0) &= x_0, \quad \Phi(0) = n(0, x_0) = n^{(0)}(x_0). \end{aligned}$$

Here $X(t)$ is Gaussian, with the following pdf:
$$p(x, t; x_0) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{|x - x_0|^2}{2\sigma^2}\right), \ \sigma = \sqrt{2Dt}\ . \tag{19}$$

Since $p(x,t;x_0)$ is symmetric with respect to x and x_0, the function $F(t,x)$ in the inequality (11) can be represented as follows:

$$F(t,x) = \sum_{i\geq 1}\sum_{j\geq 1} K_{ij} \left| \int\limits_G \Phi_i p(x_0,t;x)dx_0 \int\limits_G \Phi_j p(x_0,t;x)dx_0 - \int\limits_G \Phi_i\Phi_j p(x_0,t;x)dx_0 \right| \tag{20}$$
$$= \sum_{i\geq 1}\sum_{j\geq 1} K_{ij} \left| \mathbb{E}[\Phi_i(t,n^0(\xi))\Phi_j(t,n^0(\xi))] - \mathbb{E}[\Phi_i(t,n^0(\xi))]\mathbb{E}[\Phi_j(t,n^0(\xi))] \right|.$$

Here $\Phi(t,n^0(\xi))$ is the solution to the spatially homogeneous coagulation equations (7) with the initial conditions

$$\Phi(0,n^0(\xi)) = n^{(0)}(\xi),$$

where ξ has the gaussian distribution with $\mathbb{E}[\xi] = x$ and $\mathrm{Var}[\xi] = 2Dt$.

One can find from (20) that $\|\alpha(t,x)\|_0 = 0$ in the case of uniform initial distribution $n^{(0)}(x) \equiv \text{const}$. While in general case the value of $\|\alpha(t,x)\|_0$ depends on the form of the initial conditions $n^{(0)}(x)$ and coagulation coefficients K_{ij} and on the value of the diffusion coefficient D.

We will now estimate $F(t,x)$ in one particular case of the initial conditions $n^{(0)}$. We assume that the admixture is ejected at the time instant $t=0$ and the source is concentrated in a bounded domain $\Omega_0 = G$, i.e.

$$n^{(0)}(x) = n^{(0)},\ x \in G; \qquad n^{(0)}(x) = 0,\ \text{otherwise}. \tag{21}$$

In this case, $\Phi_i(t,n^{(0)}(x_0)) = \Phi_i(t,n^{(0)})$ for each $x_0 \in G$ and $\Phi_i(t,n^{(0)}(x_0)) = 0$, when $x_0 \notin G$, hence

$$\int\limits_G \Phi_i p(x,t;x_0)dx_0 = \Phi_i(t,n^{(0)}) \int\limits_G p(x,t;x_0)dx_0$$

and

$$F(t,x) \leq \frac{3}{2}\sum_{i\geq 1}\sum_{j\leq 1} K_{ij}\Phi_i(t)\Phi_j(t) \left| \left(\int\limits_G p(x,t;x_0)dx_0 \right)^2 - \int\limits_G p(x,t;x_0)dx_0 \right| \leq FR(t,x); \tag{22}$$
$$FR(t,x) = \frac{3}{2}\left(n^{(0)}\right)^2 \text{const} \int\limits_G p(x,t;x_0)dx_0 \left(1 - \int\limits_G p(x,t;x_0)dx_0 \right).$$

Here const is the constant from (2).

Thus, one can conclude, that $F(t,x)$ decreases, as $\int\limits_G p(x,t;x_0)dx_0$ tends to 0 or to 1.

To understand, when such situation occurs, let us assume for simplicity that G is a cube with the edge of size of $2R$ and centered in the origin of the coordinates. In this case

$$\int\limits_G p(x,t;x_0)dx_0 = \Pi_{i=1}^3 f_i(t,x_i);\ f_i(t,x) = \frac{1}{\sigma\sqrt{2\pi}} \int\limits_{-R}^{R} \exp\left(-\frac{(x_i - x_{0i})^2}{2\sigma^2} \right) dx_{0i},\ \sigma = \sqrt{2Dt}. \tag{23}$$

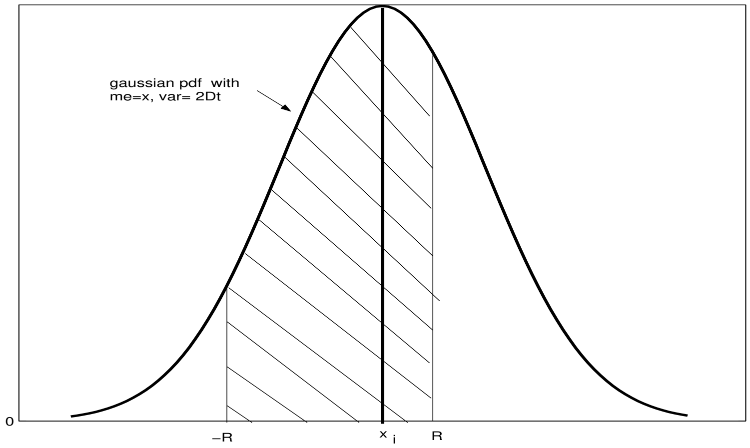

Figure 1: To the definition of the function $f_i(t, x)$.

The function $f_i(t, x)$ has a clear geometrical sense: it is equal to the area of the shaded domain under the curve of the gaussian pdf with the expectation x and variance $2Dt$, see Fig. 1.

One can find that, for fixed point x_i, the function $f_i(t, x_i)$ tends to 1 as t tends to 0, and tends to 0, as t tends to infinity.

Thus, for this particular case the right hand side of the inequality (22), estimating the value of $F(t, x)$, is small enough both for sufficiently small and sufficiently large times t. To illustrate this, we plotted in Fig. 2 $FR(t, x)$ as a function of time t (plane case) at $x = (0, 0)$, for different values of the diffusion coefficient D.

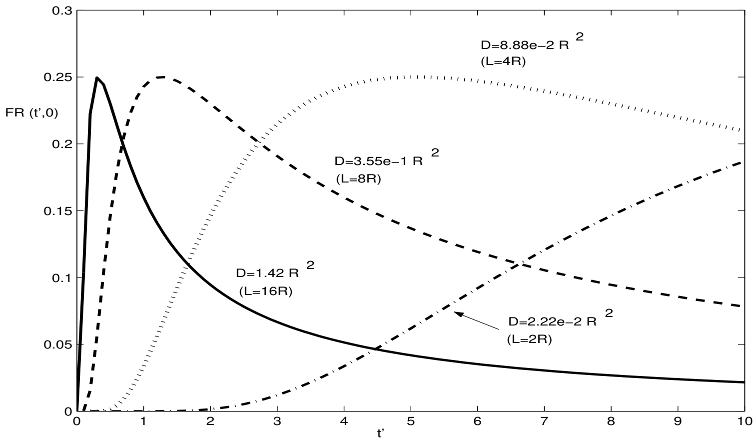

Figure 2: The function $FR(t', x)$ for $x = (0, 0)$ and different values of the diffusion coefficient D.

It is more convenient to use the dimensionless time

$$t' = t/T_c \ , \tag{24}$$

where $T_c = \dfrac{1}{K_{11} n^{(0)}}$ is the characteristic time scale of the coagulation process. It can be interpreted as the mean time of the collision at the initial time moment in the domain of the source action.

The value of L indicates the size of the domain, in which 99.7% of admixture particles are concentrated up to the moment $t' = 10$ for the corresponding diffusion coefficient. To provide this, we have taken the diffusion coefficient from the relation $3\sigma = L$, where σ is defined in (23).

The time $t' = 10$ has been chosen regarding the following condition: to this time instant, the coagulation process with the constant coagulation coefficient leads to a 20% decrease of the number of particles in the fluid element.

6 Comparison of the Eulerian and Lagrangian models.

From the previous section one can conclude, that for the considered particular case the term $\alpha(t, x)$ in the statement of the theorem can be small enough for some values of the diffusion coefficient D and time intervals. An interesting issue is the comparison of the functions $n^E(t, x)$ and $n^L(t, x)$, which in fact means the comparison of the Eulerian and the Lagrangian models of the coagulation of particles, which undergo the diffusion process.

It is important to understand, when the difference between the function $n^L(t, x)$ and the solution $n^E(t, x)$ to the problem (6) is small enough, so that the solution to inhomogeneous Smoluchowski equation can be approximated by solving the homogeneous problem along the Lagrangian trajectories. On the other hand, the question: when these functionals are quiet different is also of great interest. One can expect, that the difference between the functions $n^E(t, x)$ and $n^L(t, x)$ is small for small values of $\alpha(t, x)$ while it might be quite pronounced for large values of $\alpha(t, x)$.

Let us again assume that

$$v(t, x) = 0$$

and let us consider the two-dimensional case of the problem (6) with $K_{ij} = \text{const}$ and the following initial conditions:

$$n^{(0)}(x) = n^{(0)}, \ x \in G; \qquad n^{(0)}(x) = 0, \ \text{otherwise.} \tag{25}$$

Here G is a square of size $2R$ centered in the coordinates origin.

Eulerian model

To solve the coagulation-diffusion equation in the Eulerian coordinates (6) with the initial conditions (25) we have extended the finite element method developed in [9] to the inhomogeneous case.

It is reasonable to choose a particle size λ, which is large enough, so that all $n_l^E(t, x)$ for $l \geq \lambda$ are assumed to be equal to zero. Then we can take in the interval $[1; \lambda]$ a finite set of basis functions $\{\varphi_k(l)\}_{k=1}^N$ and approximate $n^E(t, x)$ as follows:

$$n_l^E(t, x) \approx \sum_{m=1}^{N} y_m(t, x)\varphi_m(l), \quad l = 1, \ldots, \lambda \ . \tag{26}$$

To reduce the dimension of the obtained system we consider only the equations in the set of collocation points $\{q_p\}_{p=1}^{N}$. Substituting (26) in (6) yields the following system of equations for $\{y_m(t,x)\}_{m=1}^{N}$:

$$\sum_{m=1}^{N} \varphi_m(q_p) \frac{\partial y_m(t,x)}{\partial t} = D \sum_{m=1}^{N} \varphi_m(q_p) \Delta_x y_m(t,x) + \sum_{m=1}^{N} \sum_{n=1}^{N} B^p_{mn} y_m y_n, \quad p = 1, \ldots, N, \tag{27}$$

where

$$B^p_{mn} = \frac{1}{2} \sum_{i+j=q_p} K_{ij} \varphi_m(i) \varphi_n(j) - \varphi_m(q_p) \sum_{i=1}^{\lambda} K_{q_p,i} \varphi_n(i).$$

For simplicity, we have used the piecewise-linear basis functions. In this case the approximation of $n^E(t,x)$ reads as follows:

$$n^E_l(t,x) \approx y_{\nu(l)} \varphi^1_{\nu(l)}(l) + y_{\nu(l)+1} \varphi^2_{\nu(l)}(l), \quad \nu(l) = \sup\{p |\, q_p \le l\},$$

where

$$\varphi^1_m(l) = \frac{q_{m+1} - l}{q_{m+1} - q_m}, \quad \varphi^2_m(l) = \frac{l - q_m}{q_{m+1} - q_m}.$$

Then, the system (27) takes the form:

$$\frac{\partial y_p(t,x)}{\partial t} = D \Delta_x y_p(t,x) + \frac{1}{2} \sum_{i=1}^{q_p - 1} K_{i,q_p - i} B_{i,q_p - i} - y_p \sum_{i=1}^{\kappa} K_{i,q_p} C_i , \quad p = 1, \ldots, N, \tag{28}$$

where

$$\begin{aligned} B_{ij} = {} & \varphi^1_{\nu(i)}(i) \varphi^1_{\nu(j)}(j) y_{\nu(i)} y_{\nu(j)} + \varphi^1_{\nu(i)}(i) \varphi^2_{\nu(j)}(j) y_{\nu(i)} y_{\nu(j)+1} \\ & + \varphi^2_{\nu(i)}(i) \varphi^1_{\nu(j)}(j) y_{\nu(i)+1} y_{\nu(j)} + \varphi^2_{\nu(i)}(i) \varphi^2_{\nu(j)}(j) y_{\nu(i)+1} y_{\nu(j)+1}, \end{aligned}$$

and

$$C_i = \varphi^1_{\nu(i)}(i) y_{\nu(i)} + \varphi^2_{\nu(i)}(i) y_{\nu(i)+1}.$$

To solve the system (28), the explicit finite-difference scheme has been used. The calculations have been carried out in the dimensionless variables $x' = x/R$ and t', where t' is defined in (24), with

$$\Delta t' = 0.014, \quad \Delta x' = 0.07.$$

We have taken $\lambda = 1.4e + 4$ and chosen the collocation points as follows:

$$q_p = \mathrm{round}(\gamma^p), \quad \gamma = 1.1.$$

Here the function $\mathrm{round}(x)$ equals the integer value closest to x. To check the accuracy of this method, we have solved the system of homogeneous Smoluchowski equations with $K_{ij} = 1$ and the diffusion equation without coagulation. For both of these problems the exact solution is known. The calculation shows, that the error of the scheme is less than 5% for both mentioned problems. It is expected that the same is true for the general case of the coagulation-diffusion equation.

Lagrangian model

As we noticed in the previous section, the system (8) in our case reads as follows:

$$\begin{aligned} dX(t) &= \sqrt{2D}\, dW(t), \\ d\Phi(t) &= K(\Phi)\, dt, \\ X(0) &= x_0, \quad \Phi(0) \equiv n^{(0)}. \end{aligned}$$

Here $X(t)$ is a gaussian process, with the following pdf:

$$p(x,t;x_0) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{|x-x_0|^2}{2\sigma^2}\right), \ \sigma = \sqrt{2Dt}.$$

So, the functional $n^L(t,x)$ in this case has the following representation:

$$n_l^L(t,x) = \Phi_l(t,n^{(0)}) f_1(t,x_1) f_2(t,x_2);$$

$$f_i(t,x_i) = \frac{1}{\sigma\sqrt{2\pi}} \int\limits_{-R}^{R} \exp\left(-\frac{(x_i-x_{0i})^2}{2\sigma^2}\right), \ \sigma = \sqrt{2Dt}.$$

Note that in our case an explicit representation for the solution $\Phi(t,n^{(0)})$ to homogeneous Smoluchowski equation is known. To find the integrals, we have used the trapezium rule.

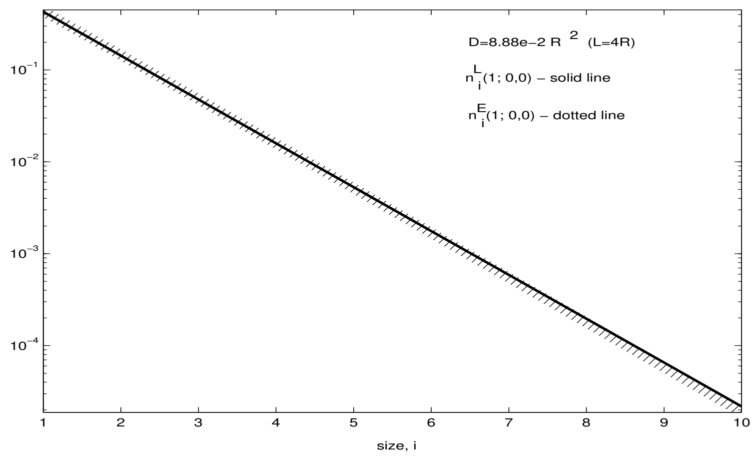

Figure 3: The size distributions $n_i^L(t',x)$ and $n_i^E(t',x)$ as functions of i for $t' = 1.0$, $x = (0,0)$ and $D = R^2 \cdot 8.88e-2$.

To present the results of calculations, we have used the same dimensionless time t', defined in (24). The calculations have been carried out for $D = R^2 \cdot 8.88e-2$. Such a value of the diffusion coefficient have been chosen to ensure that up to the moment $t' = 10$ the size L of the domain, in which 99.7% of admixture particles are concentrated, will be equal to $4R$ (see the previous section for the details). In Fig. 2, the estimation of the term $\alpha(t,x)$ is presented for the same case (dotted line).

In Figs. 3,4,5 we have plotted the size distribution of the admixture particles, given by Eulerian and Lagrangian models, in the point $x = (0,0)$, at the time moments $t' = 1$,

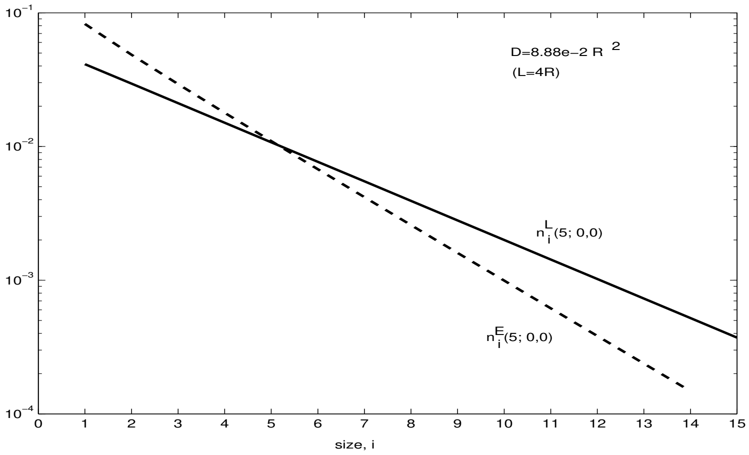

Figure 4: The size distribution $n_i^L(t',x)$ and $n_i^E(t',x)$ as a function of i for $t' = 5.0$, $x = (0,0)$ and $D = R^2 \cdot 8.88e - 2$.

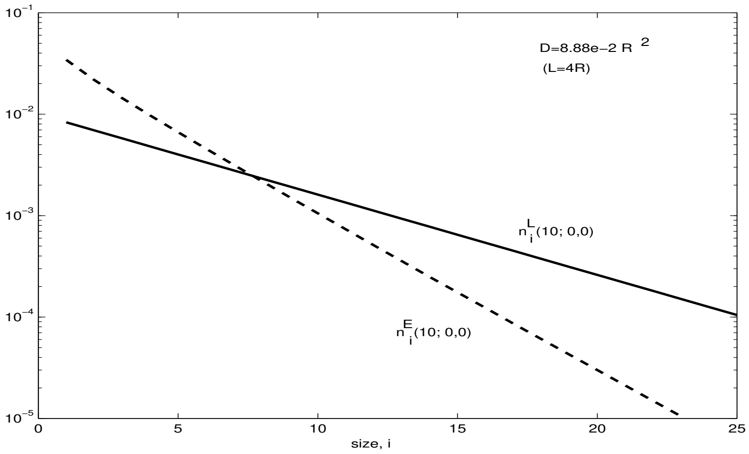

Figure 5: The size distributions $n_i^L(t',x)$ and $n_i^E(t',x)$ as functions of l, for $t' = 10.0$, $x = (0,0)$ and $D = R^2 \cdot 8.88e - 2$.

$t' = 5$ and $t' = 10$, respectively (the functionals $n_l^E(t',x)$ and $n_l^L(t',x)$ as functions of l). One can find, that these models give practically the same results for $t' = 1$. However, the difference between the functionals increases with the growth of t'. Namely, the Eulerian model provides larger number of particles of small sizes and smaller number of large particles. At $t' = 5$, this difference is about 50% for monomers and more than 100% for particles whose size is larger than 10. At $t' = 10$ the Eulerian model gives 2.5 times larger number of monomers, when comparing with the Lagrangian model. The difference between the number of particles whose size is larger than 15, is more than 400%.

In Figs. 6,7,8 we show the concentrations of particles of sizes 1, 5 and 10, respectively, given by Eulerian and Lagrangian models, as functions of time t', for $D = R^2 \cdot 8.88e - 2$. When analysing these pictures, one can conclude that the Eulerian model predicts a lower rate of growth and a lower rate of decrease of the number of particles of size $l > 1$. This leads to the effect that the number of large particles in the Eulerian model is less than that obtained by the Lagrangian model.

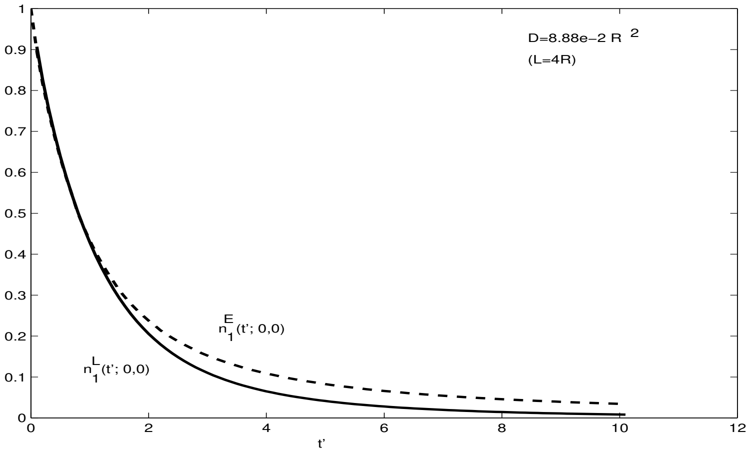

Figure 6: The concentration of clusters of size 1 $n_1^L(t', x)$ and $n_1^E(t', x)$, for $x = (0, 0)$ and $D = R^2 \cdot 8.88e - 2$.

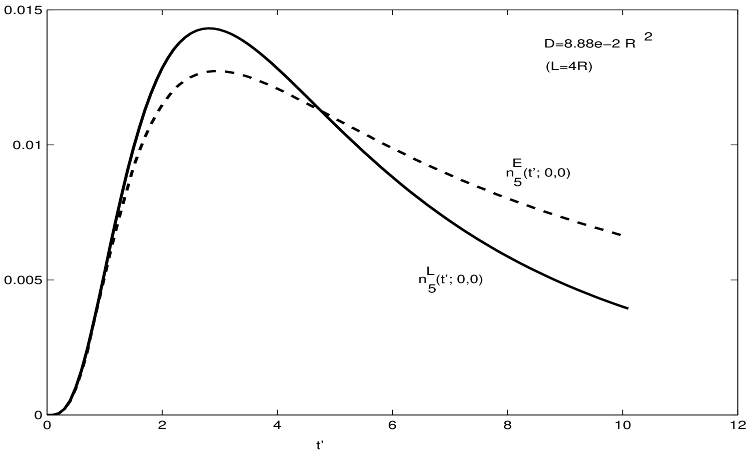

Figure 7: The concentration of clusters of size 5, $n_5^L(t', x)$ and $n_5^E(t', x)$ for $x = (0, 0)$ and $D = R^2 \cdot 8.88e - 2$.

7 Coagulation and diffusion in a fully developed turbulent flow

In this section we simulate the coagulation and diffusion processes for particles moving in an incompressible fully developed turbulent flow.

The question we are interested in is how strong the coagulation influences the number of admixture particles, under the condition that the particles are sufficiently small to be able to undergo a molecular-like diffusion. So let us assume that the admixture particles, containing 1 structural unit (monomers) have been ejected at the time instant $t = 0$ in a domain G. The particle concentration is changing in time both due to the turbulent motion of the host gas, to the diffusion of particles, and to their collisions leading to the formation of larger particles. Assuming that the turbulence is well-mixing the particles in

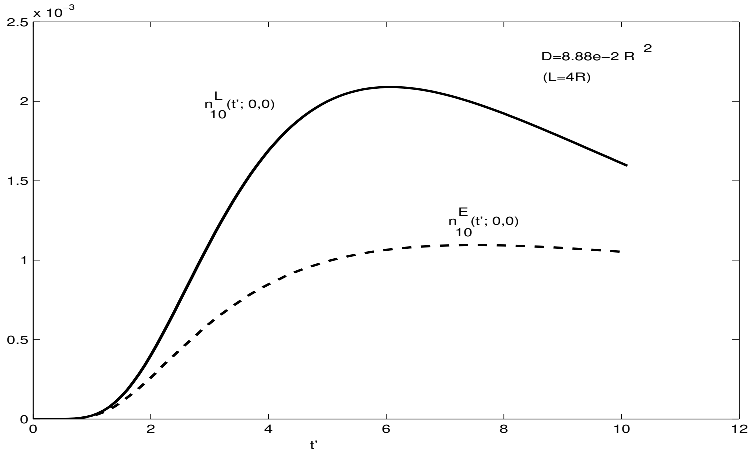

Figure 8: The concentration of clusters of size 10, $n^L_{10}(t', x)$, and $n^E_{10}(t', x)$, for $x = (0, 0)$ and $D = R^2 \cdot 8.88e - 2$.

an elementary volume, we aim at estimating under what conditions the coagulation process makes an essential contribution into the rate of decrease of the number of monomers, and when its contribution is so small, that it can be neglected?

More rigorously, we compare the solutions to the following two problems:

$$\frac{\partial n^D(t,x)}{\partial t} + v(t,x) \cdot \nabla_x n^D(t,x) = D\Delta_x n^D(t,x), \tag{29}$$

$$n_l^D(0,x) = n_l^{(0)}(x) = f(x)\delta_{1l}, \ x \in G; \quad n_l^D(0,x) = 0, \ \text{otherwise}$$

and

$$\frac{\partial n^{CD}(t,x)}{\partial t} + v(t,x) \cdot \nabla_x n^{CD}(t,x) = D\Delta_x n^{CD}(t,x) + K\left(n^{CD}(t,x)\right), \tag{30}$$

$$n_l^{CD}(0,x) = n_l^{(0)}(x) = f(x)\delta_{1l}, \ x \in G; \quad n_l^{CD}(0,x) = 0, \ \text{otherwise.}$$

The coagulation coefficients K_{ij} for the turbulent case are defined in the Introduction (see (3)).

The solution to (29) has the following probabilistic representation:

$$n_l^D(t,x) = \int\limits_G f(x_0)\delta_{1l} p(x,t;x_0)\, dx_0. \tag{31}$$

Here $p(x,t;x_0)$ is the transition density of the random process $X(t,x_0)$, governing by the following sde:

$$dX(t,x_0) = v(t,X) + \sqrt{2D}dW(t); \quad X(t,x_0) = x_0. \tag{32}$$

To calculate $n^{CD}(t,x)$, we use our Lagrangian model. Then,

$$n_l^{CD}(t,x) = \int\limits_G \Phi_l\left(t; n^{(0)}(x_0)\right) p(x,t;x_0)\, dx_0, \tag{33}$$

where $p(x,t;x_0)$ is the transition density of the solution to (32) and Φ is the solution to the homogeneous problem (7) with the turbulent coagulation coefficients (3).

In a fully developed turbulence, it is natural to assume that the mean velocity is zero:

$$v(t,x)=0.$$

Note, that in this case the function $p(x,t;x_0)$ has the form, defined in (19). We assume that the monomers at the initial time moment were uniformly distributed in the domain G where the particles were ejected.

$$n_l^{(0)}(x)=n^{(0)}\delta_{1l},\ x\in G;\quad n_l^{(0)}(x)=0,\ \text{otherwise};$$

G is a square of size $2R$ centered in the origin of the coordinates.

Let us now introduce the characteristic time scale of the diffusion as follows:

$$T_D=\frac{R^2}{D}.$$

It can be interpreted as follows: it is the time, to which the domain, containing 99.7% of admixture, becomes nearly 4 times larger, than G. In fact, according to (19), 99.7% of admixture is concentrated in the domain $[-3\sigma,3\sigma]\times[-3\sigma,3\sigma]$, while if $t=\frac{R^2}{D}$, then $3\sigma\approx 4.2R$.

We will also use the characteristic time scale of the coagulation

$$T_C=\frac{1}{K_{11}n^{(0)}},$$

which can be interpreted as the mean collision time the particles have had as they were ejected in G.

To analyse the relation between the solutions to (29) and (30) it is important to note, that these functions depend on the large number of different parameters. Actually, n^D is the function of t, x, $n^{(0)}$, R and D; while n^{CD} is the function of t, x, $n^{(0)}$, R, D, ε, ν, V_1. The following statement allows to simplify the situation.

Statement. *The functions $n^D(t,x;\,n^{(0)},R,D)$ and $n^{CD}(t,x;\,n^{(0)},R,D,\varepsilon,\nu,V_1)$ can be represented as follows:*

$$n^D(t,x;\,n^{(0)},R,D)=n^{(0)}N^D(t',x'),$$

$$n^{CD}(t,x;\,n^{(0)},R,D,\varepsilon,\nu,V_1)=n^{(0)}N^{CD}(t',x',b);$$

where

$$t'=\frac{t}{T_D},\quad x'=\frac{x}{R},\quad b=\frac{T_C}{T_D}.$$

where

$$N^D(t',x')=\frac{1}{\sigma'\sqrt{2\pi}}\int\limits_{-1}^{1}\int\limits_{-1}^{1}\exp\left(-\frac{|x'-x_0'|^2}{2\sigma'^2}\right)dx_0';$$

$$N^{CD}(t',x',b)=\frac{u(bt')}{\sigma'\sqrt{2\pi}}\int\limits_{-1}^{1}\int\limits_{-1}^{1}\exp\left(-\frac{|x'-x_0'|^2}{2\sigma'^2}\right)dx_0',\quad \sigma'=\sqrt{2t'}.$$

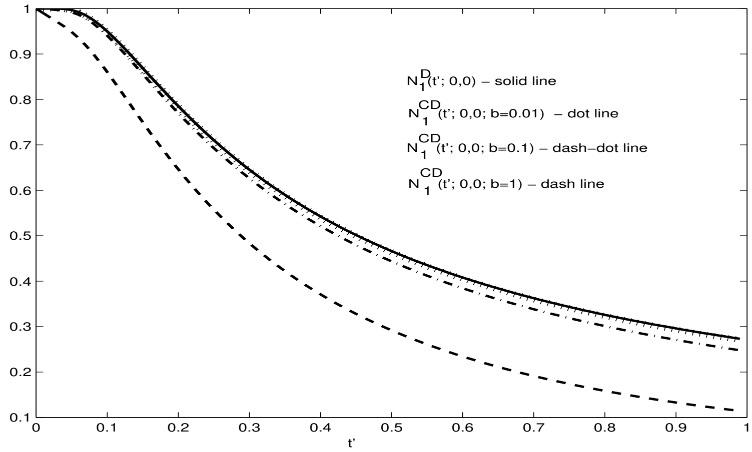

Figure 9: The functions $N_1^D(t', x')$ and $N_1^{CD}(t', x', b)$ for $b = 0.01$, $b = 0.1$ and $b = 1$ at the point $x = (0, 0)$.

Here $u(t)$ is the solution to the normalized homogeneous Smoluchowski equation with the coefficients

$$K_{ij} = \frac{1}{8}\left(i^{1/3} + j^{1/3}\right)^3.$$

The proof of the statement follows from the representations (31), (33) and (19) (using the change of the variables of the integration) taking into account that

$$\Phi\left(t, n^{(0)}(x)\right) = n^{(0)} u\left(K_{11} n^{(0)} t\right)$$

in the case of monodisperse initial conditions.

It is now more convenient to work with the functions N_1^D and N_1^{CD} instead of n_1^D and n_1^{CD}. Using the statement, the following relation between these functions in a time interval $t' \in [0, \gamma]$ can be given:

$$\sup_{t' \in [0,\gamma]} \left| \frac{N_1^{CD}(t', x', b) - N_1^D(t', x')}{N_1^{CD}(t', x', b)} \right| = \sup_{t' \in [0,\gamma]} \left| \frac{1}{u_1(bt')} - 1 \right| \to 0, \text{ as } b \to 0.$$

One can see that the difference between the functions decreases, as the ratio $\dfrac{T_D}{T_C}$ of the time scales becomes smaller. It means that the influence of the coagulation process on the behaviour of the admixture concentration decreases with the decrease of the relative rate of the coagulation, compared with the rate of the diffusion.

To illustrate this, we show the functions $N_1^D(t', x')$ and $N_1^{CD}(t', x', b)$ in the points $x' = (0, 0)$ (fig. 9) and $x' = (1.5, 0)$ (fig. 10). For both cases the following values of b have been taken: $b = 0.01$, $b = 0.1$ and $b = 1$. From these pictures one can clearly see the decrease of the difference between the functions with the decrease of the parameter b. In fact, these functions practicaly coincide for $b = 0.01$, while for $b = 1$ their difference becomes greater than 100%.

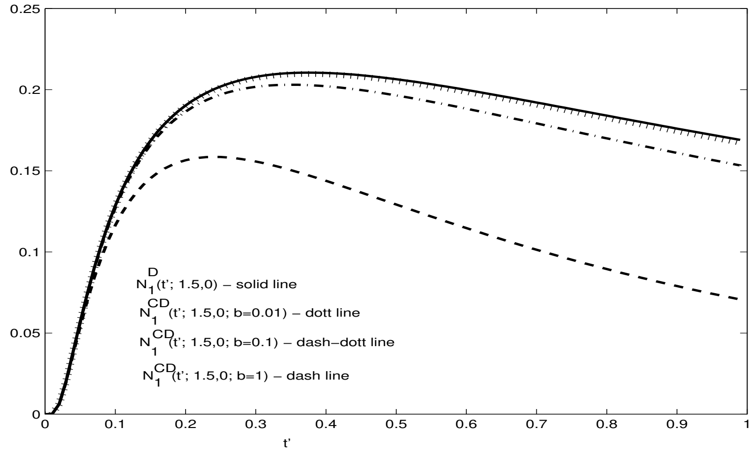

Figure 10: The functions $N_1^D(t', x')$ and $N_1^{CD}(t', x', b)$ for $b = 0.01$, $b = 0.1$ and $b = 1$ at the point $x = (0.5, 0)$.

8 Conclusion

We developed a new stochastic model for simulation of coagulating particles in a mean host flow whose diffusion activity is characterised by a constant diffusion coefficient not depending on the particle's size. This model leads to a Smoluchowski type equation, one difference to the classical Smoluchowski coagulation equation being an additional effective source. We have analysed the behaviour of this source in some particular cases.

We compared our new model with the results obtained by a finite-element method we developed for solving the classical inhomogeneous Smoluchowski equation. The results have confirmed the different predictions of two models, but also have shown regions where the results are quite close.

We have analysed, using the method developed, the relative contributions to the concentration of monomer particles moving in a fully developed turbulent flow made by the coagulation and diffusion processes.

It should be noted that the cost of the new algorithm is so dramatically decreased, compared to the conventional deterministic algorithm (a few tens of hours drop down to several minutes) that many practical problems like the formation of soot particles in flames or chemical reactions coupled to formation of a new phase can be solved in a reasonable computer time.

However it should be also mentioned that this method works only if the diffusion coefficient of all particles is the same which can be a reasonable approximation only for special systems. The problem of generalisation of the method presented to the case when the diffusion coefficient depends on the particle's size is open.

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