

# ON A MATHEMATICAL MODEL DESCRIBING THE MOTION OF SOLID PARTICLES OF MICRO- AND NANO-SIZE IN GAS FLOW

Prof. Dr.Sc.Math. Guseynov Sh.E.<sup>1,2,3,a</sup>, B.Sc.Phys. Zaimis U.<sup>1,2,b</sup>, Dr.Sc.Biol. Aleksejeva J.V.<sup>2,c</sup>, Prof. Dr.Sc.Phys. Kaupuzs J.<sup>1,2,d</sup>,  
 Assoc. Prof. Dr.Sc.Comp. Jansone A.<sup>1,2,e</sup>, Assoc. Prof. Dr.Sc.Eng. Grickus A.<sup>1,2,f</sup>  
 Faculty of Science and Engineering, Liepaja University, Liepaja, Latvia<sup>1</sup>  
 Institute of Fundamental Science and Innovative Technologies, Liepaja University, Liepaja, Latvia<sup>2</sup>  
 "Entelgine" Research & Advisory Co., Ltd., Riga, Latvia<sup>3</sup>

sh.e.guseinov@inbox.lv<sup>a</sup>, uldiss.z@inbox.lv<sup>b</sup>, jekaterina.v.aleksejeva@gmail.com<sup>c</sup>, kaupuzs@latnet.lv<sup>d</sup>, anita.jansone@liepu.lv<sup>e</sup>,  
 armands.grickus@liepu.lv<sup>f</sup>

**Abstract:** In the present article, a mathematical model is developed to describe the motion of solid particles of micro- and nano-size in a gaseous medium. The model is represented by certain integro-differential equation with appropriate initial and boundary conditions. A probabilistic interpretation of the model is provided and its solvability is studied. We find that unique solution exists at certain sufficient condition. It is shown that the Fokker-Planck equation can be obtained from the integro-differential equation. Finally, a generalization to the 2D case is performed.

**Keywords:** NANOPARTICLES, GAS FLOW, MATHEMATICAL MODEL, FOKKER-PLANCK EQUATION

## 1. Introduction

Modelling the thermophoretic force acting on the flow of solid micro- and nanoparticles is difficult due to the challenge of developing a trap to ensnare the particles and agglomerates without the use of electromagnetic and chemical influences. In this paper, the construction of a 1D model of the behaviour of micro- and nanoparticles in the gaseous medium is proposed following three major assumptions ([1]):

- ◆ the influence of micro- and nanoparticles on the gas is negligible;
- ◆ the direct influence of micro- and nanoparticles on each other is negligibly small in comparison to the influence of the gas on the particles;
- ◆ micro- and nanoparticles in the gaseous medium can move both forward and backward. This restriction is imposed so that the changing current location of micro- and nanoparticles may be performed at every fixed period of time to move the micro- and nanoparticles in the gaseous medium only to a neighbouring position.

These three assumptions are quite natural assumptions, for example, if the volume and the mass concentration of micro and nanoparticles in the gaseous medium is small enough, and if there are no external system interactions (e.g., electromagnetic), which is typical for many practical applications. In addition, in this paper, we assume that the main factor affecting the micro- and nano-sized particles from the gas is Brownian motion due to thermal pressure fluctuations in the gas. If the temperature around the micro- and nanoparticles is distributed uniformly, the time average of the Brownian fluctuations is zero. If the surrounding micro- and nanoparticles have a temperature gradient, the thermal fluctuations affect the particle in different ways from different sides, and there is a thermophoretic force, biasing the average position of the particle (see, for instance, [2], [3] and the corresponding references therein). Obviously, with the assumptions made, various solid micro- and nanoparticles in the gaseous medium may have the same coordinates.

In this paper, under the above assumptions, we first construct a discrete 1D model, and then under certain additional assumptions, the purpose of which is provisioning mathematical rigor, we make a limiting process from a discrete model into a continuous, non-deterministic model, constructed in the form of an initial-boundary value problem with an integro-differential equation. Then, the solvability of the resulting integro-differential model is investigated; it is the condition of a qualitative nature in the form of

an integral inequality, the satisfaction of which ensures the existence and uniqueness of the constructed mathematical models; given the probabilistic interpretation of the constructed model and the results obtained. In addition, in the paper it is shown that under certain conditions of the constructed integro-differential model, we can obtain the initial-boundary value problem for the Fokker-Planck equation (see [3]).

## 2. Mathematical models

**Construction of particular discrete 1D model and the question of the correct limiting process in preparing the continuous 1D model**

So we begin with the behaviour of solid particles of micro- and nano-sized in a gaseous medium. We make the following two basic assumptions:

**Assumption A:** At any time moment  $t = 0, \Delta t, 2 \cdot \Delta t, 3 \cdot \Delta t, \dots$  any micro- or nanoparticle may have one of the arbitrary coordinates  $0, \pm \Delta x, \pm 2 \cdot \Delta x, \pm 3 \cdot \Delta x, \dots$ ;

**Assumption B:** If any micro- or nanoparticle has a time coordinate  $n \cdot \Delta t$ , then at a subsequent time moment  $(n+1) \cdot \Delta t$  the same micro- and nanoparticle can have either  $(i-1) \cdot \Delta x$  or  $(i+1) \cdot \Delta x$  with the probability of finding micro- and nanoparticles at these two points being equal, i.e.

$$P\{x = (i-1) \cdot \Delta x\} = P\{x = (i+1) \cdot \Delta x\} = \frac{1}{2}.$$

Thus, with the two assumptions outlined above, we examine the problem of non-deterministic movements of micro- and nanoparticles, assuming that each micro and nanoparticle through each point in time may be randomly in one of two adjacent points (the distance between the points equals to  $\Delta x$ ), regardless of the behaviour of the rest of the micro- and nanoparticles and regardless of the history of their own behaviour. As accurately predicting the location of each individual micro- and nanoparticles is not possible, the question arises whether we can find a pattern in the behaviour of the "particle-gas" system as a whole? In other words, can we determine the gas flow distribution of the micro- and nanoparticles, having only information about the initial distribution of the micro- and nanoparticles in the stream?

Consider each point / particle from the general system of micro and nanoparticles with coordinates  $m \cdot \Delta x$  ( $m = 0, \pm 1, \pm 2, \dots$ ). Let the number of micro- and nanoparticles in the gas flow at each point  $m \cdot \Delta x$  be much greater than one. Then, with relative high

accuracy, we can assume that half of the micro- and nanoparticles, which are at time moment  $n \cdot \Delta t$  at point  $m \cdot \Delta x$ , during  $\Delta t$  will move forward on the axis  $OX$  at a distance  $\Delta x$ , and the other half will move in the opposite direction. If we introduce a new feature  $U(m, n)$ ,  $m = 0, \pm 1, \pm 2, \dots$ ;  $n = 0, 1, 2, \dots$  that means the number of micro nanoparticles at a time  $n \cdot \Delta t$  at the point with coordinates  $m \cdot \Delta x$ , then assuming that the above assumption is performed accurately, the following is obtained:

$$U(m, n+1) \approx \frac{U(m-1, n) + U(m+1, n)}{2}. \quad (1)$$

The equation (1) indicates that at any given time and coordinate, there are half the number of micro and nanoparticles that were in the previous time station at the points to the left and right combined. In the formula (1) the left and right sides cannot be equated, as this assumption is not always unconditionally true. For example, if the value of  $U(m, n)$  is small, then the formula (1) with the strict equality sign is in conflict with the fact that the values of  $U(m, n)$  must be integers and, moreover, the number of micro and nanoparticles on the edge of the considered gas flow volume for each time step  $\Delta t$  must be divisible in half, i.e. it should be an even number.

So, if we know the initial distribution  $U(m, 0)$  of micro- and nanoparticles in a volume of gas flow, then the recursive formula (1) can approximately find the required distribution of micro- and nanoparticles in all subsequent time moments. The equation (1) implies a property that determines the behaviour of the distribution of micro- and nanoparticles with time. Indeed, when the number of micro- and nanoparticles at a certain some point becomes smaller than the arithmetic mean values of neighbouring points, then the number increases, and vice versa. In addition, because of (1) it is clear that if an interval number of micro- and nanoparticles obeys a linear distribution law, then the interior points of the segment number of micro- and nanoparticles for some time remained constant. Indeed, if  $U(m, 0) = C_1 \cdot m + C_2$ , where  $C_1, C_2$  are some constants, the recursive formula (2) gives us  $U(m, i) = U(m, 0), \forall i \in \mathbb{N}$ . In other words, the number of micro- and nanoparticles included in the considered interval left / right is equal to the number of micro- and nanoparticles, leaving the left / right of this segment. It should be emphasized that this property is only true in the case, when the segment is not "washed out" at the edges. However, in the process of this scheme the possible initial asymmetry between the points with even and odd numbers cannot be aligned. This becomes especially clear if we consider that all of the micro- and nanoparticles at the initial time moment were concentrated at a single point. To eliminate this asymmetry we can, for example, consider scheme of walks in which micro- and nanoparticles can not only move to adjacent points, but with a certain probability stay in the same place. This circumstance does not allow us to go without some updates from the discrete formula (1) to the process under study, the continuous model, as  $\Delta x$  and  $\Delta t$  go to zero.

As we know, in physics, at the transition from the system consisting of a large number of particles in a continuous medium the concept of the linear density of a medium  $\rho_m = \lim_{\Delta x \rightarrow 0} \frac{\Delta m}{\Delta x} = \frac{dm}{dx}$ , is introduced, that is the mass "portion" of micro- and nanoparticles, going over a small portion of the axis per length unit of the segments  $OX$ . It is obvious that the linear density of a medium is different at various points of the axis  $OX$  and at various times  $t$ , i.e.  $\rho = \rho(x, t)$ . On the other hand, we can enter this density as the "density of micro- and nanoparticles"

$\rho_U = \lim_{\Delta x \rightarrow 0} \frac{\Delta U}{\Delta x} = \frac{dU}{dx}$ , where  $U$  is the number of micro- and nanoparticles in a small segment of the considered gas flow. Another method of introducing the concept of linear density  $\rho_U$  synthesizes a discrete (as  $U$  is considered) and continuous (as  $U$  is differentiated by the variable  $x$ ) approach to the system of "particles-gas." In both cases, it is obvious that  $dx$  should be sufficiently small compared to the characteristic length of the system as a whole, i.e.  $dx \ll l$ , but much larger than the characteristic distance between adjacent micro- and nanoparticles, i.e.  $dx \gg \frac{l}{U}$ . To continue, we were able, without loss of

understanding, to use a linear density introduced through the  $m$  - "mixing intensity of the of micro- and nanoparticles", and, through "the number of micro and nanoparticles", prove that the linear density of the number of micro- and nanoparticles is proportional to the mass density (i.e. the intensity of the mixing capacity) of the micro- and nanoparticles. In other words, we need to make sure that the linear density of the number of micro- and nanoparticles and the mass density of micro- and nanoparticles are linearly dependent. In fact, if all of flow particles have the same mass,  $m_{const}$ , then

$$dm = m_{const} \cdot dU. \text{ Hence, we obtain } \rho_U = \frac{dU}{dx} = \frac{1}{m_{const}} \cdot \rho_m, \text{ i.e.}$$

$\rho_U$  and  $\rho_m$  differs by a constant  $m_{const}$ , which is the proportionality factor.

It was said above about the "hollowing out" of the edges of the considered segment and the inapplicability of the initial asymmetry between the points with even and odd numbers. As already noted above, the recursive formula (1) cannot go to the limits for  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$ , without requiring the fulfilment of certain conditions in the case when on the axis  $OX$  edges of the boundaries of the segment with the passage of time, as it were "blurred". It is necessary to mathematically formulate the condition referred to in the recursive formula (1), for it to be possible to carry out the limiting processes for  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$ . Thus, we require that the value is such that "jumps" (if there are such jumps) in the initial distribution of micro- and nanoparticles have time to dissipate so that the change in the gas flow of micro- and nanoparticles in a single time step will be substantially smaller than the characteristic values of this number. This requirement means mathematically that  $n \gg 1$ . The second requirement is that the boundaries of the segment are not "sprawling" on the axis  $OX$  over time, or if such a "spread" borders takes place, we (i.e. foreseeable part of the segment) are far from it. The second requirement mathematically means that  $(n - |m|) \gg 1$ . These two requirements enable us to realize the limiting processes in the formula (1). Indeed, if we rewrite (1) in the form

$$U(m, n+1) - U(m, n) = \frac{1}{2} \cdot [U(m-1, n) - 2 \cdot U(m, n) + U(m+1, n)],$$

then we obtain

$$\frac{U(m, n+1) - U(m, n)}{\Delta t} = \frac{(\Delta x)^2}{2 \cdot \Delta t} \cdot \frac{U(m-1, n) - 2 \cdot U(m, n) + U(m+1, n)}{(\Delta x)^2}.$$

Further, taking into account in this equation the notation  $x = m \cdot \Delta x, t = n \cdot \Delta t$  and

$$\rho(x, t) = \frac{m_{const}}{\Delta x} \cdot U(m, n), \quad (2)$$

(the physical meaning of (2) is obvious: the density of the medium composed of micro and nanoparticles), and implementing the limit as  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ , we get

$$\frac{\partial \rho(x, t)}{\partial t} = \frac{h^2}{2 \cdot \omega} \cdot \frac{\partial^2 \rho(x, t)}{\partial x^2}, \quad (3)$$

where  $\frac{h^2}{2 \cdot \omega} \stackrel{def}{=} \lim_{\substack{\Delta x \rightarrow 0 \\ \Delta t \rightarrow 0}} \left( \frac{\Delta x}{\sqrt{2 \cdot \Delta t}} \right)^2 > 0$  is called the coefficient of sensitivity.

Obviously, the sensitivity factor may be interpreted as the number of micro- and nanoparticles passing per time unit through a length unit of a segment (area) density gradient of micro- and nanoparticles equal to one. In this interpretation, the sensitivity factor reflects the rate of the random motion of micro and nanoparticles, which is determined by the properties of the 1D gaseous medium.

If the movement of micro- and nanoparticles is not included in its equilibrium state, i.e. if the number of micro- and nanoparticles arriving / to any segment included consideration of gas flow per volume unit per time unit is not equal to the number of micro- and nano particulate departing from this segment, the sensitivity factor is a function of time:  $\frac{h^2}{2 \cdot \omega(t)}$ . Generally speaking, the coefficient

of sensitivity to the actual process of random motion micro- and nanoparticles is an unknown factor. Moreover, considering it constant, we are quite strongly limiting the assumption of unchanged during the entire interval of time sensitivity factor of observations, and the assumption of a known value of this constant is a purely statistical assumption not fully reflects the characteristics of the process of random motion of micro and nanoparticles in the gaseous medium. Therefore, there is just only the problem of determining the sensitivity factor under some additional conditions on the distribution and micro- and nanoparticles. This question, which is an independent inverse problem, is not considered in this paper.

Note that the equation (3) can also be obtained in another way if we use the notation (2) and the recursive relation (1). Indeed, by multiplying (1) by  $\frac{m_{const}}{\Delta x}$ , and using the item (2), we obtain

$$\rho(x, t + \Delta t) = \frac{1}{2} \cdot [\rho(x - \Delta x, t) + \rho(x + \Delta x, t)].$$

Hence we have the equality

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(\Delta t)^n}{n!} \cdot \frac{\partial^n \rho(x, t)}{\partial t^n} &= \\ = \frac{1}{2} \cdot \left[ \sum_{n=0}^{\infty} \frac{(-1)^n (\Delta x)^n}{n!} \cdot \frac{\partial^n \rho(x, t)}{\partial x^n} + \sum_{n=0}^{\infty} \frac{(\Delta x)^n}{n!} \cdot \frac{\partial^n \rho(x, t)}{\partial x^n} \right], \end{aligned}$$

in which the values of the function  $\rho$  and its derivatives, are taken with the values of the arguments  $x$  and  $t$ . In the last equation, in view of the uniform convergence of the present series, we can combine these terms series. Then we get

$$\Delta t \cdot \frac{\partial \rho(x, t)}{\partial t} + o((\Delta t)^2) = \frac{(\Delta x)^2}{2} \cdot \frac{\partial^2 \rho(x, t)}{\partial x^2} + o((\Delta x)^4), \quad (4)$$

or ignoring small quantities of higher order  $\Delta x$  and  $\Delta t$ , we finally obtain the equation (3). The equation (3) is an equation for the

density  $\rho(x, t)$  of the micro- and nanoparticles in the 1D gaseous medium. As mentioned above, the sensitivity coefficient (3), in general, depends on time and is an unknown to be determined. If we assume that the sensitivity coefficient is constant and is known, by the same token, we accept that  $h$  and  $\omega$  are constants. In this case, it is easy to formulate some interesting consequences:

- ♦ parameter  $\omega$  is of the order  $h^2$  (it is also seen from (4));
- ♦ if we assume that at the initial time all micro- and nanoparticles are concentrated in a finite interval under consideration per volume unit of the gas flow, as time increases the edge of the "front" of the segment will diverge at a rate of  $\varrho = \lim_{\substack{\Delta x \rightarrow 0 \\ \Delta t \rightarrow 0}} \frac{\Delta x}{\Delta t} = \lim_{\Delta x \rightarrow 0} \frac{\Delta x}{o((\Delta x)^2)} = \infty$ , i.e. in a

small time interval velocity increases indefinitely. In other words, in the limit, it can be found out that micro- and nanoparticles are moving per unit of time as far as desired. In fact, the mean absolute coordinate increment value of micro- and nanoparticles per time unit is finite, as in conditions where the direction of movement is random, the probability that all these movements are performed in one direction (in the limit to one point), tends to zero as  $\Delta t \rightarrow 0$ .

So, we have constructed a continuous 1D model (3) to uniquely identify the density of micro and nanoparticles in the gaseous medium. Now, we find out if built spared continuous 1D model from unsmoothed of initial asymmetry between the points with even and odd numbers, which was mentioned in the derivation of the discrete model (1). For this purpose, suppose that for some  $t = t'$ ,

the density  $\rho(x, t)$  of micro- and nanoparticles at some point  $x = x'$  is lower than the arithmetic mean value of the density  $\rho(x, t')$ , then for all symmetric points of small  $\varepsilon$ -neighbourhood of the point under consideration  $x = x'$ , i.e.

$\forall x'' \in B_\varepsilon(x') \stackrel{def}{=} \{x: |x - x'| < \varepsilon \square 1\}$ , we have the inequality

$$\rho(x', t') < \frac{\rho(x' + x'', t') + \rho(x' - x'', t')}{2}. \quad \text{Since}$$

$$\rho(x', t') = \rho\left(\frac{(x' - x'') + (x' + x'')}{2}, t'\right), \quad \text{we have}$$

$$\rho\left(\frac{x' - x''}{2} + \frac{x' + x''}{2}, t'\right) < \frac{\rho(x' - x'', t') + \rho(x' + x'', t')}{2}, \quad \text{which}$$

shows the convexity of the function  $\rho(x, t')$ ,  $x \in B_\varepsilon(x')$  in at the specified time moment  $t = t'$ . If the function  $\rho(x, t')$  is convex

downwards, then  $\frac{\partial^2 \rho(x, t')}{\partial x^2} > 0$ . Having regard to this inequality

$$\text{in the equation (3), we obtain the inequality } \left. \frac{\partial \rho(x, t)}{\partial t} \right|_{t=t'} > 0,$$

which means an increase in the function  $\rho(x, t)$  (here argument  $t'$  is replaced by  $t$  because of its arbitrariness). Similarly, if for

$\forall x'' \in B_\varepsilon(x') \stackrel{def}{=} \{x: |x - x'| < \varepsilon \square 1\}$  we have

$$\rho(x', t') > \frac{\rho(x' + x'', t') + \rho(x' - x'', t')}{2}, \quad \text{then by identical}$$

reasoning we find that the function  $\rho(x, t')$  is convex upwards, i.e.

$$\frac{\partial^2 \rho(x, t')}{\partial x^2} < 0. \quad \text{Consequently, } \left. \frac{\partial \rho(x, t)}{\partial t} \right|_{t=t'} < 0 \quad \text{and the density}$$

$\rho(x, t)$  decreases. So, we get that in both cases the function  $\rho(x, t)$  as a function of a variable  $x$  is either flattened out to the linear dependence not being a constant, or to a constant. In the first case it is obvious that for  $t \rightarrow \infty$  the density and flux of micro- and nanoparticles at each point are not time dependent, i.e. the process goes into a stationary state, and in the second case the mass flow of micro- and nanoparticles at each point is equal to zero, that is the process proceeds in a statistical equilibrium again. It is obvious that the continuous 1D model (3) will possess an above-described stationary state, if, for instance, at the left / right endpoint of the concerned line segment micro- and nanoparticles enter into the system "particles-gas" with constant intensity, and at the right / left endpoint of this segment micro- and nanoparticles leave the system "particles-gas" with the same intensity. The resulting flux of micro- and nanoparticles will be the same at all points of the volume unit of gaseous medium.

#### Probabilistic interpretation of constructed particular models and their solutions

As the continuous 1D model (3) under certain assumptions has been obtained from the discrete model (1), and the discrete model (1) is a non-deterministic model of the walks of the micro- and nanoparticles in a gaseous medium with the assumptions A and B (precisely the assumption B makes the constructed models particular), then the discrete function  $U(m, n)$  and the continuous function  $\rho(x, t)$  obtained from  $U(m, n)$  should have probabilistic interpretations. Furthermore, other functions and parameters of the constructed mathematical models introduced above (the discrete model (1) and the continuous model (3)) must also have probabilistic characteristics. Indeed, if it is assumed that the initial distribution of the micro- and nanoparticles in a gaseous medium is unknown and the value  $U(m, 0)$  is the mean value of the number of the micro- and nanoparticles in the position  $m \cdot \Delta x$  at the initial time moment  $t = 0$ , then this will mean that the value of  $U(m, 0)$  is the mathematical expectation of a random variable, which is the "number of micro- and nanoparticles" at any node of the discrete grid  $\{m = 0, \pm 1, \pm 2, \dots; n = 0, 1, 2, \dots\}$ . Then the mean value  $U(m, 1)$  of the number of micro- and nanoparticles at time moment  $t = \Delta t$  in the position  $m \cdot \Delta x$  is expressed in terms of the initial values for the recurrent formula (1), in which is taken  $n = 0$ . Consequently, by the newly found mean values we can calculate the mean value  $U(m, 2)$ , etc. It is obvious that with such probabilistic interpretation these mean values  $U(m, n)$  are no longer required to be integers. Summarizing, we can say that the recurrent relation (1) is the exact relation (i.e. there is strict equality sign in the (1)) between the mathematical expectation of the number of micro- and nanoparticles at the fixed time moment in the fixed place. If there is only a micro- and nanoparticle and if it is studied its "single motion" on the axis  $OX$ , then  $U(m, n)$  will be signified the probability of detection of this micro and nanoparticle at the time moment  $n \cdot \Delta t$  in the position  $m \cdot \Delta x$ . Since for the "single jump" from one node to another neighbouring node of the discrete grid, the average value of the increment of spatial coordinates is zero  $((\Delta x + (-\Delta x))/2)$ , then the variance of such "single jump" would be equal to  $(\Delta x)^2$ . Since summing up independent random variables their variances are summed up, and, obviously, during the time  $t \square \Delta t$  the micro- and nanoparticle will perform exactly  $\frac{t}{\Delta t}$  independent jumps, then the variance of total increment of the spatial coordinate of the micro- and nanoparticle at time moment  $t$

will equal to  $\frac{t}{\Delta t} \cdot (\Delta x)^2 = 2 \cdot t \cdot \left(\frac{\Delta x}{\sqrt{2} \cdot \Delta t}\right)^2 = \frac{h^2 \cdot t}{\omega(t)}$ . Therefore,

per time unit the variance of this total increment is equal to  $\frac{h^2}{\omega(1)}$ .

In other words, the sensitivity factor can be interpreted as half the variance of the total increment of coordinates of micro- and nanoparticle with the independent "jumps" in nodes of a discrete grid  $\{m = 0, \pm 1, \pm 2, \dots\}$  per time unit. Now we can interpret from the probabilistic point of view also the nature of the limiting process  $\Delta x, \Delta t \rightarrow 0$  from discrete 1D model (1) to a continuous 1D model (3). Indeed, as mentioned above, the parameter  $\omega$  in the expression the sensitivity coefficient has the order  $h^2$ , i.e.  $\omega \square h^2$ . And that, by the virtue of the described above probabilistic interpretation, is equivalent to the total variance of the increment of the spatial coordinates of micro- and nanoparticle in a fixed time  $t$  remaining a constant during the implementation of a limiting process  $\Delta x, \Delta t \rightarrow 0$ . This property is really a bit of a surprise and at the same time we find that the total path traversed by each micro- and nanoparticle in a fixed time  $t$  (all movements of micro- and nanoparticles, irrespective of their directions of movement, are

summed over their absolute values), is  $\Delta x \cdot \frac{t}{\Delta t} = \frac{(\Delta x)^2}{\Delta t} \cdot \frac{t}{\Delta x}$  and,

therefore, for the limiting process  $\Delta x, \Delta t \rightarrow 0$  the length of this path tends to infinity. This shows that the closer to the limit (of course, figuratively speaking), the greater the "instantaneous speed" of the micro- and nanoparticle. That is why in the limit the edge of the "sprawling" segment diverges completely, instantly "leaving" to infinity. After performing the limiting process from the discrete model (1) to the continuous model (3), the probabilistic interpretation of the sensitivity coefficient is the same as interpreted above. Note that the density  $\rho(x, t)$  of micro- and nanoparticles in the gaseous medium after the above probabilistic interpretation of the discrete model (1) can be interpreted as the density of the mathematical expectation of "the mass of micro- and nanoparticles". In the case studying "random motion" of only one micro- or nanoparticle, the function  $\rho(x, t)$  implies the probability density, i.e. is understood as a function of the probability distribution of finding this micro and nanoparticle: then, of course, should be satisfied the necessary condition of normalization  $\int \rho(x, t) dx \equiv 1$ .

In particular, if we formulate for the equation (3) the initial boundary value problem

$$\left. \begin{aligned} \frac{\partial \rho(x, t)}{\partial t} &= \frac{h^2}{2 \cdot \omega} \cdot \frac{\partial^2 \rho(x, t)}{\partial x^2}, \quad 0 < x < l, \quad 0 < t \leq T; \\ \rho(x, t) \Big|_{t=0} &= \rho_0(x), \quad 0 \leq x \leq l; \\ \left[ \frac{\partial \rho(x, t)}{\partial x} - \lambda_i \cdot \rho(x, t) \right] \Big|_{x=x_i} &= \rho_i(t), \quad 0 \leq t \leq T \\ \left[ \rho'_0(x) - \lambda_1 \cdot \rho_0(x) \right] \Big|_{x=x_1} &= \rho_i(t) \Big|_{t=0+0} \\ x_1 &= 0+0, \quad x_2 = l-0, \end{aligned} \right\}, \quad i = 1, 2, \quad (5)$$

then Green's Function

$$G^{(Newton)}(x, \xi; t, \tau) = \sum_{n=1}^{+\infty} \frac{G_n \cdot \sqrt{(\lambda_1^2 + \theta_n^2) \cdot (\lambda_2^2 + \theta_n^2)}}{\theta_n^2} \times \\ \times \cos(\theta_n \cdot x - \beta_1) \cdot \cos(\theta_n \cdot \xi - \beta_2) \cdot e^{-\frac{(h \cdot \theta_n)^2 \cdot (t - \tau)}{2 \cdot \omega}},$$

$$G_n = \frac{2 \cdot \theta_n^2 \cdot (\theta_n^2 + \lambda_2^2)}{\lambda_1 \cdot (\theta_n^2 + \lambda_2^2) + \lambda_2 \cdot (\theta_n^2 + \lambda_1^2) + l \cdot (\theta_n^2 + \lambda_1^2) \cdot (\theta_n^2 + \lambda_2^2)},$$

$$\theta_n > 0: \operatorname{tg}(\theta_n \cdot l) = \theta_n \cdot \frac{\lambda_1 + \lambda_2}{\theta_n^2 - \lambda_1 \cdot \lambda_2},$$

$$\beta_i (i=1,2): \cos \beta_i = \frac{\theta_n}{\sqrt{\lambda_i^2 + \theta_n^2}},$$

present in the solution of the boundary value problem (5)

$$\rho(x, t) = \int_0^l G(x, \xi; t, 0) \cdot \rho_0(\xi) d\xi - \frac{h^2}{2 \cdot \tau} \cdot \left( \int_0^l G(x, 0; t, \tau) \cdot \rho_1(\tau) d\tau - \int_0^l G(x, l; t, \tau) \cdot \rho_2(\tau) d\tau \right) \quad (6)$$

as a function of instantaneous sources (or as an influence function for  $\xi = 0$  и  $\tau = 0$ ) equals the probability density of finding a micro- or nanoparticle at time moment  $t > 0$ , only if that the micro- or nanoparticle at time moment  $t = 0$  was located in a sufficiently small neighbourhood of point  $x = 0$ .

Considering for the equation (3), the Cauchy problem

$$\begin{cases} \frac{\partial \rho(x, t)}{\partial t} = \frac{h^2}{2 \cdot \tau} \cdot \frac{\partial^2 \rho(x, t)}{\partial x^2}, & x \in \square^1, 0 < t \leq T, \\ \rho(x, t)|_{t=0} = \rho_0(x), & x \in \square^1, \end{cases} \quad (7)$$

then for  $\forall t > 0$  and  $\forall x \in \square^1$  the corresponding influence function

$$G^{(Cauchy)}(x, \xi; t, \tau) = \sqrt{\frac{\omega}{2 \cdot \pi \cdot h^2 \cdot (t - \tau)}} \cdot e^{-\frac{\omega(x - \xi)^2}{2 \cdot h^2 \cdot (t - \tau)}}$$

(this function is a solution of the problem (7) with the initial condition  $\rho_0(x) = \delta(x - \xi)$ ) at point  $(\xi = 0, \tau = 0)$  equals

$$\sqrt{\frac{\omega}{2 \cdot \pi \cdot h^2 \cdot t}} \cdot e^{-\left(\frac{x}{h}\right)^2 \frac{\omega}{2t}}, \text{ i.e. the influence function is the}$$

probability density of the micro- and nanoparticle in the gaseous medium at time moment  $t > 0$ , only if the micro- or nanoparticle initially at time moment  $t = 0$  was located at point  $x = 0$ . Further, it is easy to calculate the average absolute increment of the coordinates of the micro- and nano-particle in the gaseous medium

$$\text{during } t: \int_{\square^1} \sqrt{\frac{\omega}{2 \cdot \pi \cdot h^2 \cdot t}} \cdot e^{-\left(\frac{x}{h}\right)^2 \frac{\omega}{2t}} \cdot |x| dx = \sqrt{\frac{4 \cdot t}{\pi}} \cdot \sqrt{\frac{h^2}{2 \cdot \omega}}.$$

other words, the average absolute increment of coordinate for the considered "single" micro- and nanoparticle is proportional to the square root of the proportionality coefficient (between the intensity and density gradient of micro- and nanoparticles in the 1D gaseous medium) and to the value  $\sqrt{t}$ . This result is consistent with the mean square increment of coordinate of micro- and nanoparticle found above.

Returning to the recurrent formula (1), we emphasize again that it describes a discrete "wandering" of micro- and nanoparticles in an unit of volume of the 1D gaseous medium and was derived from the assumption that in each subsequent time moment in any point of the considered unit of volume of the gas flow there will come exactly half of the micro- and nanoparticles which were in the previous time moment in the adjacent points to the left and exactly half of the micro- and nanoparticles which were in the previous time moment in the adjacent points to the right. In other words, as the discrete model (1), and the continuous model (3) (or initial boundary value problem (5) for this model) derived from this discrete model by the

use of a limiting process (under certain additional restrictions), describe the dynamics of the distribution of micro- and nanoparticles in an unit of volume in the gas flow of the 1D medium, when the random walk of micro- and nanoparticles are allowed only to available adjacent locations on the left or right of the current location of each micro- and nanoparticle. In other words, the constructed discrete model (1) and continuous model (3) (or (5)) are mathematical models of the walk of micro- and nanoparticles in an unit of volume of the gas flow "with equally probable preference." However, in the future, we will use the term "wandering with preference" instead of a more correct term "wandering with equally probable preference", although it should be emphasized that the case, when the movement "with preference" of micro- and nanoparticle is not equally probable to neighbouring nodes of the discrete grid, the discrete model (1) (and, therefore, the continuous model (3)) will not describe this case – instead of the recurrent formula (1) there will be another recurrent formula, that differs significantly from the formula (1).

To conclude this subsection, using (5), (6) we can explain the mechanism of behaviour of the continuous 1D model (5) derived from the discrete model (1) with the strict equality sign. Indeed, taking  $t = 0$ , we can say that the solution of the discrete model (1) at the left end of the considered segment, i.e. at point  $x = 0$ , identically equals to zero, since the model (1) with the sign of the strict equality is the model of the evolution of density of micro- and nanoparticles in the gaseous medium "concentrated" for  $t = 0$  in a small neighbourhood of the left edge of the considered segment. At the same time, as it can be seen from the formula (6), for all values  $x \in [0, l]$  the solutions  $\rho(x, t)$  are strictly positive. Hence, near the edges of the "blurred" segment, the continuous 1D model (6) loses its adequacy of being the true model, even if approximate, to determine the density of micro and nanoparticles in an unit of volume of the gas flow.

#### **Construction of the general discrete 1D model and the question of the correct limiting process in obtaining the appropriate continuous 1D model**

As has been mentioned in the previous sub-section, constructed particular models are models describing the dynamics of "with preference" micro- and nanoparticles in the gas flow of the 1D medium. Now we abandon the previous assumptions that are allowed the micro- and nanoparticles to locomote in the gaseous medium only to the neighbouring free places with respect to the current location of each micro- and nanoparticles per a volume unit of gas flow. Namely, we will make the following four basic assumptions:

**Assumption C:** At each time moment  $t = 0, \Delta t, 2 \cdot \Delta t, 3 \cdot \Delta t, \dots$  each of the micro- and nanoparticles per volume unit of the gaseous medium can have one of coordinates  $0, \pm \Delta x, \pm 2 \cdot \Delta x, \pm 3 \cdot \Delta x, \dots$ ;

**Assumption D:** If any of the micro- or nanoparticles in the volume unit of the 1D gas flow has coordinate  $i \cdot \Delta x$  ( $i \in \square$ ) at time moment  $n \cdot \Delta t$  ( $n \in \{0 \cup \square\}$ ), then at the next time moment  $(n+1) \cdot \Delta t$  ( $n \in \{0 \cup \square\}$ ) the same micro- or nanoparticle can have any of the coordinates  $j \cdot \Delta x$  ( $j \in \square$ ) (not only neighbouring with the cell  $i \cdot \Delta x$  coordinates  $(i-1) \cdot \Delta x$  or  $(i+1) \cdot \Delta x$ ) with probability

$$p_{n;i,j} \stackrel{def}{=} p(n; i, j) \quad (n \in \{0 \cup \square\}; i, j \in \square); \quad (8)$$

**Assumption E:** The transition probabilities correspond to the Markovian process: for each micro- and nanoparticle in the volume unit of the gaseous medium the probability  $p_{n;i,j}$  of its location in

the cell  $i \cdot \Delta x$  ( $i \in \square$ ) at the time moment  $n \cdot \Delta t$  ( $n \in \{0 \cup \square\}$ ), and in the cell  $j \cdot \Delta x$  ( $j \in \square$ ) at the next time moment  $(n+1) \cdot \Delta t$  ( $n \in \{0 \cup \square\}$ ), obeys Markov property. It means that the probabilities  $p_{n;i,j}$  ( $n \in \{0 \cup \square\}$ ;  $i, j \in \square$ ) do not depend neither on the "gas-particles" system state at the previous time moments, nor on the behaviour of other micro- and nanoparticles in the same volume unit of the gaseous medium;

**Assumption F:** In the considered "particle-gas" system the micro- and nanoparticles are assumed to be almost homogeneous, and it is believed that the physical properties of the system do not depend on the direction of the walk of the micro- and nanoparticles in the gaseous medium.

Obviously, that the first of the listed four assumptions coincides with the principal assumption A made in the first subsection deriving the discrete model (1): namely the assumption A, which generates the linearity property (for the addition of initial distribution of micro- and nanoparticles in the gas flow, distribution at arbitrary time moment and subsequent time moment are summed up too), allowing to apply the principle of superposition. Looking ahead, we note that the latter assumption (i.e. assumption F), unlike the other assumptions, will not be active for the construction of the mathematical model, however, this assumption will be essential for the investigation of the constructed mathematical model, namely, for the proof of the constructed mathematical model having versatility in a certain sense (see the following subsection). Assumptions D and E, as it will be shown below, radically change the base of the considered probabilistic process of random walk of micro- and nanoparticles in the gas flow, which was also used as a base in the previous subsection for construction of mathematical models (1) and (3) (or (5)). Indeed, due to the fact that in this system of "particle-gas" each micro- or nanoparticle must be somewhere, we can write

$$\sum_{j=0,\pm 1,\pm 2,\dots} p_{n;i,j} \equiv 1 \quad \forall n \in \{0 \cup \square\}; \quad \forall i \in \square. \quad (9)$$

However, by analogy with the identity (9) we cannot say that  $\sum_{i=0,\pm 1,\pm 2,\dots} p_{n;i,j} = 1$ , since the value of  $\sum_{i=0,\pm 1,\pm 2,\dots} p_{n;i,j}$  can take a value larger than one if the point  $j \cdot \Delta x$  ( $j \in \square$ ) of the considered segment  $[-l, +l]$  is preferable for specific micro- and nanoparticle in the gas flow; and this sum may be less than one if, on the contrary, the point  $j \cdot \Delta x$  ( $j \in \square$ ) is not preferable for specific micro- and nanoparticle in the gas flow. By analogy with the function  $U(m, n)$  introduced in the first subsection we introduce a new function  $U(m, n) \stackrel{\text{def}}{=} U(m \cdot \Delta x; n \cdot \Delta t)$ ,  $\Delta x \equiv \text{const.}$ ;  $\Delta t \equiv \text{const.}$ ;  $m \in \square$ ;  $n = \{0\} \cup \square$ , which is the number of micro- and nanoparticles in the gas flow at a time moment  $n \cdot \Delta t$  in the point with coordinate  $m \cdot \Delta x$ . Within time interval  $[n \cdot \Delta t, n \cdot \Delta t + \Delta t]$ ,  $n \in \{0\} \cup \square$  the number of micro and nanoparticles, passing from point  $m_1 \cdot \Delta x$  ( $m_1 \in \square$ ) on the considered segment of length  $2 \cdot l$  to any other point  $m_2 \cdot \Delta x$  ( $m_2 \in \square$ ;  $m_2 \neq m_1$ ) of the same segment will be equal to  $U(m_1, n) \cdot p_{n;m_1,m_2}$ . Within the same time interval, in the opposite direction, i.e. from the point  $m_2 \cdot \Delta x$  ( $m_2 \in \square$ ) to the point  $m_1 \cdot \Delta x$  ( $m_1 \in \square$ ;  $m_1 \neq m_2$ ), there will go exactly  $U(m_2, n) \cdot p_{n;m_2,m_1}$  micro- and nanoparticles. Therefore, we can

write the "micro- and nanoparticles balance" by the following recursive relation:

$$\begin{aligned} U(m_1, n+1) &\approx U(m_1, n) - U(m_1, n) \cdot \sum_{\substack{m_2 \in \square \\ m_2 \neq m_1}} p_{n;m_1,m_2} + \\ &+ \sum_{\substack{m_2 \in \square \\ m_2 \neq m_1}} \{U(m_2, n) \cdot p_{n;m_2,m_1}\} = U(m_1, n) + \\ &+ \sum_{\substack{m_2 \in \square \\ m_2 \neq m_1}} \{U(m_2, n) \cdot p_{n;m_2,m_1}\} - \{1 - p_{n;m_2,m_1}\} \cdot U(m_1, n) = \\ &= \sum_{m_2 \in \square} \{U(m_2, n) \cdot p_{n;m_2,m_1}\}. \end{aligned}$$

So;

$$U(m_1, n+1) \approx \sum_{m_2 \in \square} \{U(m_2, n) \cdot p_{n;m_2,m_1}\} \quad (\forall m_1 \in \square). \quad (10)$$

Sense of (10) is quite obvious: any micro- and nanoparticle in the considered volume unit of gas flow at time moment  $n \cdot \Delta t + \Delta t$  ( $n = 0, 1, 2, \dots$ ) must come from somewhere to the point with coordinate  $m_1 \cdot \Delta x$  ( $m_1 \in \square$ ). It is appropriate to note that the discrete model (1) built in the first subsection is a special case of the discrete model (10). Indeed, assuming in (10) that

$$\forall m_1, m_2 \in \square : p_{n;m_2,m_1} = \begin{cases} \frac{1}{2}, & \text{if } |m_1 - m_2| = 1; \\ 0, & \text{if } |m_1 - m_2| \neq 1, \end{cases}$$

we get the recurrence formula (1).

Absolutely in the same manner as in the first subsection in the discrete model (1) the limiting processes  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$  were performed, we can also implement the relevant limiting processes  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$  in the discrete model (10). This can occur together with the following two situations:

**Situation A:** If the average "jump" of each micro- and nanoparticle in the considered gas flow for one time step also tends to zero for  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$ , then the limiting processes  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$  in the discrete model (10) again lead to a differential equation with respect to the required density  $\rho(x, t)$  of micro- and nanoparticles in the gas flow, and in the equation (in particular, equation (3)) only those micro- and nanoparticles of the gas flow will be "connected" which form a kind of a continuous medium in which the micro and nanoparticles do not collide (do not interact), but are "infinitely close" to each other. For example, if determined by the formula (8) discrete function  $p_{n;i,j}$  does not depend on  $n \in \{0 \cup \square\}$  (i.e.  $p_{n;i,j} \equiv p_{i,j}$  for  $\forall n \in \{0 \cup \square\}$ ) and has the form  $p_{i,j} = p(i-j)$ ,  $i, j \in \square$ , then, obviously, the average "jump" of each micro- and nanoparticle in the given volume unit of the gas flow for one time step tends to zero;

**Situation B:** If the average "jump" of each micro- and nanoparticle for one time step does not obligatory tend to zero for  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$ , then the limiting processes  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$  in the discrete model (10) will lead to an integral (total) ratio relative to the required density  $\rho(x, t)$  of micro- and nanoparticles in the gas flow, i.e. in this case for  $\Delta x \rightarrow 0, \Delta t \rightarrow 0$  sums will turn into not into partial derivatives, but integrals.

We will not examine the situation A, but study the situation B. However, after examining this situation we will return to the situation A in two different ways, namely, in the results obtained in the situation B, we will directly assume that the situation A holds.

So, we assume that the situation B holds. Then, we rewrite the discrete model (10) in the following form:

$$U(m_1, n+1) - U(m_1, n) \approx \sum_{\substack{m_2 \in \mathbb{Z} \\ m_2 \neq m_1}} \{U(m_2, n) \cdot p_{n; m_2, m_1}\} - \\ -U(m_1, n) \cdot \sum_{\substack{m_2 \in \mathbb{Z} \\ m_2 \neq m_1}} p_{n; m_1, m_2}.$$

Dividing this equation by  $\Delta t$ , and then taking into account the notation (2) from the first subsection in this expression, we have

$$\frac{\Delta x}{m_{const.}} \cdot \frac{\Delta \rho(m_1 \Delta x, n \Delta t)}{\Delta t} = \\ = \frac{\Delta x}{m_{const.}} \cdot \left\{ \sum_{\substack{m_2 \in \mathbb{Z} \\ m_2 \neq m_1}} \rho(m_2 \Delta x, n \Delta t) \cdot K(n \Delta t; m_2 \Delta x, m_1 \Delta x) - \right. \\ \left. - \rho(m_1 \Delta x, n \Delta t) \cdot \sum_{\substack{m_2 \in \mathbb{Z} \\ m_2 \neq m_1}} K(n \Delta t; m_1 \Delta x, m_2 \Delta x) \right\}, \quad (11)$$

where  $K(n \cdot \Delta t; p_1 \cdot \Delta x, p_2 \cdot \Delta x) \stackrel{def}{=} \frac{p(n \cdot \Delta t; p_1 \cdot \Delta x, p_2 \cdot \Delta x)}{\Delta t}$

and  $p_i \in \{m_1, m_2\}$ ,  $i = 1, 2$ .

Now, denoting in the equation (11)  $x = m_1 \cdot \Delta x$ ,  $y = m_2 \cdot \Delta x$ ,  $t = n \cdot \Delta t$ , and then performing limiting processes  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ , we obtain the following integro-differential equation with the respect to the required density  $\rho(x, t)$  of micro- and nanoparticles in the 1D gas flow:

$$\frac{\partial \rho(x, t)}{\partial t} = \int_{-l}^{+l} K(t; y, x) \cdot \rho(y, t) dy - \\ - \rho(x, t) \cdot \int_{-l}^{+l} K(t; x, y) dy; \quad x \in (-l, +l), \quad t \in (0, T], \quad (12)$$

where function  $K(t; z_1, z_2) \geq 0$ ,  $t \in [0, T]$ ,  $z_i \in [-l, +l]$ ,  $i = 1, 2$  is the kernel of the integro-differential equation (12), and is interpreted as follows: the probability that each micro- and nanoparticle in the gas flow which at time moment  $t \in [0, T]$  was in the point  $z_1 \in [-l, +l]$ , at the next time moment  $t + \Delta t$  will be in the interval  $[z_2, z_2 + dz_2] \subset [-l, +l]$  ( $z_1 \neq z_2$ ), is equal to  $K(t; z_1, z_2) dz_2 dt$ . In other words, kernel  $K(t; z_1, z_2)$  is defined as the probability density of "jump" (taken relative to unit of time) of micro- and nanoparticles in the gas flow from point  $z_1 \in [-l, +l]$  to point  $z_2 \in [-l, +l]$  ( $z_1 \neq z_2$ ) at time moment  $t \in [0, T]$ . In other words, the function  $K(t; z_1, z_2)$  is the relative velocity of such a random "jump" of each of the micro- and nanoparticles in volume unit of gas flow at time moment  $t$ . It is worth to note that in (12) (and further throughout this paper), the value  $T$ , which means the end of the time interval within which the random movement of the dynamics of micro- and nanoparticles in the gas flow is studied, can be equal to infinity. Note that passing from the discrete equation (10) to the continuous equation (12), a well-known principle of continuous medium was used.

Thus, the integro-differential equation (12) with the initial condition  $\rho(x, t)|_{t=0} = \rho_0(x)$ ,  $x \in [-l, +l]$  (13)

is a 1D model of random walk with "no preference" of micro- and nanoparticles in the gas flow in which the unknown function is the density  $\rho(x, t)$ ,  $x \in [-l, +l]$ ,  $t \in [0, T]$  of micro- and nanoparticles. Recall that this mathematical model was obtained under the assumption of having the situation B: the average "jump" of each micro- and nanoparticle for one time step does not tend to zero for  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ . It is interesting to find out what result can be obtained if in the integro-differential equation (12), which is obtained during implementation of the situation B, the situation A will be implemented? In fact, this question implies that we want to find out to which extent the constructed mathematical model (12), (13) is a more general model (in some sense, a universal model for the considered class of "particle-gas" models) to determine the density  $\rho(x, t)$  of micro- and nanoparticles in the gas flow.

Obviously, if the model is more general than, for instance, the continuous 1D model (3) of random walk of micro- and nanoparticles "with equally probable preference," then there appears the question of finding conditions under which a transition can be made from the model (12), (13) to other models, in particular, to the model (3). In the following subsections, along with other issues, we will investigate this question.

#### Investigation of the continuous 1D model (12), (13)

To find out whether it is possible to directly assume in the built integro-differential equation that the average "jump" of each micro- and nanoparticle in the given volume unit of the gas flow for one time step also tends to zero for  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ , we first transform the equation (12). To do this, we use the well-known formula  $f(y) = \int \delta(x-y) \cdot f(x) dx$ , where  $\delta(\square)$  is the Dirac delta function. In this formula as the function  $f(\square)$  we choose the

function  $\int_{-l}^{+l} K(t; \square, \xi) d\xi$ . Then we obtain the identity

$$\int_{-l}^{+l} \left\{ K(t; y, x) - \delta(x-y) \cdot \int_{-l}^{+l} K(t; x, \xi) d\xi \right\} dx = 0, \quad y \in [-l, +l].$$

Let's consider this identity in the equation (13):

$$\frac{\partial \rho(x, t)}{\partial t} = \int_{-l}^{+l} \tilde{K}(t; y, x) \cdot \rho(y, t) dy, \quad (14)$$

where  $\tilde{K}(t; y, x) \stackrel{def}{=} K(t; y, x) - \delta(x-y) \cdot \int_{-l}^{+l} K(t; x, \xi) d\xi$ ,

$$\forall x \in (-l, +l), \forall t \in (0, T].$$

The integro-differential equation (14) is equivalent to the integro-differential equation (12). Therefore, the model (14) is also a 1D model of random walk with "no preference" of the micro- and nanoparticle in the given volume unit of gas flow in respect with the required density  $\rho(x, t)$ ,  $x \in [-l, +l]$ ,  $t \in [0, T]$  of micro- and nanoparticles, and this model is constructed under the assumption that the average "jump" of each micro- and nanoparticle for one time step does not tend to zero for  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ . Now in (14), we assume that the average free "jump" of each micro- and nanoparticle for one time step tends to zero  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ , i.e. in (14) we assume that the kernel  $\tilde{K}(t; y, x)$  (or the kernel  $K(t; x, y)$ , if an equivalent integro-differential equation (12) is considered) for any fixed  $x$  and  $t$  as a function of one variable  $y$  is

different from zero only in a small neighbourhood of the point  $x$ : let  $t = t_0 \in [0, T]$ ,  $\forall x = x_0 \in [-l, +l]$  and

$$\tilde{K}(t_0; y, x_0) = \begin{cases} \bar{K}(y) \neq 0, & \text{if } y \in B(\varepsilon; x_0), \\ 0, & \text{otherwise,} \end{cases} \quad (15)$$

where  $B(\varepsilon; x_0) \stackrel{\text{def}}{=} \{z: \forall \varepsilon > 0 \mid |z - x_0| < \varepsilon\}$  is a  $\varepsilon$ -neighbourhood of the point  $x_0 \in [-l, +l]$ .

The assumption we just have made allows to state that the main contribution of the integral from the equation (14) in the region  $B(\varepsilon; x_0)$  is carried out over the variable  $y$ . Therefore, we can use the expansion of the density function  $\rho(y, t)$  in Taylor's series at

$$\text{point } x \in B(\varepsilon; x_0): \quad \rho(y, t) = \sum_{i=0}^{\infty} \frac{\partial \rho^i(x, t)}{\partial x^i} \cdot \frac{(y-x)^i}{i!}.$$

Substituting this expansion to the right side of the integro-differential equation (14), and then taking into account assumption F (which in the language of mathematics can be written as follows:

$$K(t; z_1, z_2) = K(t; |z_1 - z_2|), \quad \forall z_i \in [-l, +l], \quad i = 1, 2):$$

$$\begin{aligned} \frac{\partial \rho(x, t)}{\partial t} &= \rho(x, t) \cdot \int_{-l}^{+l} \{K(t; y, x) - K(t; x, y)\} dy + \\ &+ \sum_{i=1}^{\infty} \frac{1}{i!} \cdot \frac{\partial \rho^i(x, t)}{\partial x^i} \cdot \int_{-l}^{+l} K(t; y, x) \cdot (y-x)^i dy = \\ &= \sum_{i=1}^{\infty} \frac{1}{i!} \cdot \frac{\partial \rho^i(x, t)}{\partial x^i} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^i dy = \\ &= \sum_{i=1}^{\infty} \frac{1}{(2 \cdot i)!} \cdot \frac{\partial \rho^{2i}(x, t)}{\partial x^{2i}} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^{2i} dy. \end{aligned}$$

Thus, under the conditions that

- ◆ the average free "jump" of each micro- and nanoparticle for one time step tends to zero for  $\Delta x \rightarrow 0$ ,  $\Delta t \rightarrow 0$ ,
- ◆ the "particles-gas" system is homogeneous, and the physical properties of the system do not depend on the direction of random walk of micro- and nanoparticles in the gas flow,

we have obtained the following result: regardless of the particular type of kernel  $K(t; z_1, z_2)$  (recall that the kernel  $K(t; z_1, z_2)$  is defined as the probability density of the "shift" (taken relative to unit of time) of the micro- and nanoparticles from point  $z_1 \in [-l, +l]$  to point  $z_2 \in [-l, +l]$  ( $z_2 \neq z_1$ ) at time moment  $t \in [0, T]$ ), the density  $\rho(x, t)$ ,  $(x, t) \in (-l, +l) \times (0, T)$  of micro- and nanoparticles satisfies the integro-differential equation

$$\frac{\partial \rho(x, t)}{\partial t} = \sum_{i=1}^{\infty} \frac{1}{(2 \cdot i)!} \cdot \frac{\partial \rho^{2i}(x, t)}{\partial x^{2i}} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^{2i} dy. \quad (16)$$

From the equation (16), it is now easy to deduce the 1D model (3), which describes the walk "with equally probable preference" of micro- and nanoparticles in the gas flow. Indeed, from (16), it follows

$$\frac{\partial \rho(x, t)}{\partial t} = \frac{1}{2} \cdot \frac{\partial \rho^2(x, t)}{\partial x^2} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^2 dy +$$

$$\begin{aligned} &+ \sum_{i=2}^{\infty} \frac{1}{(2 \cdot i)!} \cdot \frac{\partial \rho^{2i}(x, t)}{\partial x^{2i}} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^{2i} dy = \\ &= \frac{1}{2} \cdot \frac{\partial \rho^2(x, t)}{\partial x^2} \cdot \int_{-l}^{+l} K(t; |z|) \cdot z^2 dz + o((y-x)^3) = \\ &= \frac{\partial \rho^2(x, t)}{\partial x^2} \cdot \int_0^{+l} K(t; z) \cdot z^2 dz + o((y-x)^3). \end{aligned}$$

In this equation, ignoring  $o((y-x)^3)$  (which is justified by assumption (15)) and introducing the function (at this stage, formally)  $a(t) \stackrel{\text{def}}{=} \int_0^{+l} K(t; z) \cdot z^2 dz > 0$ ,  $\forall t \in (0, T]$  we obtain the

$$\text{equation (3), in which } a(t) = \frac{h^2}{2 \cdot \omega(t)}.$$

The method by use of which we obtained model (3) from the equation (16) allows to obtain other continuous 1D models from the same equation (16). Precisely in this context, the equation (16) is (under the assumptions made) the general equation for determining the required density  $\rho(x, t)$  of micro and nanoparticles in the gas flow. It should be emphasized that, from the point of view of mathematical rigor, introducing the function  $a(t)$  was purely formal, because the issue

of the convergence of the integral  $\int_0^{+l} K(t; z) \cdot z^2 dz$  was not clarified: from the equation (12) (or (14)), only the convergence of  $\int_0^{+l} K(t; z) dz$  follows directly, but the convergence  $\int_0^{+l} K(t; z) \cdot z^2 dz$  cannot be guaranteed. That is why the question of

rate of decrease of the kernel  $K(t; z)$  with the growth of  $z$  for any fixed parameter  $t = t_0 \in (0, T]$  arises. In other words, it is necessary to find a condition satisfying which would guarantee the influence of the kernel  $K(t = t_0; z)$  concentrating in a small neighbourhood of zero (it is the same as the influence of the kernel  $K(t = t_0; y, x = x_0)$  concentrating in  $B(\varepsilon; x_0)$ ,  $\forall \varepsilon > 0$ ,  $\forall x_0 \in [-l, +l]$ ). To find this desired condition, we note that in the right-hand side of the equation (16) ignoring the term

$$\frac{\partial \rho^{2i}(x, t)}{\partial x^{2i}} \cdot \int_{-l}^{+l} K(t; |y-x|) \cdot (y-x)^{2i} dy, \quad i \in \square$$

is possible only if the following inequality holds:

$$\frac{1}{(2i)!} \left| \frac{\partial \rho^{2i}(x, t)}{\partial x^{2i}} \right| \int_{-l}^{+l} K(t; |y-x|) (y-x)^{2i} dy \square$$

$$\frac{1}{(2i)!} \left| \frac{\partial \rho^{2(i+1)}(x, t)}{\partial x^{2(i+1)}} \right| \int_{-l}^{+l} K(t; |y-x|) (y-x)^{2(i+1)} dy, \quad i \in \square.$$

Consequently, for the legitimacy of introducing the function  $a(t)$  and, consequently, for the correctness of the equation (3), it is



sufficient to satisfy the condition

$$12. \left| \frac{\partial \rho^2(x,t)}{\partial x^2} \right| \cdot \int_0^{+l} K(t;z) z^2 dz \square \tag{17}$$

$$\square \left| \frac{\partial \rho^4(x,t)}{\partial x^4} \right| \cdot \int_0^{+l} K(t;z) z^4 dz, \forall x \in [-l, +l], \forall t \in (0, T].$$

Since the resulting inequality (17) features functions  $\left| \frac{\partial \rho^2(x,t)}{\partial x^2} \right|$  and  $\left| \frac{\partial \rho^4(x,t)}{\partial x^4} \right|$ , it is obvious that condition (17) is of little use from a practical point of view: in the specific tasks checking its implementation is impossible due to the presence of two unknown functions in it, because the density function  $\rho(x,t)$  is the required function. However, in many cases the average variation range of the density  $\rho(x,t)$  of micro- and nanoparticles in the gas flow can be easily measured, and using this characteristic of the considered "particles-gas" system it is easy to obtain from the relation (17) sufficient conditions for the transition from the model (16) to the model (3). Indeed, taking the value  $\Delta x$  as the average interval of "jump" of micro- and nanoparticles in the gas flow and taking  $\Delta \rho$  as the average density variation range of micro- and nanoparticles in this interval of "jump", it can be supposed that for each  $i \in \square$  the function  $\left| \frac{\partial \rho^i(x,t)}{\partial x^i} \right|$  is of the order  $\frac{\Delta \rho}{(\Delta x)^i}$ .

Therefore, instead of unsuitable conditions (17) we can write the easily verifiable condition

$$12. (\Delta x)^2 \cdot \int_0^{+l} K(t;z) z^2 dz \square \tag{18}$$

$$\square \int_0^{+l} K(t;z) z^4 dz, \forall x \in [-l, +l], \forall t \in (0, T].$$

Despite the fact that conditions (17) and (18) look similar, they have another significant difference (apart from the above difference that in (17), in contrast to (18), there are no unknown functions): condition (18) connects the kernel  $K(t; y, x)$  to the average range of change in the density of micro- and nanoparticles, and from condition (17) this fact cannot be established, because functions  $\left| \frac{\partial \rho^2(x,t)}{\partial x^2} \right|$  and  $\left| \frac{\partial \rho^4(x,t)}{\partial x^4} \right|$  appearing in it are unknown, consequently, they do not lend themselves to the comparative analysis.

Condition (18) is a sufficient condition for obtaining the model (5) from the integro-differential equation (16). In addition to it, condition (18) allows one to establish the following useful property of the equation (16): even if the kernel  $K(t; |y-x|)$  remains unchanged (see the probabilistic interpretation of the kernel, which was made immediately after deducing the equation (12)) for two random walk problems of micro- and nanoparticles in one of which, the value of the average interval  $\Delta x$  of "jump" of micro- and nanoparticles in the gas flow is relatively smaller than the corresponding values of  $\Delta x$  in the other problem, then the integral-differential equation (16) can lead to completely different models.

**Extension of results for the 2D gaseous medium**

In this subsection, generalizing the results obtained in the previous subsections, we offer a 2D model with respect to the probability density  $\rho(x_1, x_2, t)$  of micro- and nanoparticles in the

gas flow in the 2D medium:

$$\left\{ \begin{aligned} \frac{\partial \rho(x_1, x_2, t)}{\partial t} &= \int_{-l_1}^{+l_1} dy_1 \int_{-l_2}^{+l_2} K(t; y_1, y_2; x_1, x_2) \rho(y_1, y_2, t) dy_2 - \\ &- \rho(x_1, x_2, t) \int_{-l_1}^{+l_1} dy_1 \int_{-l_2}^{+l_2} K(t; x_1, x_2; y_1, y_2) dy_2, \\ (x_i, t) &\in (-l_i, +l_i) \times (0, T] \quad (i=1, 2); \\ \rho(x_1, x_2, t) \Big|_{t=0} &= \rho_0(x_1, x_2), \quad (x_1, x_2) \in S, \\ S &\stackrel{def}{=} [-l_1, +l_1] \times [-l_2, +l_2]. \end{aligned} \right. \tag{19}$$

In (19), the function  $\rho_0(x_1, x_2)$  is the primary distribution of micro- and nanoparticles of gas flow in the considered volume unit in the 2D medium; function  $K(t; z_1; z_2) \geq 0$ , where  $z_j = (z_1^j, z_2^j) \quad (j=1, 2), \quad z_i^j \in [-l_i, +l_i] \quad (i, j=1, 2),$

$t \in [0, T]$ , is the kernel of the integro-differential equation (19), which can be interpreted as follows: the probability that a micro- or nanoparticle in the 2D gas flow which at time moment  $t \in [0, T]$  is at point  $z_1 \in S$ , at next time moment  $(t + \Delta t)$  will be at area  $s \stackrel{def}{=} [z_2, z_2 + dz_2] \subset S \quad (z_2 \neq z_1)$  is equal to the value

$K(t; z_1; z_2) dz_1^2 dz_2^2 dt$ . In other words, the kernel  $K(t; z_1; z_2)$  is defined as the probability density of "jump" (taken relative to unit of time) of the micro- and nanoparticles in the gas flow from 2D point  $z_1 \in S$  to point  $z_2 \in S \quad (z_2 \neq z_1)$  at time  $t \in [0, T]$ . This means that the function  $K(t; z_1; z_2)$  describes the relative speed of such random "transfer" of micro- and nanoparticles in volume unit of 2D gas flow at time moment  $t$ . Next, having similar arguments and calculations, as it was done in the previous subsection in the preparation of (18) now we can write the following:

$$12 (\Delta s)^2 \int_0^{+l_1} dz_1 \int_0^{+l_2} \tilde{K}(t; z_1; z_2) (z_1^2 + z_2^2) dz_2 \square$$

$$\square \int_0^{+l_1} dz_1 \int_0^{+l_2} \tilde{K}(t; z_1; z_2) (z_1^2 + z_2^2)^2 dz_2, \forall s \in S,$$

which allows to obtain a 2D equation of heat and mass transfer from the model (19), and

$$\exists t \in [0, T] \quad \forall x = x_0 = (x_2^0, x_2^0) \in S \quad \text{such that}$$

- ◆ if  $y \in B(\varepsilon; x_0) \subset S$ , then

$$0 \neq \tilde{K}(t; y) \stackrel{def}{=} K(t; y; x_0) - \delta(x_0 - y) \int_{-l}^{+l} K(t; x_0; \xi) d\xi;$$

- ◆ if  $y \notin B(\varepsilon; x_0) \subset S$ , then

$$K(t; y; x_0) = \delta(x_0 - y) \int_{-l}^{+l} K(t; x_0; \xi) d\xi.$$

Here  $B(\varepsilon; x_0) \stackrel{def}{=} \{z = (z_1, z_2) : \|z - x_0\|_{R^2} < \varepsilon, \forall \varepsilon > 0\}$  denotes  $\varepsilon$ -neighbourhood of  $(x_2^0, x_2^0) \in S$ ; the function  $\delta(\cdot)$  is the Dirac function.

### 3. Conclusions

In the present work, first we built up a discrete 1D model based on the following assumptions: the influence of the gas on the micro- and nanoparticles is negligible; the influence of the micro- and nanoparticles on each other is negligibly small as compared to the influence of gas on the particles; micro- and nanoparticles can move in the gas flow in different directions. At each time step a particle moves by certain distance, not necessarily to the next position. These assumptions are quite natural if, e.g., the concentration of solid particles is sufficiently small, and if external forces are absent. This situation is typical in many important applications dealing with dilute particle flows. Further in the present work, we laid down some conditions under implementation of which it is possible to carry out limiting process in the built discrete 1D model: as a result we obtain a continuous 1D model as an initial-value boundary problem for certain integro-differential equation. A probabilistic interpretation of the obtained 1D model is provided, and its solvability is studied. We find that unique solution exists at certain sufficient condition. It is shown that the Fokker-Planck equation can be obtained from the integro-differential equation. Finally, a generalization to the 2D case of the investigated problem is performed.

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