Nanobiotech 2015

IOP Conf. Series: Materials Science and Engineering 98 (2015) 012022

Danger due to the translocation of nanoparticles in soil: mathematical modeling

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Abstract. A necessary step was taken towards the formation of a migration model of nanoparticles (NPs) from the surface deep into the soil, taking into account the frequency of precipitation and the processes of adsorption and desorption which occur in the soils. An equation for migration of nanoparticles in soil is proposed. A method of obtaining the averaged equations for long-term migration of NPs in the soil profile has been developed. Similarly, partial differential equations may be obtained which describe more complex models, for example, including capillary phenomena, etc. The obtained equations allow the use of integral transformations in order to find solutions. The model can be used to plan natural experiments in different types of soils.

1. Introduction

Over the last two decades an increase in diversity and overall production of nanomaterials, along with exponential growth in the number of goods which contain engineered nanoparticles and the extension of their application areas has been observed. The extension of nanotechnological manufacturing leads to an inflow of substantial amounts of nanomaterials to the environment, their accumulation in biota and the abiotic environment followed by their possible transmission to humans. The soil is a natural accumulator of NPs both from industrial aerosols and in the process of turnover of nanomaterials (including recycling). The degree of mobility of nanoparticles in the soil and their ability to migrate identifies the risk of NPs to biota, modulating the bioavailability of toxic or biologically active NPs. The possibility of NPs entering the food chains of agricultural production and the transmission of nanotoxicity to an ultimate consumer is also linked to this factor.

The development of technology for protecting agricultural production chains and assessment of the risks to agricultural production in areas of possible contamination with nanoparticles (including the migration of nanoparticles to adjacent water bodies by means of catena) is not possible without an understanding of the factors determining the intensity of migration. Mathematical modeling of physical and chemical processes which occur in the soil is the basis of effective forecasting of NPs' behavior. The study of vertical and lateral migration of substances in the soil profile for nanoparticles has so far practically not been carried out. At the same time, models of vertical migration were developed through the example of contaminants [1, 2] and they can be used for the migration modeling of NPs. In the existing literature on mathematical modeling of the migration of contaminants different models have been considered. The most complex ones take into account the hydrodynamic features of moisture movement [3-7], capillary effects, multistaging of sorption and desorption processes [8] and others [9-16].

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Nanobiotech 2015	IOP Publishing
IOP Conf. Series: Materials Science and Engineering 98 (2015) 012022	doi:10.1088/1757-899X/98/1/012022

However, all models consider the process of migration as a single one. This approach corresponds to the mode of humidification and it is far from the description of a real migration process. Thus, the influence of the factor of repeated wetting and drying on the migration process of substances in mathematical models appears to have been totally excluded from consideration. In other words, the influence of natural climatic factors is almost ignored.

In our opinion, a correct account of natural climatic factors even in the framework of a simple model of the elementary migration process is more important than an increase in complexity of the migration process model since this is the only way to achieve adequate compliance of the modeling results with the real natural process. In this work, on the basis of natural assumptions, partial differential equations were obtained. They describe the spatial and temporal distribution of nanoparticles in the soil profile from the source of NPs which appeared on the surface of the soil.

2. The model of the migration process

It is evident that a long-term process of migration is the result of overlap of a large number of elementary acts of migration which occur during each act of humidification.

In this paper we shall use the simplest physical and mathematical description of these elementary migration processes. In particular, some factors are not taken into consideration, namely, the presence of stagnant zones, possible variety of sorption centers, nonlinear motion of the humidification front, dissimilarity of humidification (within the humidified area), capillary phenomena, the hierarchy of structural organization of the soils, etc. In the future these factors can be taken into consideration if the model should require developing.

Thus we assume that on the surface of a soil profile there is a source of accrual of NPs with a surface density N. When humidified, the nanoparticles migrate down the soil profile along with the filtered moisture. Moving with the flow of the filtered moisture, the nanoparticles make chaotic diffusive motions together with the moisture and they are also adsorbed onto the soil particles. After being desorbed, the NPs again continue moving along the profile.

The main components of the flow of nanoparticles in the soil profile are convective and diffusive. The convective component prevails at the first stage. At the second stage, the diffusive component starts to prevail with the termination of the directional filtering movement of the moisture. When this stage of migration is described mathematically, the initial conditions for moving and adsorbed components of NP should be considered the distribution of them at the end of the first stage of humidification. The sum of moving and adsorbed components of NP after a period of diffusion is the initial distribution for the adsorbed component of the act of humidification n+1. For the n+1 act at the initial time the moving component equals 0 everywhere apart from the origin of coordinates.

Thus, in order to obtain a general long-term image of migration of NPs, it is necessary to consider the phenomenon of consistent overlap of individual acts of humidification. Moreover, it is evident that for simplification, the stage of diffusion spreading achieved at the stage of filtration of the distribution of moving and adsorbed components can be rejected.

We shall assume that the movement of moisture and the NPs occurs only vertically.

We shall use the following designations.

T – the macroscopic time of migration,

t – the time inside the time interval of an individual act of humidification $(T-T_0+t_{01}-t_{02})$,

 t_{01} – the duration of an elementary act of humidification until the moment when the movement of the water front ceases,

 t_{02} – the duration of the whole act of humidification until the moment of drying,

 t_{02} - t_{01} - the duration of the mainly diffusive movement inside the humidified profile after the filtrational movement has stopped,

t – the current time inside the interval of elementary humidification,

Obviously: t_{02} , $t_{01} << T$,

 Δ – the length of the free path of the NPs between collisions,

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V – the movement speed of the moisture being filtered (to simplify, we assume that V does not depend on x_1t_1 ; generalizations are obvious),

u – the speed of the chaotic diffusive movement,

x – the distance from the surface of the soil profile,

 c_1 – the density of the NPs which move with the moisture, c_2 – the density of the adsorbed NPs,

D – diffusion coefficient c_1 ,

 τ – the "lifetime" of the NPs in a free condition, which determines the decrease c_1 inside the flow under filtration due to adsorption

$$\frac{dc_1}{d_1t} = -\frac{c_1}{\tau}$$

 γ – the value which determines the speed of change N due to destruction of NPs by moisture (or trapping soil particles with NPs by moisture),

 γ_2 – the speed of desorbtion

$$\frac{dc_1}{d_1t} = -\gamma_2 c_2$$

 τ - the average time of collisionless motion of the NPs during diffusive motion.

3. The equation of migration during an elementary act of humidification

For convenience, we shall temporarily omit the dependence of c_1 , c_2 from T within one act of humidification, i.e. we shall assume

$$c_1(T+t) \equiv \bar{c}_1(t) c_2(T+t) \equiv \bar{c}_2(t)$$

We obtain the expression for the flow of the component c_1 including directional filtrational movement of the component c_1 , I_1 .

The flow density can be depicted as:

$$I \equiv \frac{1}{\tau_0} \int_{-\infty}^{t} e^{\frac{-(t-t')}{\tau_0}} \bar{c}_1(\dot{x}, \dot{t})(V+u) * \delta(x - (\dot{x} + (V+u)(t-\dot{t}))) dt' dx \int_{-\infty}^{+\infty} W(u) du$$
(1)

In (1) $\delta(z)$ - Dirac delta function, which equals zero everywhere except the point z=0, where it is equal to infinity,

Its integral is

$$\int_{-\infty}^{+\infty} \delta(z) dz = 1$$

t' - the moment of collision with complete chaotization of speed u; W(u) - distribution function of chaotic speed u.

Obviously:

$$\int_{-\infty}^{+\infty} W(u)udu = 0$$

The formula (1) reflects the fact of summation of contributions into the flow of all the NPs which arrive at the chosen point (x, t) and they experienced the last collision at the moment t' and they have the speed (V+u) after this collision.

The presence of the δ function allows us to perform the integration in (1) over *x*:

$$I \equiv \frac{1}{\tau_0} \int_{-\infty}^{\infty} e^{-\frac{(t-t')}{\tau_0}} \bar{c}_1(x - (t-t')_1 t') W(u) du dt$$

The average time between collisions is a very small value; that is why it is possible to consider t' as coinciding with t in the time dependence c from t'. The dependence from x can be depicted as:

$$\bar{c}_1(x - (V+u)(t-t')_1 t) \cong \bar{c}_1(x_1 t) - \frac{\partial \bar{c}_1(x_1 t)}{\partial x}(V+u)(t-t')$$

Then:

$$I = \frac{1}{\tau_0} \int_{-\infty}^{t} e^{-\frac{t-t'}{\tau_0}} \left[c_1(x_1 t) - \frac{\partial c_1(x_1 t)}{\partial x} (V+u)(t-t') \right] dt' \int_{-\infty}^{\infty} (V+u) W(u) du dt$$
(2)

Performing the required integration in (2), considering (3) we obtain:

$$I \equiv \bar{c}_1 V - D \frac{\partial \bar{c}_1}{\partial x} \tag{3}$$

Where: $D = \bar{u}^2 \tau$

 u^2 – the average square speed of the chaotic movement.

The second summand in (3) is a diffusion component of the flow. The larger it is, the higher the spatial heterogeneity c_1 . Its influence can be evaluated by comparing both summands in (3).

$$\bar{c}_1 V = D \frac{\partial \bar{c}_1}{\partial x}$$

which implies that under equilibrium conditions

$$\bar{c}_1 \sim e^{\frac{V}{D}}$$
, or $\bar{c}_1 \sim e^{\frac{Vx}{v\Delta}}$

Since the length of the free path Δ is a small value, then even where *V* and *u* are equal the diffusion component plays its role only when the distribution *c* is highly heterogeneous. However, the influence of diffusion can be affected when there is a long-term period of humidification without filtration.

In view of (3) the balance equation can be written as:

$$\frac{\partial \bar{c}_1}{\partial t} + \gamma_2 \bar{c}_2 - \frac{\bar{c}_1}{\tau} = -divI$$

Or

$$\frac{\partial \bar{c}_1}{\partial t} - \gamma_2 \bar{c}_2 + \frac{\bar{c}_1}{\tau} + V \frac{\partial \bar{c}_1}{\partial x} - D \frac{\partial \bar{c}_1}{\partial x^2} = 0$$
(4)

The equation (4) must be supplemented by the equation for c_2 :

$$\frac{\partial \bar{c}_2}{\partial t} = -\gamma_2 \bar{c}_2 + \frac{\bar{c}_1}{\tau} \tag{5}$$

The first summand in (4) describes the desorption of the absorbed NPs, the second describes the speed of adsorption.

It should be noted that the equations (4) and (5) are true when the humidification front has reached the considered point x, i.e. when x < Vt. Otherwise $c_1, c_2 \neq f_{1,2}(x, t)$ and then in (4) and (5) we have

$$c_1, c_2, \frac{1}{\tau}, \gamma_2, D, V = 0$$

Thus, the equations under consideration (4) and (5) are equations with variable coefficients which are not solved in a standard way by Laplace and Fourier integral transformations, and which require a different approach.

In accordance with the aforementioned, it rational to divide the time of humidification into 2 parts: the time of directionally moving moisture during filtration (from 0 to t_{10}) and the time of the drying of the moistened profile (from t_{10} to t_{20}). The value t_{20} is indefinite to a large degree, but it can be useful for completeness of modeling studies.

Thus, in the area from 0 to t_{01} we have:

$$\frac{\partial \bar{c}_1}{\partial t} - D \frac{\partial^2 \bar{c}_1}{\partial x^2} + \frac{\bar{c}_1}{\tau} + \bar{c}_2 y_2 = 0$$

$$\frac{\partial \bar{c}_2}{\partial t} + \frac{\bar{c}_1}{\tau} + \bar{c}_2 \gamma_2 = 0$$
(6)

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Similarly, in the area *t* from t_{01} to t_{02} we write:

$$\frac{\partial \bar{c}_1}{\partial t} - D \frac{\partial^2 \bar{c}_1}{\partial x^2} + \frac{\bar{c}_1}{\tau} + \bar{c}_2 y_2 = 0$$

The initial condition for the equations (7) are the values $c_1(x, t_{01})$ and $c_2(x_1, t_{01})$ which have been obtained as a result of solving the equations (12).

$$\frac{\partial \bar{c}_2}{\partial t} - \frac{\bar{c}_1}{\tau} + \bar{c}_2 \gamma_2 = 0 \tag{7}$$

In this work we neglect the influence of diffusion in order to simplify it and we obtain long-term equations for the component of NP which is averaged over the external conditions.

4. The boundary conditions

We determine the boundary conditions for $c_1(0,t)$ (i.e. on the surface of the soil profile).

It can be assumed that:

$$c_1(0,t) = \gamma N(t) \tag{8}$$

where γ is a constant which does not depend on time. It can be assumed that $\gamma \sim 1/V$, since the higher saturability of the soil solution of NP, the lower the speed of movement through a thin but ultimate layer of soil with NPs. So far we leave aside the dependence of γ on the temperature.

On the other hand, we can write:

$$\frac{\partial N}{\partial T} = -\bar{c}_1 V \tag{9}$$

(8) and (9) give

$$N(T + t) = N_{0e}^{-\gamma V(T+t)} = N_0(T)e^{-\gamma Vt}$$

where T_0 is the initial value of N (when T=0).

The boundary condition for c_1 :

$$c_1(0, T+t) = \gamma N_0(T) e^{-\gamma V t}$$
(10)

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Since during the drying of the soil profile c_1 disappears, transforming in accordance with the accepted model into c_2 the boundary condition (9) is true at any stage of humidification.

The boundary conditions for c_2 can be determined using balance equations (5). We depict c_2 in the form:

$$c_2(0, T + t) = c_2(0, T)\bar{c}_2(0, t)$$

The equation (5) then gives

$$\frac{\partial \bar{c}_1(0,t)}{\partial t} = -\gamma_2(c_2 + \bar{c}_2(0,t)) + \frac{c_1(0,T+t)}{\tau}$$

Taking into account the small change of c_1 and c_2 during the act of humidification, for the increment c_2 during the whole act of humidification can be recorded (including the component c_1 , which transforms into c_2 at the end of the humidification cycle t_0):

$$c_{2}(t_{0}) = -t_{0}\gamma c_{2}(T) + \frac{\gamma N(T)t_{0}}{\tau} + \gamma N(T)$$
(11)

The boundary condition for $\Delta c_2(0,t)$ depicts the relation (19) without the last summand:

$$\bar{c}_2(x,t) = -\gamma c_2(T)t + \frac{\gamma N(T)}{\tau}t$$
(12)

In (11) the assumption that there is little desorption during humidification ($\gamma V t_0 << 1$) is used.

Of interest are only the values of concentration c_1 and c_2 averaged over a long period of time. We average (12) over t_0 (the time of humidification or the relation $Vt_0=l_0$, of wetted depth l_0).

$$\bar{c}_2(t) = -\gamma_2 c_2(T) \nabla + \frac{\gamma N(T) \nabla}{\tau} + \gamma N$$

or

$$\frac{\bar{c}_2(t)}{\nabla} = -\gamma_2 c_2(T) + \gamma N(T) \left(\frac{1}{\tau} + \frac{1}{\nabla}\right)$$
(13)

Where ∇ is the average time of humidification. The left part (13) in fact depicts a derivative

$$\frac{\partial c_2(0,T)}{\partial T}$$

Then:

$$\frac{\partial c_2(0,T)}{\partial T} = -\gamma_2 c_2(T) + \frac{\gamma N(T)}{\tau}$$
(14)

The integration (14) gives:

$$c_2(0,T) = Ae^{-\gamma_2 T} + \frac{\gamma N_0(\frac{1}{\nabla} + \frac{1}{\tau})}{\gamma V - \gamma_2} (e^{-\gamma_2 T} - e^{-\gamma VT})$$
(15)

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The initial value for border density $c_2(0,0)$ is zero. This determines A in (15) and we finally obtain the boundary condition for c_2 .

$$c_2(0,T) = \frac{\gamma N_0(\frac{1}{\nabla} + \frac{1}{\tau})}{\gamma V - \gamma_2} (e^{-\gamma_2 T} - e^{-\gamma V T})$$
(16)

This boundary condition is necessary in order to obtain a unique solution of the partial differential equation found below, which describes the spatio-temporal dynamics of migration of the NPs.

We note that according to (16) $c_2(0,T)$ has a maximum, as the function of "large" time T. Its appearance reflects the obvious fact of accumulation of the NPs in the surface region and further flushing of it with a soil solution of low concentration with gradual depletion of the surface source of NPs.

5. Averaged (climate-oriented) equations of migration

The increment of the adsorbed component c_2 is considered small during one act of humidification and can be found. The total increment Δc_2 during several acts of humidification can be considered small as well. This allows us to average the obtained c_2 (during one humidification) in accordance with the statistics of precipitation. Then, considering it the differential increment per unit time (the gap between two humidifications), the differential equation for the value $c_2(x,T)$, averaged over the statistics of humidification, can be obtained. Here we practically do the same as when deriving the boundary conditions for $c_2(0,T)$. Since the component $c_2(x,T)$ does not accumulate with an increase in time by means of its transformation into c_2 , we can depict c_2 as:

$$c_2(x, T+t) = c_2(x, T) + c_2(x, t)$$
(17)

Where c_2 is the increment of c_2 during the investigated humidification $c_2 \ll c_2$ (T).

We write down these equations neglecting the small values c_2 in the first equation (6):

$$V\frac{\partial c_1}{\partial x} + \frac{\partial c_1}{\partial t} + \frac{c_1}{\tau} = \gamma_2 c_2(x, T)$$
(18)

$$\frac{\partial c_2}{\partial t} + \gamma_2 c_2 = \frac{c_1}{\tau} \tag{19}$$

The equation (18) is heterogeneous. Its solution can be presented as a general solution of the homogeneous equation and a specific solution of the heterogeneous equation $c_{11}+c_{12}$. The general solution c_{11} is found by separation of variables:

$$c_{11} = Ae^{-\alpha t} * e^{-\left(\frac{1}{V\tau} - \frac{\alpha}{V}\right)x} \left(Al^{-\alpha t}e^{-\left(\frac{1}{V\tau} - \frac{\alpha}{V}\right)x}\right)$$

Where A is the arbitrary constant determined from the boundary conditions when x=0, α is a yet unknown constant determined also from the boundary condition (10).

After the required calculations are completed, we obtain:

$$c_1(x, T+t) = \gamma N_0 e^{-\gamma V(T+t) + \left(\gamma - \frac{1}{\tau V}\right)x} + \frac{\gamma_2}{V} ex \int_0^x c_2(x', T) e^{(\gamma - \frac{1}{V\tau})(x-x')} dx'$$
(20)

Where $\tilde{t} = \frac{x}{v}$

For the NPs we consider that their solvability or transition into another mobile form C_1 during one act of humidification is small.

$$\gamma V t_0, \ \gamma_2 t_0 <<1$$

Then:

$$C_1(x_1T + t) = \gamma N_0 e^{-\gamma V t + \left(\gamma - \frac{1}{tV}\right)x} + \frac{\gamma_2}{V} \int_0^x c_2(x'_1T) e^{-\frac{1}{V\tau}(x - x')} dx'$$
(21)

The equation (19) including (17) can be rewritten:

$$\frac{\partial C_2}{\partial t} + \gamma_2 C_2(x_1 T) = \frac{C_1}{\tau} \frac{(x_1 T + t)}{t}$$
(22)

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Where C_1 is determined by the relation (20), and the boundary condition for ΔC_2 is given by the relation (11). The integration (22) taking into account the weak time dependence C_2 and C_1 within one humidification gives

$$C_{2} = -\gamma_{2}C_{2}(x,T)(t-\tilde{t}) + \frac{\gamma N_{0}e^{-\gamma VT + \left(\gamma - \frac{1}{\tau V}\right)x}}{\tau}(t-\tilde{t}) + \frac{\gamma_{2}}{V_{\tau}}(t-\tilde{t}) \int_{0}^{x} c_{2}(x',t)e^{-(x-x')\frac{1}{\tau V}}dx'$$
(23)
$$\tilde{t} = \frac{x}{V}$$

It is necessary to remember that the expressions for c_1 and c_2 in the formulas (21) and (23) are true, when x and t correspond to the point x with the water front which has reached this point. In other words, (21) and (23) are true when

$$\frac{x}{V} < t < t_0$$

During drying of the profile, c_1 is transformed into C_2 and the total increment of the related component c_2 (which equals $C_1(x,t_0)+C_2(x,t_0)$ then:

$$\bar{c}_2 = -\gamma_2 c_2 \left(t_0 - \frac{x}{V} \right) + \frac{\gamma N_0}{\tau} \left(1 + \frac{t_0 - \frac{x}{V}}{\tau} \right) e^{-\gamma V T - \frac{x}{\tau u}} + \frac{\gamma_2}{\tau V} \left(1 + \frac{t_0 - \frac{x}{V}}{\tau} \right) \int_0^x c_2(x', T) e^{-\frac{(x-x')}{\tau V}} dx' \quad (24)$$

In (24) t_0 can be changed into l_0/u , where *l* is the depth of wetting. It is obvious that not every wetting provokes the change of the c_2 component; it is reasonable to consider in (24) only $x < t_0 u$. For subsequent (24) it is convenient to depict as follows:

$$\bar{c}_2 = -\gamma_2 c_2 \left(\frac{l-x}{V}\right) + \gamma N_0 \left(1 + \frac{l-x}{V\tau}\right) e^{-\gamma V T - \frac{x}{V\tau}} + \frac{\gamma_2}{V} \left(1 + \frac{l-x}{\tau V}\right) \int_0^x c_2(x',T) e^{-\frac{(x-x'_1)}{\tau V}} dx'$$

Individual wetting at the pace of migration of the NPs plays a minor role. Notable changes in the distribution of the NPs can occur only after multiple humidifications (remembering that we are

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considering the migration of slightly soluble and slightly destructible NPs). This imposes calculation of the average increment during multiple humidifications Δc_2 . Averaging can only be performed in accordance with the function of power distribution of precipitation (or, to be more exact, the depth of wetting *l*). We determine the distribution function w(l). Then the averaged value of increment c_2 is:

$$\bar{\bar{c}}_2 = \int_x^\infty w(l) dl \bar{c}_2 \tag{25}$$

Where w(l) is a normalized distribution function.

The integration in (25) is spread from x for the reasons given above. The spread of the interval of integration to ∞ is insignificant because

$$\frac{l}{\tau V} \gg 1$$
, $(\bar{l} = Vl)$

 c_2 is nothing other than the average increment c_2 during one humidification.

We can write it as:

$$\overline{\overline{c}_2} = \frac{\partial c_2(x,T)}{\partial T} \nabla$$

We obtain the differential equation:

$$\frac{\partial c_2(x,T)}{\partial T} \nabla = \int_x^\infty w(l) dl \left\{ -\gamma_2 c_2(x,T) \left(\frac{l-x}{V}\right) + \gamma N_0 \left(1 + \frac{l-x}{V\tau}\right) e^{-\gamma V T \frac{x}{V\tau}} + \frac{\gamma_2}{V_\tau} \left(1 + \frac{l-x}{\tau V}\right) \int_0^x c_2(x',T) e^{\frac{(x-x')}{V\tau}} dx' \right\}$$
(26)

The equation (26) depicts an integro-differential equation, the solution of which depends on the particular kind of w(l). The solution of the equation (26) with the boundary condition (16) and zero, for example, the initial condition (c(x, 0)=0) uniquely determines the spatial and temporal distribution of c_2 .

The exponential distribution function w(l) is good because, in its main features, it reasonably describes the distribution function of humidification: the probability of weak humidifications is higher than strong ones. In addition to this, it is convenient for calculations.

For the exponential distribution function

$$w(l) = \frac{e^{-\frac{l}{l^{-}}}}{l^{-}} = \frac{1}{l^{-}}exp\left(-\frac{l}{l^{-}}\right)$$

the equation (26) will have the form:

$$\frac{\partial c_2(x,T)}{\partial T}\nabla = \frac{\gamma_2}{V} \left(1 + \frac{\bar{l}}{\tau V}\right) e^{-\frac{x}{\bar{l}}} \int_0^x e^{-\frac{(x-x')}{\tau V}} c_2(x'T) dx - \gamma_2 c_2(x,T) \frac{e^{-\frac{x}{\bar{l}}} * \bar{l}}{V} + e^{-\gamma VT - \frac{x}{V\tau}} \gamma N_0 \left(1 + \frac{l}{\tau V}\right) e^{-\frac{x}{\bar{l}}}$$
(27)

After differentiating over *x*, we obtain the partial differential equation of the second order:

$$\frac{\partial^2 c_2(x,T)}{\partial x \partial T} - \frac{1}{l} * \frac{\partial c_2}{\partial T} + \frac{1}{\tau V} * \frac{\partial c_2}{\partial T} + \frac{\gamma_2 \bar{l}}{\nabla V} * \frac{\partial c_2}{\partial x} * e^{\frac{x}{l}} - \frac{\gamma}{V \nabla} c_2(x,T) e^{\frac{x}{l}} = 0$$
(28)

Thus, we obtained a differential equation which describes the long-term migration of NPs. This equation takes into account multiple wettings of the soil profile in accordance with statistical distribution of precipitation.

The equations (27) and (28) are spread over the whole plane x, T. The known methods of solving can be applied to them.

We must note that the time T in the equations is the total time of humidification and not the absolute time.

6. Conclusion

A necessary step has been taken towards the formation of the migration model of NPs in the soil profile, which adequately reflects actual physical and chemical processes occurring in the soil profile and the influence of natural and climatic factors on them. The method of obtaining averaged equations for the description of the long-term migration of NPs in the soil profile has been developed. In the same way partial differential equations, which describe more complex models, for example, those using diffusion, capillary phenomena and others, can be obtained. This will be the subject of our further research. The obtained equations permit the use of integral transformations in order to find solutions. The obtained model will be applied in the design of field studies on the migration of marker nanoparticles in different types of soils.

Acknowledgments

This study (research grant No 8.2.57.2015) was supported by Tomsk State University Academic D.I. Mendeleev Fund Program in 2015.

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