ANALYTICAL DEPENDENCE OF POLLUTION DENSITY ON THE POWER-TYPE DIFFUSION COEFFICIENT IN DISSIPATIVE SYSTEMS

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Abstract. In environment engineering, there exists a wide class of systems belonging to the so-called dissipative type. Investigation of such systems allows determining the basic dynamical properties and peculiarities of pollution expansion. The most interesting properties appear in the case of nonlinear dissipative systems, which may exhibit bifurcations and irregular solitonic waves. Concrete examples of dissipative environment engineering systems allowing an analytical assessment of pollution density are considered. In the case when the external impact is negligible and the diffusion coefficient is of a special kind, it is possible to trace the dependence of pollution density and, for example, of its irregular waves on the diffusion coefficient in an analytical aspect.

Keywords: dissipative environment engineering systems, pollution dynamics, diffusion–convection model.

1. Introduction

Pollution is a serious problem in almost all countries, especially those with high population density and large industrial centers. The mathematical modelling is one of the basic instruments to analyse the distribution of pollution. The idea of using diffusion to study the biological systems described by the diffusion–convection model was introduced by J.G. Skellam in the early 1950s [1]. General discussions and references on diffusion–convection equations in biological aspects may be found in [2-8]. Nearly at same time, the diffusion–convection systems have been employed for modelling of pollution dynamics. As early as 1960s, an extensive survey appeared on the results of air pollution dynamics in New York [9]. The ever-increasing possibilities offered by computers allow a mathematical modelling of the nature and dynamics of pollution in aerial and water environments [10]. Large metropolises become interested in studying the nature and dynamics of air and soil pollution [11, 12]. The new generation of computers allow the mathematical modelling of pollution dynamics in a medium by parallel computation [13]. Lately, attention has been focused on studying the dynamics of pollution by heavy metals [14, 15].

We understand diffusion as the spontaneous net movement of particles from an area of high concentration to an area of low concentration in a given volume of fluid (either liquid or gas) down the concentration gradient. Therefore, there will be a net movement of particles from high to low concentration. Initially, a concentration gradient leaves a smooth decrease in concentration from high to low which will form between the two regions. As time progresses, the gradient will grow increasingly shallow until the concentrations are equalized.

Diffusion is a spontaneous process. It is simply the statistical outcome of random motion. This process increases entropy, decreasing Gibbs free energy, and therefore is thermodynamically favorable. Diffusion operates within the boundaries of the Second law of thermodynamics because it demonstrates nature's tendency to wind down, as evidenced by increasing entropy.

The diffusion equation provides a mathematical description of diffusion. This equation is derived from Fick's law, which states that the net movement of diffusing substance per unit area of section (the flux) is proportional to the concentration gradient (how steeply the concentration changes in space), and is toward lower concentration. (Thus if the concentration is uniform there will be no net motion.) The constant of proportionality is the diffusion coefficient, which depends on the diffusing species and the material through which diffusion occurs. Fick's law is an assumption that may not hold for a...
given diffusive system (e.g., the diffusion may depend on concentration in addition to concentration gradient), in which case the motion would not be described by the normal (simple, Fickian) diffusion equation. An analogous statement of Fick’s law, for heat instead of concentration, is Fourier’s law.

The mechanism of diffusion is "Brownian motion" whereby a molecule makes a random walk about a central location since by kinetic theory the mean velocity of a particle is zero if it is not subject to any external forces. Due to collisions with neighboring molecules the motion of the particle is characterized by a mean free path which tends to confine the particle. But since there is no potential field acting to restore a particle to its original position, it is still free to move about the vessel or liquid in which it is located. The Laplacian in the diffusion equation indicates that the dispersion of the particles is second order effect, i.e., due to changes in the concentration gradient.

Consider a large balloon of 10 meters in diameter. Imagine this large balloon in a football stadium or any widely crowded area. The balloon is so large that it lies on top of many members of the crowd. Because they are excited, these fans hit the balloon at different times and in different directions with the motions being completely random. In the end, the balloon is pushed in random directions, so it should not move on average. Consider now the force exerted at a certain time. We might have 20 supporters pushing right, and 21 other supporters pushing left, where each supporter is exerting equivalent amounts of force. In this case, the forces exerted from the left side and the right side are imbalanced in favor of the left side; the balloon will move slightly to the left. This imbalance exists at all times, and it causes random motion. If we look at this situation from above, so that we cannot see the supporters, we see the large balloon as a small object animated by erratic movement.

Now return to Brown’s pollen particle swimming randomly in water. One molecule of water is about 0.1 to 0.2 nm, (a hydrogen-bonded cluster of 300 atoms has a diameter of approximately 3 nm) where the pollen particle has a diameter of roughly 1 µm in diameter, roughly 10,000 times larger than a water molecule. So, the pollen particle can be considered as a very large balloon constantly being pushed by water molecules. The Brownian motion of particles in a liquid is due to the instantaneous imbalance in the force exerted by the small liquid molecules on the particle.

Contrary to Brownian motion, which is the diffusion of a single particle, interactions between particles may have to be considered, unless the particles form an ideal mix with their solvent (ideal mix conditions correspond to the case where the interactions between the solvent and particles are identical to the interactions between particles and the solvent will amount for the following effects:

- the diffusion coefficient $D$ in the particle diffusion equation becomes dependent of concentration. For an attractive interaction between particles, the diffusion coefficient tends to decrease as concentration increases. For a repulsive interaction between particles, the diffusion coefficient tends to increase as concentration increases.
- In the case of an attractive interaction between particles, particles exhibit a tendency to coalesce and form clusters if their concentration lies above a certain threshold. This is equivalent to a precipitation chemical reaction (and if the considered diffusing particles are chemical molecules in solution, then it is a precipitation).

Now let go to the diffusion–convection systems. The simplest example of the nonlinear diffusion–convection equation is the one-dimensional diffusion logistic equation

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x} \left( D(N) \frac{\partial N}{\partial x} \right) + F(N),$$

where $N = N(x,t)$ is the pollution density, $F(N)$ is the external impact, and $D(N)$ is the diffusion coefficient.

In this paper, we restrict the consideration to the problem of the existence of solutions of a nonlinear reaction diffusion model for a single-species pollution moving in one space dimension. A single-species pollution dynamics with dispersal in a spatially heterogeneous environment is modelled by a nonlinear diffusion–convection equation with a nonlinear term of diffusion coefficient. Each nonlinear kinetics describes the relation between the growth rate and the density of a steady-state pollution distribution. Our main concern is investigation of the possible appearance of the area and time restrictions and the phenomenon of travelling waves. The existence of nonlinear kinetics realizing the diffusion coefficient terms is established. It is shown that the freedom of such kinetics in some cases is restricted by the nonlinear behaviour of the diffusion coefficient.

2. Power dependence of the diffusion coefficient

For simplicity, we will consider a one-dimensional area. In the case when the diffusion coefficient is a power function from pollution density and the external impact is not large,

$$D(N) = aN^n, \quad F(N) << 1,$$
the type (1) system allows a complete analytical solution. Employing the method of similarity we will introduce a new variable \( \xi = x/(at)^{(2+v)} \).

The solution of equation (1) under conditions (2) has the form

\[
N = (at)^{-\frac{1}{2+v}}\left[ \frac{v}{2(2+v)} (\xi_0^2 - \xi^2) \right]^{\frac{1}{v}},
\]

where \( \xi_0 \) is the integration constant. The behaviour of this solution essentially depends on the sign of the power \( v \).

For \( v > 0 \), solution (3) gives the distribution of pollution density \( N(x,t) \), peculiar to an area with the borders \( x = \pm x_0 \) defined by the equality \( \xi = \pm \xi_0 \); beyond these borders, \( N(x,t) = 0 \). Hence it follows that with time the pollution borders expand according to the law

\[
x_0 = \text{const} \cdot t^{\frac{1}{2+v}}.
\]

Note here that power \( v \) in the diffusion coefficient \( \nu \) is an unknown in advance and free parameter of the model. The dependence \( (\xi(x))^v \) allows us to determine the power \( v \). This remark is useful for applications.

The integration constant \( \xi_0 \) is determined by the condition of normalization of the whole volume of pollution:

\[
\int_{-x_0}^{x_0} N(x)dx = \int_{-\xi_0}^{\xi_0} f(\xi)d\xi = 1,
\]

hence

\[
\xi_0^{2+v} = \frac{(2+v)\Gamma^{2+v} \Gamma^{1/2+1/v}}{v^\frac{2}{v+2} \Gamma^{v}(1/2+1/v) \Gamma^{v}(1/v)},
\]

where \( \Gamma(x) \) is the Euler gamma-function.

The irregular wave solution describes the motion of pollution with a constant velocity. Such solution is a special case of the travelling wave. For the travelling wave, i.e. in the case when \( N = N(x+vt) \), equation (1) turns into

\[
\frac{\partial N}{\partial x} = \frac{\partial}{\partial x} \left( N^v \frac{\partial N}{\partial x} \right),
\]

whence, after a double integration, we obtain the following solution:

\[
N = N_0 [x+vt]^{-\frac{1}{v}},
\]

where \(|x|\) is the distance from the boundary of the inhabited area.

For \( v < 0 \), the solution (2.2) can be expressed as

\[
N = (at)^{\frac{1}{2+v}} \left[ \frac{v}{2(2-v)} (\xi_0^2 + \xi^2) \right]^{\frac{1}{v}}, \quad v \to |v|
\]

where \( v \to |v| \) in expression (9) means substitution of the positive value of \( v \).

In this case, the pollution density is distributed all over the area, and for large distances \( N \) diminishes obeying the power law: \( N \sim x^{-2} \). This solution is valid only if \( v < 2 \); if \( v \geq 2 \), the normalization integral (5) which now is taken on the whole real axis becomes diverged, implying an instantaneous distribution of pollution at an infinite distance. The integration constant \( \xi_0 \) in expression (2.8)

\[
e^{-2/v} \xi_0^2 = \frac{2(2-v)\pi^{\frac{v}{2}}}{v} \Gamma^v(1/v - 1/2) \Gamma^v(1/v),
\]

For \( v < 0 \), the equation for an irregular wave (8) has no solutions turning into zero at a finite distance, i.e. pollution is distributed at any given moment throughout the whole space. Thus, such solution should be rejected.

Finally, for \( v \to 0, \xi_0 \to 2/\sqrt{v} \), and the solution determined by expressions (3) gives the ordinary Gaussian distribution.

Sometimes, we do not know the integration constant \( \xi_0 \), which depends on power \( v \) (6). In this case, instead of solution (3), we may use a solution of the form

\[
N(x,t) = A [ |t+B|^{-v/2} \frac{v}{2a(\nu+2)} (x+C)^2]^{-\frac{1}{v}},
\]

where \( A, B \) and \( C \) are arbitrary constants.

![Fig 1. The dependance of solution (3) on dimensionless variable \( \xi \) for parameters \( \nu = 1, \ldots, 6 \).](image)

3. **Inhomogeneous generalization of power dependence**
In the case when the diffusion coefficient \( D = D(x,t,N) \), we deal with the presence of inhomogeneous diffusion coefficient in an environment engineering system. In the general case, the problem of the evolution of the density of a pollution with an inhomogeneous diffusion coefficient can be solved only numerically. Nevertheless, in some cases an exact analytical solution can be found. Let us consider an inhomogeneous generalization of the evolution of pollution \( N(x,t) \) in the form

\[
\frac{\partial N}{\partial t} = x^{-\mu} \frac{\partial}{\partial x} \left[ x^\mu N^\nu \frac{\partial N}{\partial x} \right] + F(N) \quad (11)
\]

This equation offers a rather wide detailing of equation (1.1) in the case of the power dependence \( D(N) \); the properties of its solutions essentially depend on the magnitude of the constituent parameters \( \mu, \nu, \rho \). The introduction of an explicit dependence of the diffusion coefficient on the coordinate \( x \), on the one hand, is determined by the consideration of non-homogeneity and, on the other hand, by investigation of the process of evolution in a cylindrical or spherical system of coordinates, where the operator \( \text{div} \) explicitly depends on the coordinate \( r \).

We will single out the following three groups of the solution of equation (11): a) of the rapid \((v < 0)\), b) slow \((v > 0)\), and c) normal \((v = 0)\) evolution, and consider the solutions of the equation of evolution (1) separately for each group.

Let \( \mu = \rho \) in the case of rapid evolution \((v < 0)\). We will search for the solution of the pollution density function in the form

\[
N(x,t) = x^{\frac{2}{\nu}} f(t) \quad (12)
\]

The substitution into the initial equation (11) and integration takes the following expression of the solution \( N(x,t) \):

\[
N(x,t) = x^{\frac{2}{\nu}} \left[ \frac{x^2}{N_0 t} - \frac{4 + 2v(1 + \rho)}{\nu} \right]^{\frac{1}{\nu}} \quad (13)
\]

where \( N_0 = N(x,0) \) is the initial value of \( N(x,t) \). For \( v = -2/(1 + \rho) \) we have a stationary solution \( N(x,t) = N_0 \).

Note an important circumstance: the expression in brackets in solution (13) must be non-negative. This means that the evolution of pollution density, although not limited in space, proceeds in a finite time period \( 0 \leq t \leq t_{\text{max}} \):

\[
t_{\text{max}} = \frac{v}{4 + 2v(1 + \rho)} \frac{x^2}{N_0^v} \quad (14)
\]

In any point of space, the pollution density diminishes from its initial value \( N_0(x) \) to zero.

Now, let us consider the case of slow evolution \((v > 0)\). We will seek the solution of the pollution density function in the form

\[
N(x,t) = t^{-\frac{k}{2}} f(s), \quad s = xt^{-\frac{1}{2v}} \quad (15)
\]

Thus, the solution of the initial equation (3) may be expressed as

\[
N(x,t) = N_0 t^{-\frac{k}{2}} (s_n^2 - s^2)^{\frac{1}{2v}}, \quad s = xt^{-\frac{1}{2v}} \quad (16)
\]

for \( 0 < s < s_m \), or in the dimensionless form

\[
N(x,t) = N_0 \left[ 1 - \left( \frac{x}{s_m} \right)^2 \right]^{\frac{1}{2v}} \quad (17)
\]

At a fixed value of the spatial variable \( x \), from expressions (16) or (17) it follows that solution \( N(x,t) \) exists only for \( t > t_{\text{min}} \). Thus, we observe a "delayed" response of the pollution evolution.

In the case of slow evolution, the presented solution is not the only possible one. Indeed, let us consider the obtained solution (13) for \( v > 0 \). This solution is valid for the interval \( 0 \leq t \leq t_{\text{max}} \), where \( t_{\text{max}} \) is determined by expression (17); however, in this case, for \( t \to t_{\text{max}} \) the solution gains an unlimited increment.

Finally, in the case of normal evolution \( v = 0 \), the solution of the pollution density function can be expressed as

\[
N(x,t) = C t^{\frac{k}{2}} e^{-\frac{kx^2}{4t}} \quad (18)
\]

where \( k \) is an arbitrary constant. For \( k = 1 \) we obtain a solution corresponding to a normal or Gaussian distribution. The solution (18) exists in the whole region of the determination of the variables \((x,t_0)\).
Fig 2. The dependence of solution (3) on space and time variables $x, t$ for parameter $\nu = 0$

4. Exponential type of the diffusion coefficient

From the obtained solutions of the initial equation (2) we see that the essential properties of the asymptotic behaviour depend on the diffusion coefficient $D(N)$. In the case of the constant $D(N) = D$ we have a Gaussian type of solution, in the case of the power law $D(N) = aN^\nu$ we have an essentially different blow-up type of solution.

The coefficient of diffusion depends on the porosity of the medium. The porosity, in turn, usually inversely depends on the quantity of the filtered matter. Thus we are expecting the exponential type of the dependence of the diffusion coefficient.

$$D(N) = ae^{\lambda N}, \quad (19)$$

where $a$ and $\lambda$ are arbitrary constants. The evolution equation for the concentration has the form

$$\frac{\partial N}{\partial t} = a \frac{\partial}{\partial x} \left[ e^{4N} \frac{\partial N}{\partial x} \right]. \quad (20)$$

This type of diffusion again has the analytical solution. The direct verification of the expression

$$N(x, t) = \frac{2}{\lambda} \ln \left( \frac{\pm x + A}{\sqrt{B - 2at}} \right), \quad (21)$$

where $A$ and $B$ are arbitrary constants shows that expression (21) obeys equation (20). Note here that we obtain one more qualitatively different type of solution. Indeed, along the time variable $t$, solution (21) takes place only up to the time value $t_* = B/(2a)$. Thus, in this case we have a time-bound solution.

5. Some properties of the solution with the diffusion coefficient of the general form

After such a successful consideration, the next natural question arises: is it possible to derive some general properties of the evolution equation in the form

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x} \left[ f(N) \frac{\partial N}{\partial x} \right], \quad (22)$$

where $f(N)$ is an arbitrary function?

The first note concerns the self-similar solution. In the variable $\xi = x/\sqrt{t}$, when $N(x, t) = N(\xi)$, equation (22) turns into the ordinary differential equation

$$\left[ f(N)N^\prime \right]_\xi + \frac{1}{2} \xi N^\prime_\xi = 0. \quad (23)$$

As we have seen above, this equation in some special cases has exact analytical solutions.

The next note deals with the traveling wave solution. From equation (22) it follows that the implicit form of the traveling wave solution

$$k^2 \int f(N) dN \frac{\partial N}{\partial \lambda} + \lambda N + C_1 = kx + \lambda t + C_2, \quad (24)$$

where $k$, $\lambda$, $C_1$, $C_2$ are arbitrary constants. There, the special case of $\lambda = 0$ corresponds to a stationary solution.

6. Discussion

A comparison of the results of Parts 1 and 2 allows concluding that the power nonlinearity and non-homogeneity exerts an influence on the behaviour of the solution of a diffusive dissipative system.

In both cases, the pollution density $N(x, t)$ essentially depends on the index of power dependence: for $\nu < 0$ the solution is determined on the entire numerical axis, while for $\nu > 0$ the solution is compact in the region $|x| < x_0$, the limits of the region expanding with time in accordance with the law $x_0 = ct^{2\nu}$. A traditional way of presenting the subject of the paper would be to take concrete results of pollution dynamics measurements and to apply to them the proposed theoretical results. However, the aim of the present paper is somewhat different: we want to show the great possibilities contained in the classical diffusion–convection system. One of these possibilities is the nonlinear characteristic of the diffusion coefficient which, to our knowledge, has not been this far used for investigating environment engineering models [9-15]. The usual way of treating the results obtained from observations is to “squeeze” them into the known mathematical diffusion–convection model which has proven correct in a
number of cases. In our opinion, the procedure deserves a more “creative” approach involving consideration of the inherent possibilities of the diffusion–convection model. This would allow not only to improve the qualitative correspondence between the model and the results, but also to account for the intrinsic qualitatively new phenomena. In the classical diffusion–convection model, the border of a pollution area changes its position obeying the dependence \( x_0 = \text{const} \cdot t^{1/2} \). In case we account for the possible power characteristic of the diffusion coefficient \( D(N) = aN^\nu \), this dependence can take another form: \( x_0 = \text{const} \cdot t^{1/(2+\nu)} \). The power index \( \nu \) modifies the pollution area expressed through the constant \( 0 < \xi_0 \leq \xi \leq \xi_0 \), i.e. throughout all the dynamics the pollution is distributed not in the whole area but only in its expanding, though always limited, part. In our opinion, this property could be useful while explaining the high density of pollution.

The solutions themselves of the concentration and traveling excitation wave qualitatively differ from the respective case of the constant characteristic of diffusion coefficient \( D(N) = a = \text{const} \).

The diffusion–convection model is closely related to the theory of active media. At present, this theory is based on the diffusion–convection type evolution equation

\[
\frac{\partial X}{\partial t} = F(X) + \sum_{i} \left( D_{ij}(X) \left( \frac{\partial X}{\partial R_j} \right) \right),
\]

(25)

where \( X = X(R,t) \) is a set of macroscopic functions, which characterizes a system under study, e.g., substance concentration of the chemically active media; \( F(X) \) is a nonlinear function determined by the structure of the process under study, \( D_{ij} \) are the coefficients of the space diffusion of the system elements.

Concrete examples of such equations were introduced rather long ago (see, for instance, Murray, 1977). It is important to note that various modifications of the Ginsburg–Landau equation also belong to type (19) equations. These modifications are widely used in the theory of equilibrium and non-equilibrium phase transitions.

To elucidate the effect of the nonlinear function of the diffusion coefficient \( D(N) \) on pollution concentration, we have deliberately limited ourselves by a negligibly low effect of the external impact. In case the total effect of the diffusion coefficient and external impacts is accounted for, we see that due to the nonlinearity of the diffusion coefficient \( D(N) \) such effect is not a mere sum total of separate contributions, but presents a complicated nonlinear effect.

When applying the diffusion–convection model to the assessing of pollution dynamics, the general peculiarities of the diffusion process should be accounted for. Their effect can essentially change the properties of the model [16, 17]. For instance, even linear diffusion, because of various effects of nonlocality, may be more rapid or slower than the normal Gaussian diffusion, thus imposing considerable changes in the properties of the pollution dynamics model.

7. Conclusions

Thus, the finite size of the molecules that diffuse through the medium and the inhomogeneous character of the latter provide a sufficient theoretical basis for changing the mathematical model of passive concentration transport. As a consequence, in the new model we obtain:

- a power change of the concentration in the thick of the porous media instead of the conventional linear change;
- a changed dependence of the flow value on the concentration;
- a changed expression of the first Fick’s law.

Passive transport through a homogeneous medium is modified by the concentration and transport rate of a substance, whereas in the case of inhomogeneous medium it depends on the pressure gradient. These two types of transport (diffusive and convective) may be regarded as two theoretical limit cases. In real cells they are superimposed. Therefore, the proposed model of the fractional Fick’s law is well applicable to real dissipative environment engineering systems.

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References


