An Active-Medium Model of Organic Substance Transformation in Soil and Its Dynamic Properties

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Abstract. An analysis of the behaviour of the soil system considered as an active medium with distributed energy sources was undertaken. This approach enabled the authors to build a heuristic model of soil which accounts for processes of organic substance production, migration and utilisation. The soil body is presented as a spatially distributed trophic chain with non-linear interactions of adjacent links. The level of this non linearity appears to be the key parameter determining the dynamic behaviour of the model system in one-, two- and three-dimensional cases. The conditions for the existence of pulse-generating and autowave modes in this system were determined by computer simulations. Of particular interest is the behaviour of damaged soil, especially its self-regeneration potential. Inoculation autowave was proven to restore the initial state of the soil if two adjacent or separated trophic links fall out. Possible ways of the further development of the proposed model are also discussed.

Key words: Soil model — Trophic chain — Organic substance distribution — Autowave

Introduction

When compared to the atmosphere and the inland waters, soil is much more vulnerable to anthropogenic influences due to the heterogeneity of its physicochemical structure and diversity of processes responsible for the migration of different compounds. This fact makes theoretical studies of soil systems greatly important while significantly complicating such investigations.

The essential results obtained from models of soil are expected to be estimations of the spatio-temporal characteristics of pollutants migration and soil selfpurification in local areas with peculiar physicochemical parameters, the evidence for the dynamic behaviour of the system and some recommendations on the regeneration of the initial state of soil biocenosis

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The fragmentary nature of the information available on the structure and the concentration dynamics in soils presents invincible difficulties when one attempts to construct an imitative model of the soil body. That's why in this paper we put forward a heuristic model of the soil system which takes into account the basic mechanisms of organic substance transformation and makes it possible to analyse this process and accompanying phenomena in detail

Methods

Theoretical model of distributed trophic chain

The basic approach to the development of the quantitative soil model is to consider it as an active medium, i.e. a system with distributed energy sources where metabolic processes of organic substance production and utilization play a key role in their migration. To be more specific, we will assume that 1) primary organic substance is produced only in a thin surface layer which gives start to trophic chain penetrating downwards into the soil, 2) the distribution of organic substance is non-uniform in space and time, and 3) the destruction processes involve biological as well as physicochemical stages, especially chemical degradation and transfer with hydrodynamic flows (often of turbulent nature)

The authors of the block model of organic substance transformation in soil (Kerzhentsev et al 1988, Kovda et al 1990) assumed that the role of the transformer links is played by soil horizons. In that case, a major part of organic substance processed at a given level is transferred to the next one while a minor part is mineralized and moved to the atmosphere, hydrosphere or phytome

When modelling the transformation of organic substance in soil we used similar assumptions (Zaikin and Rudyakov 1989) but, contrary to the aforementioned papers, "functional units" in our model are presented by trophic chain links rather than by soil horizons. In this case organic substrate while being partially mineralized is transferred from one link to another. The mineralization process is described by single term with no detailed specification of its paths (the final state of mineralized substance, for instance). Contrary to Kovda et al. (1990), the mobility of transformers as well as the rate of the formation of transformers "igniting" densities (i.e., densities guaranteeing the possibility to restore catabolic chain functions in reasonable time after an interruption in anabolism) have been added. Basically, the resulting model can be considered as a modified distributed Lotka's scheme (Lotka 1910) adapted for a large (and infinitely large in the limit) ensemble of predators and preys.

The mobility of chemical links in the chain of transformers can be properly allowed to by diffusion terms with coefficients of molecular or turbulent diffusion (Kadantsev et al 1997) In the absence of significant taxis, random components of movements of separate individuals in each biological link can also be taken into consideration by diffusion terms. Therefore the system of the model equations for trophic chain with n links takes the form

$$\frac{\partial U_1}{\partial t} = -F_2(U_1, U_2) - \beta_1 U_1 + D_1 \Delta U_1 \frac{\partial U_2}{\partial t} = \alpha_2 + F_2(U_2, U_1) - F_3(U_2, U_3) - \beta_2 U_2 + D_2 \Delta U_2 \frac{\partial U_k}{\partial t} = \alpha_k + F_k(U_k, U_{k-1}) - F_{k+1}(U_k, U_{k+1}) - \beta_k U_k + D_k \Delta U_k$$

$$(1)$$

$$\frac{\partial U_n}{\partial t} = \alpha_n + F_n(U_n, U_{n-1}) - \beta_n U_n + D_n \Delta U_n$$

where $U_k = U_k(x, y, z, t)$ stands for local partial density of organic substance at the kth link, α_k is the weak influx of U_k which provides an "igniting" density of substrate utilized by that link, F_k and F_{k+1} describe the rate of exchange between adjacent links, the term $\beta_k U_k$ denotes the rate of mineralization, D_k is diffusion coefficient, and Δ is the Laplacian

The above model means that soil is considered as an active medium and therefore can be expected to demonstrate dynamic modes typical for other active media. The unique feature of this system is its successive type, that is, energy necessary for excitation to move is transferred in a step-by-step mode

Computational procedures

A thorough investigation of the model (1) was carried out by computer simulations based on mesh algorithms For the pointwise system (Eqs. (1) with no diffusion terms) the simplest explicit computational scheme was used. Let $t_i = i\tau$, i = 0, I, denote the points of the mesh along the temporal axis. Then, the set of difference equations approximating the pointwise version of model (1) takes the form

$$\frac{U_1^{i+1} - U_1^i}{\tau} = -F_2(U_1^i, U_2^i) - \beta_1 U_1^i$$

$$\frac{U_n^{i+1} - U_n^i}{\tau} = \alpha_n + F_n(U_n^i, U_{n-1}^i) - \beta_n U_n^i$$
(2)

where i = 0, I During computer simulations the latter equations were solved with the initial conditions

$$U_k|_{t=0} = \alpha_k / \beta_k \tag{3}$$

and in some cases with the additional condition

$$U_1|_{t=0}^{t=T} = (U_1)_0 \tag{4}$$

meaning that there is constant perturbation in the first link at time interval [0, T]The solution to Eqs (2) can be written in explicit form

$$U_{1}^{i+1} = U_{1}^{i} - \tau [F_{2}(U_{1}^{i}, U_{2}^{i}) + \beta_{1}U_{1}^{i}]$$

$$U_{n}^{i+1} = U_{n}^{i} + \tau [\alpha_{n} + F_{n}(U_{n}^{i}, U_{n-1}^{i}) - \beta_{n}U_{n}^{i}]$$
(5)

where the values U_k^1 , $k = 1, \dots, n$, should be obtained from initial conditions (3)

When analysing the distributed system (model (1) with diffusion terms) the main disadvantage of the explicit algorithms lies in their instability, as originally shown by Kurant et al (1940), this scheme demonstrates a stable behaviour and other "good" properties only if $\tau \leq h^2/2$ where h denotes the mesh step for the spatial coordinate Taking this into account for the distributed model we use im plicit algorithms which are rather stable over wide regions of mesh parameters If $t_i = i\tau$, i = 0, I, and $x_m = m\Delta x$, m = 0, M, stand for temporal and spatial mesh respectively, then for the two dimensional soil model (where the only spatial axis x is directed downwards) the implicit difference scheme takes the form

$$\frac{(U_1)_m^{i+1} - (U_1)_m^i}{\tau} = D_1 \frac{(U_1)_{m-1}^{i+1} - 2(U_1)_m^{i+1} + (U_1)_{m+1}^{i+1}}{h^2} - F_2((U_1)_m^i, (U_2)_m^i) - \beta_1(U_1)_m^i$$

$$\frac{(U_n)_m^{i+1} - (U_n)_m^i}{\tau} = \alpha_n + D_n \frac{(U_n)_{m-1}^{i+1} - 2(U_n)_m^{i+1} + (U_n)_{m+1}^{i+1}}{h^2} + F_n((U_n)_m^i, (U_n)_m^i) - \beta_n(U_n)_m^i$$
(6)

with the same initial conditions as for system (2) and the boundary conditions

$$U_k|_{x=0} = U_{k0}, \quad \partial U_k / \partial x|_{x=0} = V_k \tag{7}$$

The solution to this boundary problem was calculated for consequent time layers denoted by indices i Namely, Eqs. (6) were first passed along the x-axis for any fixed temporal layer. The difference equation for the arbitrary variable U_k at the (i + 1)th upper layer looks like

$$(U_{k})_{m+1}^{i+1} = 2(U_{k})_{m}^{i+1} - (U_{k})_{m-1}^{i+1} + \frac{h^{2}}{D_{k}} \{\tau^{-1}[(U_{k})_{m}^{i+1} - (U_{k})_{m}^{i}] - F_{k}((U_{k})_{m}^{i}, (U_{k-1})_{m}^{i}) + F_{k+1}((U_{k})_{m}^{i}, (U_{k+1})_{m}^{i}) + \beta_{k}(U_{k})_{m}^{i}\}$$

$$(8)$$

and calculations should proceed from the smallest values of m to the biggest ones When for a given (i + 1)th layer all values U_k have been obtained (though the boundary problem (6)–(7) was formulated for half-line $x \ge 0$, calculations along the x axis were stopped after the values U_k decreased to the base "igniting" level), the algorithm goes to the next layer

The situation is even more complicated for the three-dimensional system Since in this case the number of calculations skyrocket exponentially, we used special techniques called alternative directions (Peaceman and Rachford 1955, for more details, see Fedorenko 1994) in order to split the upper layer equations into two independent systems for coordinates x and y. The main idea of the alternative directions method when applied to two dimensional equation in partial derivatives

$$\frac{\partial U_k}{\partial t} = D_k \left(\frac{\partial^2 U_k}{\partial x^2} + \frac{\partial^2 U_k}{\partial y^2} \right) + f_k(t, x, y, U_k, U_{k+1}) \tag{9}$$

is to build a difference scheme consisting of two sets of "orthogonal" steps Let once again index m to numerate mesh cells in x-direction and index l to play the same role for y-axis. At the steps of the first kind the upper layer is involved only when differentiating with respect to x

$$\frac{(U_k)_{ml}^{i+1} - (U_k)_{ml}^i}{\tau} = D_k \frac{(U_k)_{m-1l}^{i+1} - 2(U_k)_{ml}^{i+1} + (U_k)_{m+1l}^{i+1}}{h^2} + D_k \frac{(U_k)_{ml-1}^i - 2(U_k)_{ml}^i + (U_k)_{ml+1}^i}{h^2} + f_k(t, x, y, (U_k)_{ml}^i, (U_{k+1})_{ml}^i)$$
(10)

while the next step should be constructed in much the same way but with exchange of x and y

$$\frac{(U_k)_{ml}^{i+2} - (U_k)_{ml}^{i+1}}{\tau} = D_k \frac{(U_k)_{ml}^{i+1} - 2(U_k)_{ml}^{i+1} + (U_k)_{m+1l}^{i+1}}{h^2} + D_k \frac{(U_k)_{ml-1}^{i+2} - 2(U_k)_{ml}^{i+2} + (U_k)_{ml+1}^{i+2}}{h^2} + f_k(t, x, y, (U_k)_{ml}^{i+1}, (U_{k+1})_{ml}^{i+1})$$
(11)

The upper indices at (U_k) in Eqs. (10) and (11) indicate that if all values $(U_k)^i$ are known, their values at the (i+1)th layer can be obtained in a similar manner as in the system with a single spatial coordinate (see Eq. (8)) using standard boundary conditions

We give so much place to description of computational methods used because their choice is of a prime importance in numerical solution to non-linear differential equations in partial derivatives. As it was pointed out by many authors (see, for example, Fedorenko 1994), inadequate difference schemes can lead to numerical effects which bear no relation to the system under consideration. The main criterion here consists in the convergence of meshed functions to an exact solution, but in the overwhelming majority of cases such a convergence could hardly be proven However, what we can definitely note concerning the aforementioned algorithms is that they provide a good approximation of the exact solution. Moreover, the use of implicit difference techniques while making more complicated equations for so called upper layer gives a solid ground to expect a high degree of stability of numerical solutions. An additional argument for this statement arises from computer simulations themselves: two- and fourfold decreases in the numbers of mesh steps produced only minor quantitative changes in functions U_k while their qualitative behaviour remained the same.

During computer simulations the parameter P varied from 0.7 to 1.2; typical values for α lied in the region $10^{-7} - 10^{-6}$ mol/cm³/s; variable β was changed by more than an order of magnitude (between 0.001 and 0.02 s⁻¹); for the diffusion coefficient we used different values from the interval $2 \times 10^{-5} < D < 3 \times 10^{-2}$ cm²/s. The numbers of trophic links in different variations of the basic model (see below) range from a few dozens to several hundreds. Typical numbers of mesh points for every axis were 512 or 1024, but in some cases, as it was already said, we augmented this value by a factor of two to four in order to examine the stability and reproducibility of our results. The peculiar values of model parameters in different cases are pointed out in the Figure legends.

Results

The steady-state distribution mode; characteristic time, diffusion coefficient

The exponential decrease of the total organic substance density with depth (Fig. 1, right) can be obtained from (1) without specifying the particular type of interaction functions F_k . Combining all equations of (1) with equal values of α_k , β_k and D_k for different k we have:

$$\partial M^* / \partial t = \alpha (n-1) - \beta M^* + D\Delta M^* \tag{12}$$

where M^* is the total mass of organic substance distributed in volume which is determined by the boundary conditions; n, as before, denotes the number of links. Let $M^* = \alpha(n-1)/\beta + M$ and $\Delta M = \partial^2 M/\partial h^2$, where depth h is measured from the soil surface. Then,

$$\partial M/\partial t = -\beta M + D\partial^2 M/\partial h^2 \tag{13}$$

To obtain the steady-state density distribution let's specify the boundary condition on the surface: $M|_{h=0} = M_0$. Then, the solution in the half-space h > 0 takes the form

$$M = M_0 \exp\left(-\beta^{1/2} D^{-1/2} h\right) \tag{14}$$

The depth h_e at which $M = M_0/e$ could be estimated experimentally. In (14) the parameter β equals $1/\tau$ where τ is time constant for soil community. For chernozem earth characterized by exponential density distribution similar to that presented in Fig. 1, τ equals 400 years (Kerzhentsev 1990).

A trophic link consists of a decomposer and the organic substance to be transformed (in the proper phase for subsequent processing). The mass of the decomposer is typically considerably smaller than that of the organic substance, and in many cases hardly amounts to 1% of their combined mass. The mobility of the organic substance at the given link is obviously not dependent upon the mobility of



Figure 1. Steady-state distribution of organic substance in the trophic chain after the transient process *Left* – trophic chains at different depths *h* (each point corresponds to a single link) with at least "igniting" concentration of substrate at each link. The vertical bars at each point are proportional to substrate density at the corresponding link *Right* exponential distribution of the total organic substance density with depth. The parameters of the model (1) P = 0.8, $\alpha = 10^{-7}$, $\beta = 0.0015$, D = 0.03 n = 125

the decomposer, and is largely determined by the diffusion coefficient and the level of porosity of the medium. The effective diffusion coefficient of a porous medium is determined as

$$D^* = D/c \tag{15}$$

where c is the porosity coefficient equal to the total volume of pores in a unit of the medium volume So, the highly porous, "springy" chernozem should have a longer time constant than denser soils

The dynamic modes in the pointwise trophic chain

To study the dynamic behaviour of the soil model, simulations were carried out under the following assumptions

1) The soil system is uniform meaning the parameters in Eqs. (1) are the same for all links,

2) Functions F_k were set to have the form $F_k = \gamma_k U_{k-1} U_k^P$ with $\gamma_k = 1$ for all k,

3) All trophic links except the first one are of catabolic nature The first link plays an anabolic role and the number of individuals belonging to it was set to be constant during the given time period (the latter assumption is equivalent to the boundary conditions of the first kind) Furthermore, when studying the dynamic behaviour of a trophic chain with no regard to space coordinates the system was assumed to be pointwise, namely the diffusion terms in Eqs (1) were entirely ignored (approximation of so called ideal kneading reactor)

The initial state of the trophic chain is characterized by stationary values of "igniting" concentrations in each link $U_k = \alpha_k / \beta_k$ Short-term perturbation at the first link generates moving pulses with an amplitude smoothly decreasing to zero As it is evident from computer simulations, in the case of a prolonged perturbation the system behaviour can be of different types

1) When coefficient P is below 0.9 the model displays a smooth decrease in organic substance density along the chain,

2) An increase of P to 0.95 0.97 leads to the appearance of a source of pulses that are periodically generated by first links (Fig. 2). These pulses corresponding to the excitation states of two adjacent links are attenuating with a gradual decrease in amplitude and velocity causing the density to progressively reach the "igniting" level,

3) A further increase in value of P (to the region of P > 1.05) brings about the mode of intermittent generation while periods of bursts remain the same them internal structure changes drastically from one link to another

The dynamic modes in the distributed system (two-dimensional system)

Addition of one spatial dimension to the just considered scheme makes it possible to trace the movement of organic substance downwards into the soil and the appearance of plane waves Furthermore, it allows to elucidate the influence of shortand long-term perturbations on the system, the transient processes and the steadystate mode In model (1) diffusion coefficients and parameters β_k that determine the level of mineralization are essentially the scaling factors As became apparent from numerical experiments, parameter P plays a more critical role because small variations in its value result in qualitative changes of the dynamic mode (bifurca tions)

Figure 1 (left) illustrates the steady-state distribution of organic substance with the depth of soil and the length of the trophic chain settled after the transient process Some peculiarities of this state deserve to be mentioned

1) Transformers of first trophic links localized near the soil surface process organic substance themselves thus preventing it from penetrating downwards,

2) Decomposers of last links which obtain small quantities of the substrate display effectively the same behaviour,

3) The peak of density is penetrating deep into the soil while moving along the chain and diminishing in amplitude. As a result the maximum depth is reached by substantial quantities of organic substance belonging to intermediate links



Figure 2. Steady-state mode of periodic pulses generation in a pointwise system (the organic substance density distribution is shown in an arbitrary phase of the process) U – density of organic substance, k – link number (for this Figure, the total number of links n = 200) The Parameters of the model (1) P = 0.97, $\alpha = 10^{-7}$, $\beta = 0.0015$

 $U_{k} U_{max}$

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Figure 3. Formation of waves at the edge of the trophic chain and their penetration along the chain and downwards into the soil. The vertical bars at each point are proportional to substrate density at the corresponding link. (A) An increase in value of P up to 0.95 leads to the emergence of the wave source. (B) Further increase of P (to 1.05) causes stochastization of waves and their penetration to larger depths and distances along the chain. Other parameters of the model (1): $\alpha = 10^{-7}$; $\beta = 0.0015$; D = 0.03; n = 75.

When P = 0.95 and other parameters of model (1) take their values as in Fig. 1, the system generates rapidly damping waves which move on the same trajectory as density peak in the case of P = 0.8 described above (Fig. 3A). Further increase in P to the value 1.05 leads to stochastization of waves with a concurrent slowing down of their attenuation (Fig. 3B).

Unhealthy conditions of the soil system: falling out of a link

One or more links can fall out from the trophic chain as a consequence of infec-



Figure 4. Inoculation autowave in the two-dimensional system with two missing links (k = 4 and k = 5) in the region $x > x_2$. The width of the horizontal lines is proportional to substrate density at the corresponding chain link for the given spatial point. The parameters of the model (1) P = 0.7, $\alpha = 10^{-6}$, $\beta = 0.02$, $D = 2 \times 10^{-5}$, n = 28

tions or mechanical damage during agricultural activity. In some cases selective suppression or destruction of separate links by pollutants of anthropogenic origin is observed. For the model system the falling out of one link ($\alpha_k = 0$) gives rise to accumulation of organic substance in previous ones because the lacking link forms an impermeable boundary. What's more important, the falling out of a link causes non-uniformity in functional roles of other links. As computer simulations reveal, odd links of the trophic chain (counted from the impermeable boundary towards the beginning of the chain) accumulate organic substance while even links increase the rate of its processing (see the right bottom region of Fig. 4).

Inoculation as a method of healing soil illness; inoculation autowave

For an inactive producer the most natural but rather expensive way of fallen link restoration on arable land is to sow it with an appropriate species. If the producer is in active state this procedure can be simplified by seeding the species only at the edge of the field; then an inoculation autowave will complete this process for the whole field.



Figure 5. If missing links are not adjacent (k = 6 and k = 16, as in this Figure) their inoculation takes place with a time delay. The parameters of the model (1) and the number of mesh points are identical to those in Fig. 4.

Figure 4 presents the result of computer simulations for a trophic chain with two lacking links. The model medium was chosen to be a long thin layer with a penetrating plane perturbation wave. The initial state remained practically unchanged in region $x > x_2$ except that the link with a significantly increased density was formed in front of the fallen ones. To disturb the system, small quantities of lacking species were added in the vicinity of point x = 0. After the completion of the regeneration process an inoculation autowave of a constant velocity and shape was generated in region $x_1 < x < x_2$. Behind the wavefront the state of the system was restored to its original form. In the case of a fallout of two separated links the main result of the simulations is quite predictable (Fig. 5): at the spatial region determined by the time difference between the moments at which the inoculation of the lacking links begins one can reveal an intermediate stationary state.

Inoculation autowaves in the three-dimensional system

Results similar to those presented in Fig. 5 were obtained with the full-dimensional model (three spatial coordinates). In this case circular inoculation autowaves appear in the planar layer but their major features (distribution of organic substance density, for example) remain the same. Figure 6 illustrates organic substance den-



Figure 6. A portion of the detailed organic substance density distribution during the process of missing link inoculation by circular autowaves (three-dimensional model, autowave profile is shown in projection to the radial axis of the polar coordinates) The parameters of the model (1) P = 0.7, $\alpha = 10^{-6}$, $\beta = 0.02$, $D = 2 \times 10^{-5}$, n = 12

sity distribution at the wavefront (for one missing link): the significant shortening of the trophic chain affected some quantitative characteristics of the autowave while its general nature remained unmodified.

Discussion and Concluding Remarks

The comparison of some results obtained for model (1) with observations on real soil systems makes it evident that considering soil as a distributed active medium could quantitatively forecast key parameters of toxicants' penetration into the soil and the processes of its regeneration. These results can be extended beyond the world of organic substances taking into account that many inorganic compounds and even heavy metals are involved in metabolic pathways. (A typical example: the fractional analysis of soil samples suggests that approximately 60% of lead and cadmium in soils are incorporated into organic substance (Zolotareva 1983)). Some new findings on the dynamical behaviour of soil systems as well as theoretical explanations of joint non-additive action of toxicants and their non-uniform spatial and temporal distribution observed within years after the penetration into soils can also be obtained by adapting model (1) to specific real conditions.

Leaving aside these practical implications, the different dynamic modes revealed for the non-linear model (1) are of particular value on their own. Treating of soil as an active medium made it possible to discover several modes of behaviour typical for dynamic systems, from pulse generation to penetration of stochastic waves to autowave phenomena. Amongst unexpected results it is worth to note the effect of non-uniform organic substance distribution between even and odd links of the trophic chain. This pattern, illustrated in Figs. 4 and 5, could be interpreted as the ability of the soil to form complex structures, though in this case they can be registered in, say, a community of microorganisms rather than in space. In general, such a potential is typical for dynamic systems. Considering different dynamic modes in the soil system it should be emphasized that the key role in determining its behaviour is played by the degree of non-linearity of the model; even small variations of parameter P can cause bifurcations and transition of the whole system to a new mode. At the same time other parameters can vary in rather wide regions with no catastrophic consequences (the peculiar values of α , β and D in Figs 1–6 were chosen mostly for illustrative purposes) We should also note that different dynamic modes were revealed in model system just for the simplest interactive functions $F_k(U_k; U_{k-1})$ Therefore, one could expect to uncover some new dynamic features of the model when taking these functions in a more complicated form. However, this task hes well beyond the scope of the present paper.

Another way of the further development of the model lies in the transition from the analysis of a single trophic chain to quantitative description of multiple chains acting in parallel (the model of a trophic net) additional structural components and links in this case may bring about new peculiarities of the dynamic behaviour of the system. Even more, our approach enables to extend the consideration of the soil as a distributed active medium to the trophic chain itself. From mathematical point of view such consideration is equivalent to going from Eqs. (1) to infinite number of trophic links characterised by density function

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