River water pollution assessment under climate change in Kura-Araks basin: modeling approach.

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Abstract

The discrete model for investigation of dynamics of heavy metals accumulation in rivers of Armenia is considered. One of main issues of studying the water chemical composition in a system with spatial heterogeneities and several sources of pollution is defining local parts with almost equal conditions. The boundaries for local subsystems associated with a point oscillator are identified on multidimensional statistical data for different regions. Long-term monitoring study of the quality and quantity of water in Kura-Araks watershed is used for reference and the model predictions verifying.

Based on comparable monitoring data in the region estimation of pollution levels allows application of modeling approach not only to the rivers of Armenia but also to the transboundary rivers of the entire Kura- Araks basin.

Key words: water pollution, climate change, coupled oscillators, target patterns, phase locking.

Introduction

A discrete model for investigation of dynamics of heavy metals (HMs) accumulation in rivers of Armenia is considered. The influence of spatial spread on redistribution of chemical components is presented through study of the behavior of weakly coupled oscillators. The chain topology is naturally implied for discrete models of systems such as river ecosystems. We will consider chains with the nearest-neighbor coupled oscillators where oscillatory elements are weakly coupled.

The behavior of weakly coupled oscillators in a chain has been the object of extensive work by several authors (e. g.Kopell &. Ermentrout.1990; Bressloff & Coombes 1998). A very broad framework is given for the investigation of long chains of N weakly coupled oscillators (Ermentrout 1986).

The assumption of weak coupling implies slow convergence to a steady state, i.e. that the relative position (phase) of the oscillators changes slowly with respect to their motion around the limit cycle (absolute phase).

1. Model definition.

In a discrete mathematical model the spatial system is represented by a chain of coupled oscillators. The coupling of *n* dynamical systems can lead to synchronization of their outputs. The dynamics for each of these can be either periodic or chaotic. Synchronization results from mutual adjustment of oscillators that gives rise to a common dynamical behavior.

From mathematical point of view an oscillator is a dynamical system. The dynamics of $n \geq 2$ of coupled oscillators is governed with the following system:

$$x_k' = f_k(x_k, s_1, \ldots s_n)$$
$$s_k' = \varepsilon g_i(x_k, s_k)$$

where $x_k \in R^m$ $x_k \in R^m$ describes the state of the *k* th oscillator, $s_k \in R^n$ $s_k \in R^n$ describes how it affects the other oscillators for *k*=1,…*n,* note the dimension of space for uncoupled oscillator can be different from the one for the number of oscillators. The parameter $\varepsilon \ll 1$ is small reflecting the assumption that the connecting variables are "slow". Both in cases of slowly and weakly coupled oscillators there is a continuous transformation that maps solutions of the system onto solutions of the phase system which is easier for studying the collective behavior. It is assumed that without coupling each component of the chain has an asymptotically stable limit cycle. For the nearest-neighbor coupling the equations are of the form:

$$\theta_k' = \omega_k + H^+(\theta_{k+1} - \theta_k) + H^-(\theta_{k-1} - \theta_k) \qquad (1.1)$$

Where *k*=1,…*n*, H^+ and H^- are smooth 2π-periodic functions of their arguments and ω_k is the frequency of each oscillator. The term H^+ for k=n and H^- are ignored for *k*=*n* and *k*=1 respectively. The equation (1.1) is in coordinates around the limit cycle, then the phase space of *k* oscillators lies in an *k* torus. The interaction functions H^+ and H^- can be computed provided uncoupled oscillation is known ad a formula is given for the interaction between the oscillators (for details of derivation we refer to Kopell &. Ermentrout 1990)

The dynamics of the total system components essentially depends from the strength of coupling. Coupled oscillators interact via mutual adjustment of their amplitudes and phases. When coupling is weak, amplitudes are relatively constant and the interactions could be described by phase models**.**

Almost all analysis to date has been carried out for chains of oscillators in the weak-coupling regime where averaging methods can be used to reduce the model to a system of phase equations.

If the coupling is not sufficiently weak but is of a pulse in nature, the methods for pulse-coupled oscillators can be utilized. In the river system model the waves will take the form of one-dimensional target waves, originating at the center and propagating the right edge. Damping will lead to a new steady state.

It is known that the connectivity functions *H* are different for different types of individual oscillators, which could include Van der Pol relaxation oscillators. Dynamics of coupled oscillators systems is determined by the existence of commensurability relations between frequencies of oscillations of individual oscillations, such as $\omega_1 = 2\omega_2, \omega_1 = 4\omega_4$, which bring to resonances between oscillations. Pumping of energy in the system brings to establishing of some periodic or almost periodic solutions, such as it takes place in throphic chains, where species on subsequent levels are connected with prey- predator relationship. Conditions under which traveling wave solutions in a chain of pulse-coupled integrate-and-fire oscillators with nearest-neighbor interactions and distributed delays can be generated are derived in (Bressloff & Coombes 1998). Traveling waves destabilize when the detuning between oscillators increases.

River ecosystems are continuous. On the first stage mathematical models in one-dimensional statement are used for estimation of conservative admixture transfer. Most often such calculations are based on using of the Saint Venant classical equations for nonlinear diffusion wave. For the case of a conservative admixture spread along the river flow the following transfer equation is used

$$\frac{\partial \omega}{\partial t} = \frac{\partial}{\partial x}\left(\psi(x.y)\left|\frac{\partial y}{\partial x}\right|^{\frac{1}{2}} sign\frac{\partial y}{\partial x} \right) + q(x,t),$$

$$\omega\frac{\partial s}{\partial t} + Q\frac{\partial s}{\partial x} = \frac{\partial}{\partial x}\left(E\omega\frac{\partial s}{\partial x} \right) + f(x,t) \qquad (1.2).$$

The following notation are used here: x-spatial coordinate, t- time, $s = s(x,t)$ is the concentration of a conservative admixture, ω-the estimate of the river flow section, Q-is the river water discharge defined in terms of the flow speed and ω, E -- the coefficient of longitudinal dispersion, $f(x,t)$ - estimate of the admixture input from external sources defined proportion of the flow length per time units, $q(x,t)$ is the term water input from external sources counted on unit length, $\psi(x,y)$ is a function depending variables, called hydraulic radius, Manning's coefficient and the cross section surface. The boundary conditions for solving the equation (1.2) are:

$$s(x,0) = s_0(x); s(0,t) = s_1(t); s(L,t) = s_2(t)$$

A structure of a computer system is described for the analysis of the state-of-the environment information about water resources and carrying out the forecast calculations is described in (Belolipetsky, Genova & Gurevich 2001).

The models based on solution of equation (1.6) allow incorporating river morphometry information; define impact of change in dispersion on the rate of transfer. Its discrete approximation described by forced oscillations in chains of coupled harmonic oscillators, where oscillations are generated under some external force application provides less exact terms.

Let $s(x,t)$ be the concentration of some HM at space point x and time t. Assume $\partial s/\partial x = p$ and p =const, i.e. the change of concentration is linear along the river flow. Let us recall that a perturbation of media in form $y = y(x-ut)$ is meant under wave, and then it defines some profile y y moving in the space with speed u. The necessary condition of toughness in this case is that the water the movement is not immediate but depends on river characteristics and the flow does not shrink. We bring the expression (1.2) to the form

$$\omega\frac{\partial s}{\partial t}=E\omega\frac{\partial^2 s}{\partial x^2}+f(x,t)-Qp \qquad (1.3)$$

Let $F = f(x,t)-Qp$ be the perturbation function in (1.3). Consider the equation (1.3) in the form:

$$\frac{\partial s}{\partial t}=D\frac{\partial^2 s}{\partial x^2}+F(s)$$

We will write $F(s)$ in the form $F(s)\approx F'(0)s'$ $F(s)\approx F'(0)s$ where we neglect the members of o(s), $u=se^{-F'(o)t}$ in the formula, $F'(0)$ denotes derivative on s evaluated in steady state. Introducing a new function $u=se^{-F'(o)t}$ we will bring the original equation to the standard heat-conduction equation, i.e.

$$\frac{\partial u}{\partial t}=D\frac{\partial^2 u}{\partial x^2} \qquad (1.4).$$

Suppose the density of concentration $s=s(x,t)$ of some HM at t=0 was zero everywhere except some small area (local burst), where it has value s_0=const. The equation (1.4) has the following solution:

$$u(x,t)=\frac{s_0\Delta x}{2\sqrt{\pi Dt}}\exp\left\{-\frac{x^2}{4Dt}\right\}$$

where Δx is the area of local burst. Turning back to variable $s=s(x,t)$ we obtain:

$$s(x,t)=\frac{s_o\Delta x}{2\sqrt{\pi Dt}}\exp\left\{-\frac{x^2}{4Dt}+F'(0)t\right\}$$

$$s(x,t)=\frac{s_o\Delta x}{2\sqrt{\pi Dt}}\exp\left\{-\frac{x^2}{4Dt}+F'(0)t\right\}.$$

Take one fixed value, $s=s_1$ to determine the speed with which such density propagates along the river.

By taking logarithms we derive:

$$\ln s_1=\ln\frac{s_o\Delta x}{2\sqrt{\pi Dt}}-\frac{1}{2}\ln t-\frac{x^2}{4Dt}+F'(0)t \qquad (1.5)$$

It is possible to define the spatial coordinate x_1 corresponding to the value s_1 from (1.5)., then the speed of wave propagation is:

$$v(t)=\frac{dx_1}{dt}=2\sqrt{F'(0)D}-\frac{1}{2}*\frac{1}{t}\sqrt{\frac{D}{F'(0)}} \qquad (1.6).$$

We can conclude from (1.6) that when $t \to \infty$ the speed tends to $2\sqrt{F'(0)D}$, which is the minimal speed of the wave propagation.

The estimate (1.6) is valid for the stationary waves. We need special characteristics of the riverbed and flow to define whether the waves will die out at some distance from source of burst or will speed up. The existence of solutions of traveling wave type $s(x+vt)$ spreading to the left with the speed v is proved for the wave on a line (Svirezhev 1987). By solving the equation (1.3) with boundary conditions for s the parameters of wave propagation. In general, the solutions of wave propagation type suppose one point of external input. The heat-conduction equation can be solved for one-dimensional heat conduction without inner source of heat corresponding to sources of local burst in our case. Thus the additional problem is definition of initial densities of concentration generating wave propagation with the river water flow. In some cases the convergence to the minimal speed defined by (1.6) can be proved.

2. Model equations of point oscillators.

The components and links are shown on the balance flow model diagram shown on figure 1. The dynamics of a point oscillator is described by the following system of ordinary differential equations:

$$\frac{dm_i(t)}{dt} = \sum_{j=1, j\neq i}^{6} l_{ji} m_i - \sum_{i\neq j, i=1}^{6} l_{ij} m_i \qquad (2.1)$$

In this system there are seven equations, i.e. i takes values from 1 to 6, since the number of compartments in the point model is seven, l_{ij} are nonnegative constants describing the strength of connection between blocks. The components in the right part correspond to the input of HMs from all j compartments external to i. The compartments are denoted in the following way: 1-atmosphere, 2- soil, 3- sediments, 4- river water, 5-overland runoff, 6-groundwater flow. In vector form the equations take the form.

$$\frac{d\mathbf{m}(t)}{dt} = \mathbf{L} \cdot \mathbf{m}(t) + f(t) \qquad (2.2)$$

$f(t)$ in (2.2) is designed to express small perturbations from random sources. There can be different restrictions on the perturbation force value, under condition that the type of stability of the solution is preserved.

The point model coincides with the one applied for the technoecosystem (Revazyan & Ajabyan 2007) and covers the processes of transfer between main aggregated blocks. The approach is classic with slight modifications in many other models. The distribution of HM flowing from a constant source is assumed periodical, all point oscillators are determined as identical.

We will model the system with the same composition of HM, for example we take the concentrations for Cu and Zn**.**

The essential features are revealed for the system in time scale of the investigation of solutions. For HM the time of decay is negligible comparing with the human lifespan, and then the main mechanisms of loss are sedimentation and transformation to soluble forms. Other factor is through getting in plants, bodies of animals, deep layers in soil. We will neglect the waste in the process of transfer between adjacent oscillators.

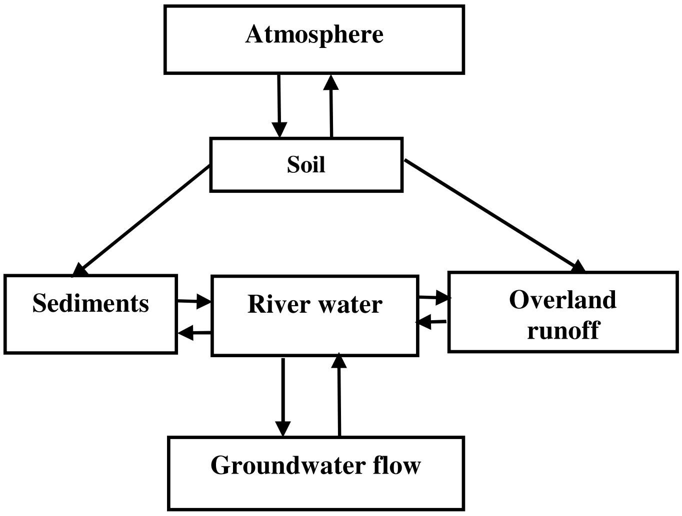

Fig. 1. The diagram of mass exchange between compartments.

In system (2) the concentration of HM in compartments *i*=1,...,6 are defined by column vector $\mathbf{m}(t)$, $\mathbf{L}$ - the matrix of coefficients, determining the intensities of change in ij,

$$\mathbf{m}(t)=\begin{pmatrix} m_i(t) \\ \cdots \\ m_i(t) \\ \cdots \end{pmatrix}; \quad \mathbf{L}=\begin{pmatrix} l_{11} & \cdots & l_{1j} & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ l_{i1} & \cdots & l_{ij} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \qquad i,j=1,...6 \qquad (1.5)$$

The parameters l_{ij}, l_{ji} in (1.5) are nonnegative as in (1.4), they can be derived from characteristics of the ecosystem. Suppose blocks on figure 1 are numbered in the following way: 1-atmosphere, 2-soil, 3-sediments, 4-river water, 5- overland runoff, 6-groundwater flow. Thus, to estimate $l_{5,4}$ we use formula $q=C_bQ_b$, where Q_b is the intensity of overland runoff, C_b - concentration of pollutants per unit of flow, i.e. it is measured in kg/m^3. Q_b is derived using formula $Q_b=C*W*J$, where C is the maximal or average intensity of precipitation, W -the surface of watershed, J -.precipitation intensity.

In more realistic approach the system parameters should be described by nonlinear functions. We can investigate the system dynamics under different hypotheses on parameter type and values.

3. Model application.

Monitoring data over five years 2004–2008 demonstrates almost similar annual variation of HM concentration. This presents evidence of local factors determining the change of concentrations.

Based on the results of research on assessment of climate change impact on river flow in Armenia the prediction can be made that under scenario, if air temperature increase 1,5-2^{o}C, 1,1P the total river flow will decrease on 5,77 % (Program "Investigation of climate change in Armenia" 2003, page 117).

Our investigations over 2004-2008 showed decreasing of total river flow in 5-7% on the territory of Armenia. The changes of river flow observed on the territory of Armenia in connection with the climate change reflected in parameters of the system (2.2) through the coefficients expressing nature and intensity of the runoff change.

The results long-term data on investigation of dynamics and behavior in basin of Rivers Pambak-Debed can be used for estimation of system (2.2) coefficients. The results include statistical analyses of data on dependence of HM concentration from volume of runoff, the estimates of the excess of any HM concentration with respect to the natural background (Saghatelyan & Nalbandyan 2008). Modeling of spatial changes allows applying data that reflects regularities of HM accumulation in each of successive water sampling points of river and compare them with the previous point characteristics (Saghatelyan, Kekelidze & Nalbandyan 2008).

Consider the task on dynamics of transfer for contents of Cu and Zn in along the river net Shirakamut-Vanadzor-Ayrum. We use mesh method for numerical solution of the equation (1.2). We use the approach with side differences on *x,* the declivity of waterbed is not taken into account, however a detailed structure of the river bottom form can be included (Abdrakhmanov, Kudriasheva & Popov 1995). We can take into account the change in concentrations resulting from sedimentation. The cross section of riverbed is of rectangular form, though natural rivers have more complex shapes. However such approximation is justified for modeling tasks on mixture dynamics in rivers. Some physical characteristics of River Debed are the following: cross section is 28.4 m^2, average water discharge is 31.3 m^3/sec. We accept stepwise function for values of $f(x,t)$. The numerical scheme is given in (Kudriashova 1993). In particular the convergence of approximate solution to the exact one under condition of infinite increase of the number of mesh nodes is proved. The finite-differences scheme is the same as used in (Abdrakhmanov, etc.1995).

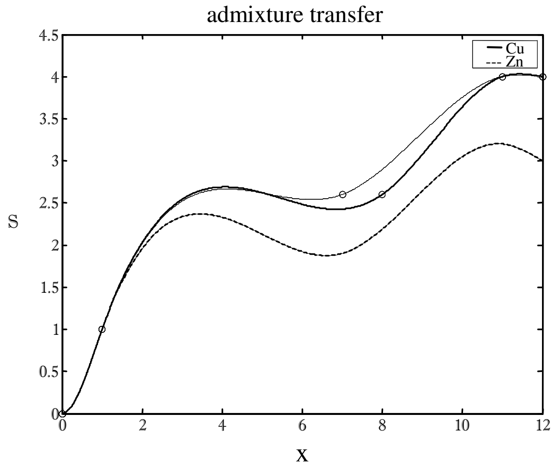

Fig. 2. Transfer of Cu and Zn along the river net.

x-axis is distance in km, scale 1 unit corresponds to 10km, solid line represents dynamics for Cu, dashed-Zn.

The lengths between successive points in rivers are brought in the table 1.

Table 1

Pambak-Shirakamut	Pambak-Vanadzor	Debed -Ayrum
3 km from the waterhead	82 km	112 km

Let us *a* be the point Pambak-Vanadzor and *b* the point at Debed-Ayrum. Boundary values are selected averaged over five years, that is why seasonal annual changes are not included. There are sources of additional input at Pambak-Vanadzor and Debed –Ayrum. The real data from monitoring showed an increase to 2,6 times with background to *a* for contents of Cu at Vanadzor and change of the contents to four times approximately at Ayrum. The same variables for Zn are 1.9 and 3.2. Debed is the largest river in northern Armenia, it is affected by several pollution sources located along the river and its two major tributaries Pambak and Dzoraget. Vanadzor, Spitak and Alaverdi towns are located in the watershed of the Debed river. The main industrial pollution sources are the Akhtala mining and dressing plant, and the Alaverdi copper smelter.

The program for numerical solution of the Saint Venants equations is performed as a program in MATLAB 7.

Mathematical models based on Saint Venants equations provide base for disposition of stations for monitoring of the river-net state and analyze dynamics of pollutants based on various scenarios of pollutants transfer.

Conclusion

In this paper a model for heavy metals balance in system atmosphere-soil-river water is proposed. Modeling approach is used for estimation of local subsystems mutual impact, considered as point oscillators for idealized models of metal accumulation in parts of the river net.

Development of a model for the polluting substances transfer is directed to solution of tasks of water quality management in Kura-Araks rivers basin. The model will allow taking into account factors of both anthropogenic and natural pollution, as well as the impact of climate change in the region.

The proposed approach to modeling will be further developed and used for applied models of spatial transportation of pollutants in Kura-Araks rivers basin.

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