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Mathematical modeling of advection- diffusive transport processes of certain pollutants from point sources in the Podu Iloaiei reservoir- Case Study

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Abstract: In this paper is analyzed the advection-diffusion mechanism of transport of pollutants from the wastewater treatment plant of Târgu Frumos city arriving through Bahlueţ watercourse in Podu Iloaiei reservoir, located downstream. Transport processes of pollutants are highlighted by a mathematical model developed in MATLAB programming software.

Keywords: advection diffusion transport, mathematical model, Podu Iloaiei reservoir.

1. INTRODUCTION

For simulating the dispersion of pollutants in reservoirs have been developed so models oriented by transport and statistical models.

In 1985, Walker has developed a series of empirical relationships for modeling potential eutrophication of lakes used later in designing kinetic models of order 1 and order 2, which are used in the study for BATHUB eutrophication of reservoirs model as developed by U.S. Army Corps of Engineers (WW Walker, 2004).

Leon et Escalante (1993) and Karahan (2001) had developed two-dimensional complex models applied in the surface waters domain.

Iscen et al. (2008) had developed a model based on multivariate statistical techniques.

Gavrilescu et. al. (2005) propose a model of order zero, applicable to biodegradable pollutants.

Chiorescu et. al. (2011) had developed a model of order zero applicable to non-biodegradable pollutants, but also considers sorption-desorption processes by introducing an appropriate term TSD (sorption-desorption term).

Chiorescu E., Roca D., (2012), took the numerical model from the previous paper, which could have improved by determination of TSD parameters by applying the method of least squares, minimizing the sum of deviations module and minimizing the sum of deviations module for the solution of Cauchy problem. For a representative case study, it was found that by applying latter method have been obtained best results in terms of accuracy to solve the Cauchy problem.

Having regard to current techniques for monitoring of water quality from the reservoirs, which requires only one or two sampling sections at certain time intervals, the samples analyzed, in this study we took the numerical model from paper Chiorescu E., Roca D., (2012) for which we obtained the best results, we completed the model with a related term- evaporation from the surface of reservoir and then we applied for a representative case study from Bahlueţ river basin even pollution of the Podu Iloaiei reservoir, caused by deficiencies occurring at waste water treatment plant Târgu Frumos city, during 04.02. ÷ 09.03.2011 period of time.

2. MATHEMATICAL MODEL

It is considered a lake supplied upstream by a conventional source of clean water (water course Bahlueţ) in which is discharging a concentrated source of pollution (Tg Beautiful WWTP). The reservoir discharge the outflows to downstream section through a floodway (bottom drain, outlet structure) from reservoir a certain water flow is taken by the inlet water station for irrigation of agricultural areas.

2.1. Basic equations

The mathematical model adopted for the dispersion of a soluble pollutant to reservoir is considered by zero order and usual approximations for density of water and polluting solutions (from lake, ρ, for source of water supply of a reservoir ρ_a; for concentrated source of pollution , ρ_p) as follows:

$$\frac{\rho}{\rho_w} \cong 1; \frac{\rho_a}{\rho_w} \cong 1 \tag{1}$$

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$$\frac{\rho_p}{\rho_w} \cong 1 + \frac{C_p}{\rho_w} \tag{2}$$

Considering and evaporation from the surface of reservoir, completing mathematical model from paper Chiorescu E., Roca D, we obtained the following system of two first order differential equations with dependent variables C and V.

$$\begin{cases} \dfrac{dC}{dt} = \dfrac{Q_a C_a + Q_p C_p - \left[\left(1 + C_p/\rho_w\right)Q_p + Q_a - Q_{evp}\right]C - Q_e\left(C - C_{sat}\right) r_0 A e^{-\alpha(t-t_0)}}{V} \\ \dfrac{dV}{dt} = Q_a + \left(1 + C_p/\rho_w\right)Q_p - Q_e - Q_{evp} \end{cases} \tag{3}$$

Where t – time (t_0 – initial time), [s], C=C(t)- concentration of water from the reservoir, [kg/m^3], V=V(t)- volume of water from the reservoir, [m^3], ρ_w –density of pure water to water temperature from the reservoir, [kg/m^3], $Q_a = Q_a(t)$ – the volume flow rate of water supply of the reservoir with clean water, [m^3/s], $Q_p = Q_p(t)$ – the volume flow rate of concentration pollution source, [m^3/s], $Q_e = Q_e(t)$ – the volume outflow rate wich is discharged to downstream or is flow rate of water retrieved by the inlet pumping station [m^3/s];

$Q_{evp} = Q_{evp}(t)$- the volume water flow rate which is evaporated from the surface of the reservoir (the concentration of evaporated water is assumed being zero), [m^3/s], $C_a = C_a(t)$ – concentration of pollutant from water supply (values under the maximum admissible level), [g/m^3], $C_p = C_p(t)$ – concentration of pollutant of the concentrated source of pollution (values above the maximum admissible level), [g/m^3], $C_e = C_e(t) \approx C(t)$ - concentration of pollutant of outflow and/or retrieved from the reservoir, [g/m^3], C_{sat} - concentration of pollutant to saturation, [kg/m^3], r_0 – the specific retard coefficient, [m^{-2}], A=A(t) – area of reservoir cuvette, corresponding to volume V (approximated by the surface area of the reservoir), [m^2], α – the sorbtion process rate (coefficient greater than zero).

Therefore, TSD, having expression

$$Q_e\left(C - C_{sat}\right) r_0 A e^{-\alpha(t-t_0)} \tag{4}$$

Is defined using the exponent α, and two coefficients, C_{sat} şi r_0.

Considering the characteristic curves of the lake - the capacity and, respectively, the water surface area, V=V(H), A=A(H), by removing of the level, H, from the two functions, was deducted the dependency of area with the volume V:

$$A = \mathrm{A}\left[\mathrm{V}^{-1}(V)\right]. \tag{5}$$

For experimental determination of the functions $Q_a(t)$, $C_a(t)$, $Q_p(t)$, $C_p(t)$, $Q_e(t)$, $C_e(t)$ şi $Q_{evp}(t)$, as well as parameters C_{sat}, r_0 şi α, we must have the following series of n couplings experimental data:

$$\left\{t_i, V_i = \mathrm{V}(H_i), Q_{pi}, C_{pi}, Q_{ai}, C_{ai}, Q_{ei}, C_{ei}, Q_{evpi}\right\} \text{cu}$$

i=1,2,…n. (6)

Over any range [ti, ti+1], the following approximations have been assumed in functions Qa(t), Ca(t), Qp(t), Cp(t), Qe(t) şi Ca(t):

$$Q_a(t) \approx \bar{Q}_{a0} + \bar{q}_a t, C_a(t) \approx \bar{C}_a, Q_p(t) \approx \bar{Q}_{p0} + \bar{q}_p t, C_p(t) \approx \bar{C}_p \tag{7}$$
$$Q_e(t) \approx \bar{Q}_e, C_e(t) \approx \bar{C}_e, Q_{evp}(t) \approx \bar{Q}_{evp},$$

And by the processing of data from series (7) resulted:

$$\bar{Q}_a = \left(\bar{Q}_a\right)_{i,i+1} = \frac{Q_{ai} + Q_{ai+1}}{2}, \bar{Q}_p = \left(\bar{Q}_p\right)_{i,i+1} = \frac{Q_{pi} + Q_{pi+1}}{2},$$
$$\bar{Q}_e = \left(\bar{Q}_e\right)_{i,i+1} = \frac{Q_{ei} + Q_{ei+1}}{2}; \tag{8}$$

$$\begin{cases} \bar{Q}_{evp} = \left(\bar{Q}_{evp}\right)_{i,i+1} = \dfrac{Q_{evpi} + Q_{evpi+1}}{2}, \\ \bar{Q}_{a0} = \left(\bar{Q}_{a0}\right)_{i,i+1} = \dfrac{Q_{ai}\, t_{i+1} - Q_{ai+1}\, t_i}{t_{i+1} - t_i}, \\ \bar{Q}_{p0} = \left(\bar{Q}_{p0}\right)_{i,i+1} = \dfrac{Q_{pi}\, t_{i+1} - Q_{pi+1}\, t_i}{t_{i+1} - t_i}; \end{cases} \tag{9}$$

$$\bar{q}_a = \left(\bar{q}_a\right)_{i,i+1} = \frac{Q_{ai+1} - Q_{ai}}{t_{i+1} - t_i}, \bar{q}_p = \left(\bar{q}_p\right)_{i,i+1} = \frac{Q_{pi+1} - Q_{pi}}{t_{i+1} - t_i}; \tag{10}$$

$$\bar{C}_a = \left(\bar{C}_a\right)_{i,i+1} = \frac{C_{ai} + C_{ai+1}}{2}, \bar{C}_p = \left(\bar{C}_p\right)_{i,i+1} = \frac{C_{pi} + C_{pi+1}}{2},$$
$$\bar{C}_e = \left(\bar{C}_e\right)_{i,i+1} = \frac{C_{ei} + C_{ei+1}}{2}. \tag{11}$$

To examine parameters Csat, r0 şi α, in TSD expression TSD was operated approx. $C(t) \approx C_e(t)$, so that resulting the following system, of n-1 eqs:

$$\left[\left(\bar{C}_e\right)_{i,i+1} - C_{sat}\right] r_0\, \bar{A}_{i,i+1}\, e^{-\alpha(t_i - t_0)}\left(\alpha\, \bar{\Omega}_{i,i+1} + \bar{\Gamma}_{i,i+1}\right) = \bar{\Theta}_{i,i+1}, \tag{12}$$

with i=1,2,...n-1,

where $\bar{\mathrm{E}} = \bar{\mathrm{E}}_{i,i+1} = e^{-\bar{a}(t_{i+1} - t_i)}$,

$$\bar{\Omega}_{i,i+1} = \bar{Q}_e\left[\bar{\mathrm{E}} + \bar{a}\left(t_{i+1} - t_i\right) - 1\right],\ \bar{\Gamma}_{i,i+1} = \bar{a}\bar{Q}_e\left(\bar{\mathrm{E}} - 1\right) \tag{13}$$

$$\bar{\Psi}_i = \left[\bar{a}\left(\bar{Q}_{a0} - \bar{Q}_{evp}\right) - q_a + q_a \bar{a} t_i\right]\bar{C}_a,$$
$$\bar{\Psi}_{i+1} = \left[\bar{a}\left(\bar{Q}_{a0} - \bar{Q}_{evp}\right) - q_a + q_a \bar{a} t_{i+1}\right]\bar{C}_a \tag{14}$$

$$\bar{\Lambda}_i = \left(\bar{a}\bar{Q}_{p0} - q_p + q_p \bar{a} t_i\right)\bar{C}_p, \bar{\Lambda}_{i+1} = \left(\bar{a}\bar{Q}_{p0} - q_p + q_p \bar{a} t_{i+1}\right)\bar{C}_p \tag{15}$$

$$\bar{\Theta}_{i,i+1} = \bar{a}^2 \bar{V}\left(C_{ei+1} - C_{ei}\bar{\mathrm{E}}\right) + \left(\bar{\Psi}_i + \bar{\Lambda}_i\right)\bar{\mathrm{E}} - \left(\bar{\Psi}_{i+1} + \bar{\Lambda}_{i+1}\right),$$

$$\bar{a} = \bar{a}_{i,i+1} = \frac{1}{\bar{V}}\left[\left(1 + \bar{C}_p/\rho_w\right)\bar{Q}_p + \bar{Q}_a\right]; \tag{16}$$

$$\bar{V} = \bar{V}_{i,i+1} = \frac{V_i + V_{i+1}}{2},\ \bar{A} = \bar{A}_{i,i+1} = \mathrm{A}\left[\mathrm{V}^{-1}\left(\bar{V}_{i,i+1}\right)\right] \tag{17}$$

For n≥4, selecting three reprezentative values for order number i: $i^I, i^{II}, i^{III} \in \{1, 2, 3, \ldots, n\text{-}1\}$ (18)

d introducing the notation (exemplified for i=i^I) of the form:

$$t_i = t^I, \bar{A}_{i,i+1} = \bar{A}^I, \left(\bar{C}_e\right)_{i,i+1} = \left(\bar{C}_e\right)^I, \bar{\Gamma}_{i,i+1} = \bar{\Gamma}^I, \bar{\Omega}_{i,i+1} = \bar{\Omega}^I$$

and $\bar{\Theta}_{i,i+1} = \bar{\Theta}^I$ (19)

From system (12) is extracted following system of ree equations, compatible determined:

$$\begin{cases}\left[(\bar{C}_e)^{I} - C_{sat}\right]\cdot r_0 \cdot \bar{A}^{I} \cdot e^{-\alpha\cdot\left(t^{I}-t_0\right)} \cdot \left(\alpha\cdot\bar{\Omega}^{I} + \bar{\Gamma}^{I}\right) = \bar{\Theta}^{I} \\ \left[(\bar{C}_e)^{II} - C_{sat}\right]\cdot r_0 \cdot \bar{A}^{II} \cdot e^{-\alpha\cdot\left(t^{II}-t_0\right)} \cdot \left(\alpha\cdot\bar{\Omega}^{II} + \bar{\Gamma}^{II}\right) = \bar{\Theta}^{II} \\ \left[(\bar{C}_e)^{III} - C_{sat}\right]\cdot r_0 \cdot \bar{A}^{III} \cdot e^{-\alpha\cdot\left(t^{III}-t_0\right)} \cdot \left(\alpha\cdot\bar{\Omega}^{III} + \bar{\Gamma}^{III}\right) = \bar{\Theta}^{III}\end{cases} \quad (20)$$

The solution of the system (20) lead to satisfying the following conditions:

$$\begin{aligned}\min\Big\{&\left|\left[(\bar{C}_e)^{I} - C_{sat}\right] r_0 \bar{A}^{I} e^{-\alpha\left(t^{I}-t_0\right)}\left(\alpha\bar{\Omega}^{I}+\bar{\Gamma}^{I}\right)-\bar{\Theta}^{I}\right| + \\ +&\left|\left[(\bar{C}_e)^{II} - C_{sat}\right] r_0 \bar{A}^{II} e^{-\alpha\left(t^{II}-t_0\right)}\left(\alpha\bar{\Omega}^{II}+\bar{\Gamma}^{II}\right)-\bar{\Theta}^{II}\right| + \\ +&\left|\left[(\bar{C}_e)^{III} - C_{sat}\right] r_0 \bar{A}^{III} e^{-\alpha\left(t^{III}-t_0\right)}\left(\alpha\bar{\Omega}^{III}+\bar{\Gamma}^{III}\right)-\bar{\Theta}^{III}\right|\Big\}\end{aligned} \quad (21)$$

The Problem (21) was solved numerically using standard external MATLAB function- **fminsearch.m,** which is based by the minimization algoritm Nelder_Mead, that calls a user scalar function, returned by the sum of the relation (21) and require the start values α_0, C_{0sat} şi r_0, which satisfying the following restrictions:

$$\alpha^{\min} \le \alpha^{0} \le \alpha^{\max},\ C_{\mathrm{sat}}^{\min} \le C_{\mathrm{sat}}^{0} \le C_{\mathrm{sat}}^{\max} \quad (22)$$

and $r_0^{\min} \le r_0^{0} \le r_0^{\max}$

where the indices „ min ” and „ max ” indicate the lower limits and upper limits, of the range where is envision searching of the solution.

2.2. Solving the Cauchy problem for system (1)

As mentioned above, the coefficients of the system (3) can be determined by relations (7) ... (11), and the parameters that define TSD from solving the problem (21).

The Cauchy problem attached to the system (3) is defined by that system and initial conditions below:

$t = t0 \ge t_1$, $C(t_0) = C_0$ şi $V(t_0) = V_0$. (23)

Usually, the Cauchy problem (1) & (22) can be solved numerically by Ruge-Kutta numerical method of variable order. Finally, using appropriate interpolation techniques, results and analytical expressions of the unknown functions:

$C=C(t)$ and $V=V(t)$, for $t \in [t_0,t_n]$. (24)

To validate the mathematical model in the line (6) we will retain $N \le n$ pairs of values:

$\{t_{i*}, C_{i*}\}$, for $i*=1,2,...,N$ and $t_0 \le t_{i*} \ge t_n$ (25)

which define the experimental functions:

$C^*=C^*(t)$, cu $C^*(t_{i*})=C_{i*}$ (26)

As a validation criterion, for the function C=C(t), was established the mean deviation of order p=1 of theoretical values C from the experimental values C*, σC.

$$\sigma_C = \frac{\sum_{1=1}^{N}\left(C_i - C_{i-1}\right)}{N-1} \quad (27)$$

2.3. The determination of TSD parameters by the minimizing the sum of deviation of order p method for solution of Cauchy problem for system (1)

The system (20) for determining the parameters of TSD is based on analytical solution of the system (3) which was determined operating in TSD the approximation $C(t) \approx C_e(t)$. The method presented in this section give up this approximation and consists in determining the unknowns terms α, C_{sat}, and r_0 from the following condition of minimization:

$$\min\left[\sum_{i^*=1}^{N}\left|C_{i*} - C\left(t_{i*}\right)\right|\right]. \quad (28)$$

Problem (28) was solved numerically using standard external function **fminsearch.m**, which is based on the Nelder_Mead minimization algoritm, that requires the begin values α_0, C^0_{sat} and $r^0{}_0$, values can be estimated with the solution of system (20); the **fminsearch.m function** calls a user scalar function given by the sum from the relation (28).

As a validation criterion for the function C=C(t), with TSD parameters determined from the condition (28), we used the average deviation of order p=1, σC, given by the relation (27).

In analyzing the accuracy of determination of the solution C=C(t), are use-full the absolute deviation δC(ti*), [kg/m³] and relative deviation δrC(ti*), [%], defined by the following relations:

$$\delta_C\left(t_{i*}\right) = C\left(t_{i*}\right) - C_{i*},\quad \delta_{rC}\left(t_{i*}\right) = \frac{C\left(t_{i*}\right) - C_{i*}}{C_{i*}}\cdot 100 \quad (29)$$

i*=1,2,...,N

If p=1, the relation (28) becomes:

$$\min\left[\sum_{i^*=1}^{N}\left|C_{i*} - C\left(t_{i*}\right)\right|\right], \quad (30)$$

And lead to minimization of the sum of deviations module for solution of the Cauchy problem mentioned above.

With the purpose to facilitate the practical application of the mathematical model presented in Chapter 2, was used **Lac_Acumulare_Zero.m** computer program.

3. THE Lac_Acumulare_Zero.m COMPUTER PROGRAM

The **Lac_Acumulare_Zero.m computer program** use the programs of the external standard function **fminsearch.m**, **ode113.m** şi **norm.m**.

3.1. The input data computer program, systematized by category, are:

1°- The general parameters (the variation time step,Δt, [h]);

2°- The geometrical characteristics of reservoir (water level in the reservoir, H, [mdMN] stored water volume, V, corresponding to level H [m³] the water surface of the reservoir area, A, corresponding to H level [m²]).

3°- The hydraulic characteristics of reservoir (the moments of monitoring of the hydraulic parameters, t_i, [h] or [d], the flows of the pollution source, Q_{pi}, [m^3s^{-1}]; the water flows of the water supply, Q_{ai}, [m^3s^{-1}], water volumes to reservoir, V_i, [m^3] or the height, H_i, [mdMN]; the outflows discharge to downstream section, Q_{ei}, [m^3s^{-1}]); the evaporated flows from the surface of the reservoir, Q_{evpi}, [m^3s^{-1}]).

4°- The water quality characteristics of the inflows/ outflows (the moments of monitoring of the quality parameters, t_i, [h] or [d], the concentration of the pollution source, C_{pi}, [gm^{-3}], the concentration of the supplying source, C_{ai}, [gm^{-3}], the concentration of the outflows, discharge to downstream or intake from reservoir, C_{ei}, [gm^{-3}]).

5°- Initial conditions and/or final (initial moment, t_0, [h], initial concentration in reservoir, C_0, [gm^{-3}], the initial volume of water stored to reservoir, V_0, [m^3], the final moment of compute, t_{Max}, [h]).

6°- Restrictions imposed to the TSD term (the minimum values for the exponent α and the coefficients C_{sat}, r_0: $\alpha^{\min}$, [h^{-1}], $C_{\rm sat}^{\min}$, [g m^{-3}] and $r_0^{\min}$, [m^{-2}]; the maximum values for the exponent α, and the coefficients C_{sat}, r_0: $\alpha^{\max}$, [h^{-1}], $C_{\rm sat}^{\max}$, [g m^{-3}] and $r_0^{\max}$, [m^{-2}]).

3.2. The output data from the **Lac_Acumulare_Zero.m computer program**, also systematized by category, are:

1°- The coefficients of the system (20), $\left\{(\bar{C}_e)^{I}, \bar{A}^{I}, \bar{\Omega}^{I}, \bar{\Gamma}^{I}, \bar{\Theta}^{I}\right\}, \left\{(\bar{C}_e)^{II}, \bar{A}^{II}, \bar{\Omega}^{II}, \bar{\Gamma}^{II}, \bar{\Theta}^{II}\right\}, \left\{(\bar{C}_e)^{III}, \bar{A}^{III}, \bar{\Omega}^{III}, \bar{\Gamma}^{III}, \bar{\Theta}^{III}\right\}$;

2° - The parameters of the **TSD** term (4) (the exponent α, [h^{-1}], the saturation concentration coefficient, C_{sat}, [g m^{-3}], the coefficient r_0, [m^{-2}]) was evaluated from solving teh system (20) and minimizing the sum of deviations module for the solution of the Cauchy problem.

3° - The solution (24) for the Cauchy problem (3) and (24) and their respective dimensions (the number of points *m*, which is rendered the solution (24), $m \geq n$; the solution (24): $\{t_j, C_j, V_j\}$, j=1,2, ..., m; the solution (26), $\{t_{i*}, C_{i*}\}$, $i* = 1, 2, \ldots, N$; the absolute deviations, $\delta_C(t_{i*})$; the relative deviations, $\delta_{rC}(t_{i*})$; the mean deviation of order p=1, σ_C);

4°- Significant graphical representations for the output data (the variations of the pollutant concentration in to the reservoir, based on the experimental measurements and by the solution (24) for the Cauchy problem (3) and (24), the variation of the absolute deviations, $\{t_{i*}, \delta_C(t_{i*})\}$, $i* = 1, 2, \ldots, N$, the variation of the relative deviations, $\{t_{i*}, \delta_{rC}(t_{i*})\}$, $i* = 1, 2, \ldots, N$).

4. THE CASE STUDY

The case study was solved with **Lac_Acumulare_Zero.m** computer program, which simulate the pollution of the Podu Iloaiei reservoir (Fig. 1), from the water course Bahlueţ river basin, caused by deficiencies occurring at waste water treatment plant Târgu Frumos during 04.02. ÷ 09.03.2011, when the concentration of the pollutant analyzed (Total nitrogen) exceeded maximum allowed limit C_{adm}=15 gm^{-3}.

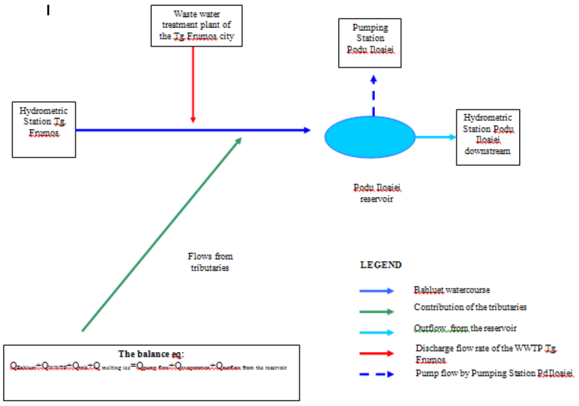


Fig. 1- Schematic diagram of the flows which are part of the balance eq.

4.1. Input data

1°- the time step for computing Δt. Was adopted Δt=1 hour;

2°- The characteristics curve of the reservoir (Tab. 1), the capacity (rows 2 and 3) and area of reservoir (rows 2 and 4);

Tab. 1- The characteristics curve of the Podu Iloaiei reservoir

Nr. pct.	1	2	3	4	5	6	7	8
H, [mdMN]	61.7	62.0	62.2	62.4	62.5	62.8	63.0	63.1
V, [m^3]	3537000	4320000	4885000	5483000	5794000	6776000	7471000	7830000
A, [m^2]	2217060	2509700	2705240	2899670	2996350	3283710	3472570	3566050

3°- The hydraulic characteristics of the reservoir (Tab. 2, in column 1...6);

Tab. 2- The hydraulic characteristics of the Podu Iloaiei reservoir şi water quality characteristics of the inflows/outflows from the Podu Iloaiei reservoir

i	t_i [h]	Q_{pi} [m^{3}s^{-1}]	Q_{ai} [m^{3}s^{-1}]	Q_{ei} [m^{3}s^{-1}]	C_{pi} [gm^{-3}]	C_{ai} [gm^{-3}]	C_{ei} [gm^{-3}]	Q_{evpi} [m^{3}s^{-1}]
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
1	0	0.0414	0.953	0.621	15.123	8.413	1.379	0.0063
2	**24**	**0.0412**	**0.967**	**0.619**	**15.593**	**8.330**	**1.406**	**0.0071**
3	**48**	**0.0411**	**1.157**	**0.618**	**16.022**	**7.688**	**1.433**	**0.0078**
4	72	0.0409	1.211	0.618	16.410	7.544	1.459	0.0083
5	96	0.0408	1.075	0.616	16.760	7.911	1.485	0.0088
6	120	0.0407	1.043	0.616	17.071	8.006	1.511	0.0091
7	144	0.0405	1.030	0.616	17.346	8.052	1.537	0.0093
8	168	0.0404	1.069	0.616	17.586	7.930	1.562	0.0095
9	192	0.0402	1.171	0.617	17.791	7.666	1.587	0.0095
10	216	0.0401	1.112	0.617	17.963	7.819	1.612	0.0094
11	240	0.04	1.119	0.618	18.102	7.810	1.636	0.0092
12	264	0.0398	1.115	0.618	18.211	7.826	1.66	0.0090
13	288	0.0397	1.070	0.619	18.290	7.941	1.684	0.0087
14	312	0.0396	1.073	0.620	18.341	7.935	1.707	0.0083
15	**336**	**0.0395**	**1.115**	**0.621**	**18.341**	**7.822**	**1.73**	**0.0078**
16	**360**	**0.0393**	**1.141**	**0.623**	**18.360**	**7.756**	**1.752**	**0.0073**
17	384	0.0392	1.180	0.624	18.331	7.663	1.774	0.0067
18	408	0.0391	1.209	0.625	18.279	7.595	1.796	0.0061
19	432	0.039	1.250	0.627	18.203	7.502	1.817	0.0054
20	456	0.0389	1.312	0.628	18.106	7.388	1.837	0.0047
21	480	0.0388	1.335	0.630	17.988	7.332	1.857	0.0040
22	504	0.0387	1.364	0.632	17.850	7.265	1.877	0.0032
23	528	0.0386	1.398	0.634	17.695	7.194	1.896	0.0024
24	552	0.0385	1.432	0.635	17.522	7.123	1.915	0.0016
25	576	0.0384	1.507	0.637	17.333	7.014	1.933	0.0008
26	600	0.0383	1.530	0.639	17.129	6.957	1.95	0.0000
27	624	0.0382	1.538	0.639	16.912	6.910	1.967	0.0000
28	648	0.0381	1.596	0.640	16.682	6.825	1.983	0.0000
29	672	0.038	1.614	0.640	16.441	6.763	1.999	0.0000
30	696	0.0379	1.660	0.640	16.189	6.690	2.014	0.0000
31	720	0.0378	1.689	0.640	15.929	6.623	2.029	0.0000
32	744	0.0378	1.717	0.640	15.660	6.718	2.043	0.0000
33	**768**	**0.0377**	**1.765**	**0.641**	**15.385**	**6.652**	**2.056**	**0.0000**
34	**792**	**0.0376**	**1.849**	**0.641**	**15.104**	**6.575**	**2.068**	**0.0000**
35	816	0.0376	1.838	0.641	14.818	6.534	2.08	0.0000

4º- The water quality characteristics of the inflows/ outflows (Tab. 2 – column 1, 2 and 7…9) from the Podu Iloaiei reservoir;

About the 3º and 4º subsections are made following specifications::

a) source of pollution is waste water treatment plant Târgu Frumos, so that Q_{pi} and C_{pi} is the flow, respectively concentration of the discharge flow from the waste water treatment plant, the water supply flow rate with conventional clean water, Q_a, has 3 components:

- Q_a^1 - the Bahlueţ water flow rate, measured in the S.H. Târgu Frumos section, with concentration of the pollutant $C_a^1 < C_{adm}$;

- Q_a^2 - the all tributary water flow rate of the Bahlueţ water course, downstream S.H. Târgu Frumos section, but upstream of the Podu Iloaiei reservoir, with mean concentration in pollutant $C_a^2 < C_{adm}$;

- Q_a^3 - the melt flow precipitation in solid form fallen directly at surface of the Podu Iloaiei reservoir, with concentration of the pollutant $C_a^3 \cong 0$.

Thus, the flow Q_a and the concentration of the pollutant of water supply, C_a, has been evaluated, with following relations:

$$Q_a = Q_a^1 + Q_a^2 + Q_a^3, C_a = \frac{Q_a^1 \cdot c_a^1 + Q_a^2 \cdot c_a^2}{Q_a} \qquad (32)$$

b) the outflow or intake flow from the reservoir,Q_e, has 3 components (because the Podu Iloaiei reservoir it is in use of approx. 35 years, because of intense silting up of cuvette with bed material with fine texture, the base flow to groundwater reservoir was negligible).

- the Bahlueţ water flow rate, measured to the S.H. Podu Iloaiei section, with concentration of the pollutant Ce ≈C;

- the intake flow from Podu Iloaiei reservoir through pumping station of the Podu Iloaiei Experimental station, with concentration of the pollutant Ce ≈C;

- the evaporation flow by water surface of the Podu Iloaiei reservoir(during summer can have a significant weight), with concentration of the pollutant $C_e^3 \approx 0$.

Thus, the flow Q_e and the concentration C_e was evaluated with the following relations:

$$Q_e = Q_e^1 + Q_e^2 + Q_e^3, C_e \cong C \qquad (33)$$

c) The experimental data series (4º) include n=35 couplers, t€[t_0,t_{max}].

5º- Initial conditions and/or final:

$t_0=t_1=0$, in period 04.02.2011;

$t_{Max}=24 \cdot 33=816$, in period 09.03.2011;

$C_0=1.379$ gm^{-3};

$V_0=V(H_0)=V(61.96)=4210900 m^3$;

6º- Iniţial values imposed on term TSD: $\alpha^0=0{,}01 [h^{-1}]$, $C^0_{sat}=0$ [g m^{-3}] şi $r^0_0=0$ [m^{-2}]

The values of the dimensions which was used at evaluation of the system coefficients (20) have been take from the Tab. 2, the rows $i^I=2$, $i^I+1=3$, $i^{II}=15$, $i^{II}+1=16$, $i^{III}=33$, $i^{III}+1=34$ (rows highlighted with bold characters), and the values of the coefficients are summarized in Tab. 3.

Tab. 3- The numerical values of the system coefficients (20)

(i, i+1)	$\left(\bar{C}_e\right)_{i,i+1}$ [gm-3]	$\bar{A}_{i,i+1}$ [106 m2]	$\bar{\Omega}_{i,i+1}$ [m3s-1]	$\bar{\Gamma}_{i,i+1}$ [m3s-2]	$\bar{\Theta}_{i,i+1}$ [g s-2]
(2, 3)	1.4195	2.4896	-0.2662	0.0221	0.2692
(15, 16)	1.7410	2.6944	-0.2477	0.0206	0.2569
(33, 34)	2.0620	3.1164	-0.3061	0.0254	0.4321

The solution of the system (20), was obtained solving numerically eq. (21), so that the verification deviations of each eq. of the system (20) are mentioned in Tab. 4.

Tab. 4- The solution of the system (20) for the TSD parameters

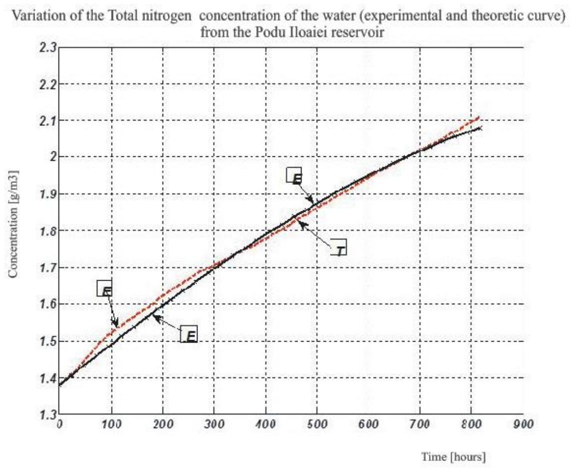
Nr. crt.	The TSD paramaters term			Verification deviations, [$\cdot 10^{-11}$]		
	C_{sat}, [gm^{-3}]	r_0, [10^{-6} m^{-2}]	α,[h^{-1}]	Ec. 1	Ec. 2	Ec. 3
1	1.4195	1.00	0.299631	-0.2692	-0.2569	-0.4321

The results on determining the TSD parameters by minimizing the sum of deviations module for the Cauchy problem solution and standard deviation σC are shown in Tab. 5

Tab. 5- Errors on TSD determination and solving the Cauchy problem for the system (3)

Nr. crt.	The TSD paramaters term			σ_C
	C_{sat}, [gm^{-3}]	r_0, [10^{-6} m^{-2}]	α,[h^{-1}]	
1	*2*	*3*	*4*	*5*
1	0.0018	2.7237e-6	5.6811e-4	0.0136

The variation of the concentration of pollutant to the reservoir based on the experimental measurements, C_{i*} (the E curve) and by solution (25) for the Cauchy problem (3)…(24), $\{t_j, C_j\}$, $j=1,2, ..., m$ (the T curve) are shown in Fig. 2.



Legend:

E ▬▬ based on the experimental measurement

T ▬ ▬ ▬ the numerical solution on the TSD being determined by minimization of the sum of deviation module for the solution of the Cauchy problem

Fig. 2- Variation of Total nitrogen concentration of the water from the Podu Iloaiei reservoir

The variation of the absolute deviation, $\{t_{i*}, \delta_C(t_{i*})\}$, $i*=1,2,\ldots,N$ and the relative deviations, $\{t_{i*}, \delta_{rC}(t_{i*})\}$, $i*=1,2,\ldots,N$, for numerical solution with TSD already determined by minimization of the sum of deviations module for solution of the Cauchy problem, are shown in Fig. 3 and Fig 4:

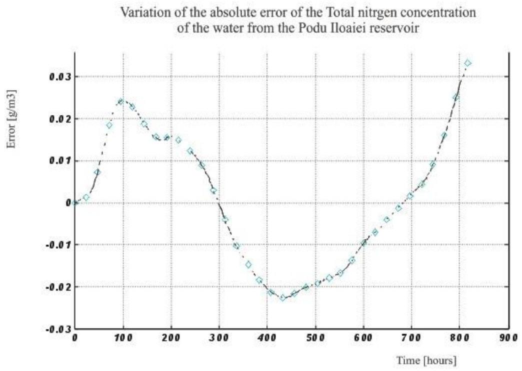


Fig. 3- Variation of the absolute error of the Total nitrogen concentration of the water from the Podu Iloaiei reservoir

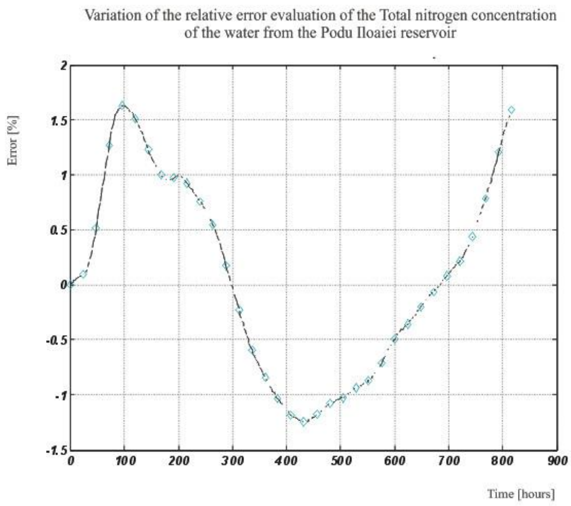


Fig. 4- Variation of the relative error of the Total nitrogen concentration of the water from the Podu Iloaiei reservoir

4. CONCLUSIONS

1. Were completed the differential equations with a term of evaporation from the water surface of the reservoir.

2. The accuracy numerical solution of the Cauchy problem for the system of differential equations (3) is in dependency precision of determination of the TSD parameters; for that reason the exponent α, as well as the two coefficients, C_{sat} şi r_0, from the TSD analytical expression being determined trough processing experimental data from the complete data set $\{t, Q_p, C_p, Q_a, C_a, Q_e, C_e, V\}$ with the optimal algoritm (Chiorescu E., Roca D., 2012), based on the minimization method of the sum of deviations module for the solution of the Cauchy problem.

3. Using same values for the TSD parameters, (shown in Tab. 5-columns 2, 3 and 4), determined for a specific case of pollution, adequately monitored, can be simulated, with high accuracy, the dispersion of a pollutant to the reservoir, in certain scenarios for de couple of the values $\{Q_p, C_p, Q_a, C_a, Q_e, V\}$ (with the purpose of carry out respective process forecasting).

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