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RESEARCH ON AQUATIC POLLUTION LEVEL OF MALEIA RIVER BY SIMULATION IN COMPUTATIONAL FLUID DYNAMICS

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Abstract

Watercourses that transit rural / urban areas are susceptible to the phenomenon of aquatic pollution due to various types of polluting species. The important issues of river pollution and of polluting species dispersion, require an approach with predictive tools (models for transport of polluting species) which can evaluate the performance of depollution measures/actions to reduce pollution and to take optimal management decisions. Thus, from January 2017 to May 2017, a monitoring investigation was carried out on the Maleia watercourse, polluting species concentrations measured by different physical-chemical methods being considered as input data for the Surface Water Modelling Systems (SMS) software in order to establish the dispersion of pollutants in the aquatic environment. The hydrodynamics of the river sector has been simulated through a module of the Surface Water Modelling Systems using the Reynolds form of Navier-Stokes equation system, along with the continuity equation for incompressible fluids in turbulent motion with free surface. The numerical simulation of advection-diffusion processes at an average depth of the studied river sector, was used for analyzing the space-time evolution of aquatic pollutants.

The originality of this paper starts from the desideratum that rivers crossing inhabited areas are subjected to discharge of pollutants which implies the analysis of the quality of the studied water course (Maleia), as well as the illustration of the dispersion of certain pollutant species by estimating the dilution times as well as the determination of the iso-concentration field.

Numerical models have been obtained for a sector of the Maleia River, providing the possibility of simulating both common and accidental pollution (related to space-time evolution of transport and dispersion of pollutants). The models obtained allowed the estimation of water quality in each finite element of the studied sector, and not just in one sampling point, as it is usually measured.

Key words: aquatic pollution, water body, dispersion, mathematical model

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1. Introduction

One of the most important environmental issues in Romania is aquatic pollution, which is an extremely complex phenomenon (Marinov et al., 2017). Fast industrial development and increased standards of living led to a corresponding increase of water supply capacity, but along with this increase, the amounts of contaminated discharges also grew significantly (Unes and Varcin, 2017; Zaharia and Jufa, 2017). Many rivers and particularly those crossing inhabited areas are subject to contaminated discharges (Costabile and Macchione, 2017).

Therefore, the aquatic environmental management decision makers need the support of reliable tools for assessing water quality and for predicting consequences of their decisions (Wurbs and Hoffpaur, 2017). This issue can be addressed through the use of computational tools for predicting the concentration of pollutants (Christopher and La Roux, 2018).

Currently, specialists use different numerical simulation software packages (Cote et al., 2016), such as Somes River in Romania the COMSOL Multiphysics program was used for predicting accidental pollution; for the Severnaia Sosiva

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watercourse from Russia ArcGIS and CE-QUAL-W2 software were used (Bicak et al., 2018) for modelling the spatial-temporal evolution of river hydrodynamics and for the Argazi-Miass-Șersni aquatic basin from Russia a dynamic modelling of the aquatic ecosystem has been performed through the Water Quality Analysis Program (WASP) (Cheema et al., 2018; Yulaev and Sukharev, 2005), on Olt river the numerical simulations were performed with the help of Surface - Water Modelling System (SMS) (Militaru et al., 2013; Ștefan et al., 2018).

The objectives of this paper are, on the one hand, monitoring the quality of the watercourse crossing areas with household settlements located around Petroșani city (characterized by pollutant species that reveal both the background pollution of the river and the pollution phenomena characteristic for the activities carried out in the area of interest), in order to obtain an ample image of the natural receiver state tributary of the Jiu river, in accordance with the household activities that can produce aquatic pollution. On the other hand, the numerical modelling of space-time evolution of physical-chemical parameters which overruns Maximum Allowable Concentration (M.A.C.) of polluting species that characterize agriculture, fruit growing as well as rural tourism on Maleia water course, by using the Navier-Stokes equation and simulation of pollutants' transport and dispersion phenomena through Computational Fluid Dynamics (CFD), as well as analysis/evaluation of the numerical simulation results.

2. Experimental

2.1. Area of interest, presentation of activities in the area and criteria for selection of pollutant species

The Jiu hydrographic basin (Fig. 1) is located in the southwestern part of the country, bordered by the Sureanu, Parâng, Retezat and Cerna mountains, which separate it from the Mureș, Sebeș, Strei and Cerna basins. The Maleia water course is located in

the Jiu river basin, about 13 km long and it is the tributary of the East Jiu River, with cadastral code: VII - 1.16.9. The Maleia watercourse has its springs at the base of the Parang massif, from the grooves formed at its base. The springs are 1,700 m high, with a high torrential character throughout the year.

When selecting the Maleia watercourse to monitor, we had in mind the situation in Petroșani Municipality, thus obtaining a bigger picture of the Jiu River natural receiver status affluent, in accordance with domestic activities that may produce aquatic pollution. The basic economic activities of the Southwest Region of Romania, including Petroșani Depression, are: agriculture (cereal crops, potato culture), fruit growing, wood exploitation and processing, and last but not least rural tourism. Agriculture, in addition to major benefits, also carries risks, sometimes having the potential of affecting human health. These must be known in order to be able to take the necessary measures.

In order to analyze water quality from their pollution point of view, monitoring points were chosen both upstream and downstream of the settlements on the Maleia watercourse. In order to characterize the water samples taken from the physico-chemical point of view, the following criteria and pollutant species were centralized in Table 1. Only dispersions of the pollutant species presenting exceedances of the reference values in the legislation in force will be presented in the paper.

2.2. Methods for investigation of aquatic polluting species concentrations

Sampling water assays represents a particularly important stage in conducting the physical-chemical water quality analysis, because the water samples must be representative (Weinberg and Teodosiu, 2012) and should not introduce errors in the composition and quality of water due to a faulty technique or incorrect material preparation conditions, knowing that errors caused by inappropriate sampling can no longer be corrected.



Fig. 1. Location of Maleia water course as well as monitoring points

Table 1. Centralization of the criteria and pollutant species used in the monitoring program

<i>Criteria</i>	<i>Pollutant species</i>
Determination of acidity / alkalinity range	pH
Quantifying biochemical decomposition of organic substances contained in the water	BOD ₅
Identification of chemical disintegration processes for sulphur-containing substances	Sulphates
Determination of solubility degree correlated with migration capacity	Chloride
Indication of processes of chemical disintegration and dissolving of dolomite, limestone and marl	Mg ²⁺
Identifying the existence of volcanic or sedimentary rocks in the river bed	Na ⁺ , K ⁺
Verifying the existence or non-existence of hydrobiontes metabolism	NH ₄ ⁺
Indication of fresh pollution processes	Nitrite
Characterization of the eutrophication process of the aquatic ecosystem	Nitrate
Identifying the presence of humic acids	Total iron ions
Indication of the presence of certain herbicides or discharges of wood residues into the watercourses	Phenols

The sampling program used was focused on several aspects, namely: setting sampling points (upstream/downstream of households), sampling time (every third day of the month) as well as the sampling frequency, respectively monthly sampling (Vasilache et al., 2012).

To quantify the pollution level, several measuring methods have been used, namely: Inductively Coupled Plasma Optical Emission Spectroscopy Analysis in accordance with SR EN ISO 11885: 2009 Water quality. Determination of selected elements by inductively coupled plasma optical emission spectroscopy (ICP-OES), Ion Chromatographic method in accordance with SR EN ISO 14911: 2003 Water quality. Determination by ion chromatography of dissolved ions. Method for water and wastewater, as well as Spectrophotometric method in UV-VIS accredited and in house developed method (SR EN ISO 14911, 2003; SR EN ISO 11885, 2009). In case of the Inductively Coupled Plasma Optical Emission Spectroscopy method, the Optima 2100 DV Perkin Elmer was used for measuring magnesium, sodium, potassium and total ferrous and ferric iron ions (Călămar et al., 2017). Through Ion Chromatography method, using the ICS 3000 - Dionex equipment, sulphate, chloride, nitrite and nitrate indicators (Velić et al., 2015) were measured. Through the spectrophotometric method, BOD₅, ammonium concentration and phenols were measured by using the Hach Lange DR 2800 equipment.

2.3. Computational analysis methodology used in the study of river aquatic dynamics

Mathematical and numerical modelling of rivers represents an essential tool in estimating the level of pollution, as well as in measuring the space-time evolution of pollutants (Militaru et al., 2013) in order to prevent exceptional situations. Lately, the computational analysis of fluid dynamics (CFD – computational fluid dynamics), which operates with numerical computing techniques (Marusic et al., 2012), is widely used in order to measure the flow parameters and to model different fluid flow processes (Yin et al., 2016), including the turbulent flow. The advantage of using CFD is the possibility to obtain high accuracy detailed information on the simulated system (Petrilean et al., 2017). Solving a problem with

CFD, involves modelling the geometry of the studied field, meshing the domain, defining the model, setting the properties, establishing the initial and limit conditions, solving as well as interpreting the results (Beşliu et al., 2011), among others.

Nowadays, more and more companies, most of them in the USA, elaborate and develop software in the field of pollutant dispersion analysis in the aquatic environment. These companies include, among others (Cretescu et al., 2013):

- the United States Environmental Protection Agency (WASP and QUAL2E programs, WASP, 2017);
- ANSYS company from Canonsburg, Pennsylvania, SUA (ANSYS CFX program, ANSYS, 2019);
- Research Centre for Agriculture and the US Natural Resources Centre (AGNPS program, AGNPS, 2019);
- MapTech Company from Blacksburg, Virginia, USA (GWLF program, GWLF, 1992);
- Institute of Ecology of Fresh Waters and Fisheries in Inland Waters, Berlin, Germany (MONERIS program, MONERIS, 2000);
- US Army Hydrological Engineering Centre (WQRRS program, WQRRS, 1989);
- Aquaveo company (Aquaveo, 2016a) in the USA (WMS, SMS).

In order to measure the pollution level of Maleia watercourse, Surfacewater Modelling System (SMS) software was used, which measures the hydrodynamics of the studied sector, modelled by the Reynolds form of Navier-Stokes equations (Ani et al., 2012) and the evolution of pollutant concentration using the fundamental advection-dispersion equation.

For modelling turbulent flow in Maleia watercourse, it was necessary the solving of numerical flow equations. In the first stage, the hydrodynamics of the modelled sector was determined through the Navier-Stokes equation system in the Reynolds form after the Cartesian coordinates *x* and *y* together with the continuity equation for incompressible fluids in turbulent motion with free surface. In the second stage, at the resulting hydrodynamics, the evolution of the pollutant concentration field was determined by numerical simulation of advection - diffusion processes at an average depth of the aquatic system. The transport equation also was solved through finite

element method, applying the Galerkin residual weighting method.

2.4. Input data used for simulations

To begin the simulation process, it is necessary to centralize the measurements performed, to set limit conditions on flow and water level, as well as the initial conditions (data used by the RMA2 subprogram within the SMS program).

Using the method of monitoring by investigation (Kovács et al., 2012), representative results were obtained for the measurement campaign conducted on the Maleia watercourse. It consisted in sampling water assays, analysis thereof with the aim of identifying the exceeding of water quality limits, as well as identifying the magnitude and impact of pollution. The upstream sampling point was located at 1.8 km away from the households, and the downstream sampling point set 200 m away from the households, these points being fixed by geographic coordinates shown below:

- Lat 45.252263 E (Upstream) Lat 45.251864 E (Downstream);
- Long 23.241571 N (Upstream) Long 23.222669 N (Downstream).

Table 2 shows the synthesis of Maleia watercourse monitoring during January 2017 - May 2017, both upstream and downstream of household settlements.

The concentration values presented in Table 2 represent the average concentrations obtained from the physico-chemical analysis of 10 water samples in different days. Analyzing Table 2 it is noted that all the quality indicators are within the normal limits governed by the legislation in force.

In order to determine the pollution level of Maleia watercourse by means of numerical simulation, such as Computational Fluid Dynamics, a sample of water was taken from a sampling point from a settlement that discharges the waste water directly into the water stream, located upstream (10 m) of the area for which the dispersion maps were drawn (Giurma et al., 2013).

Values of physical-chemical analysis of the sample taken from the pollution source of Maleia water stream are summarized in Table 3. The concentration values presented in Table 3 represent the average concentrations obtained from the physical-chemical analysis of 10 water samples in different days during January 2017 - May 2017.

Table 2. Quality indicators values on Maleia watercourse sampling points

No.	Indicator	M.A.C.*	January		February		March		April		May	
			U.S.P. [†]	D.S.P. [‡]	U.S.P. [†]	D.S.P. [‡]	U.S.P. [†]	D.S.P. [‡]	U.S.P. [†]	D.S.P. [‡]	U.S.P. [†]	D.S.P. [‡]
1	pH	6.5-8.5	7.42	7.85	7.28	7.43	6.83	7.43	7.36	7.85	7.42	7.96
2	BOD ₅ [mg O ₂ /dm ³]	20	6.82	5.14	6.86	5.18	6.93	5.07	8.89	5.02	8.72	5.13
3	Sulphates [mg/ dm ³]	600	11.37	11.28	11.34	11.26	11.38	11.25	11.39	11.21	11.36	11.27
4	Chloride [mg/ dm ³]	500	4.46	4.44	4.47	4.44	4.32	4.27	4.35	4.31	4.29	4.27
5	Mg ²⁺ [mg/ dm ³]	100	1.04	1.03	1.04	1.03	1.04	1.03	1.04	1.03	1.04	1.03
6	Na ⁺ [mg/ dm ³]	-	3.01	3.01	3.01	3.01	3.01	3.01	3.01	3.01	3.01	3.01
7	K ⁺ [mg/ dm ³]	-	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67
8	NH ₄ ⁺ [mg/ dm ³]	2.0	0.36	0.52	0.33	0.51	0.39	0.62	0.37	0.59	0.31	0.53
9	Nitrites [mg/ dm ³]	1.0	0.23	0.18	0.25	0.19	0.29	0.17	0.36	0.27	0.40	0.38
10	Nitrates [mg/ dm ³]	25.0	3.39	3.42	3.47	3.53	3.39	3.47	3.42	3.61	3.38	3.45
11	Total iron ions [mg/ dm ³]	5.0	0.021	0.07	0.021	0.07	0.021	0.07	0.021	0.07	0.021	0.07
12	Phenols [mg/ dm ³]	0,3	0.08	0.11	0.07	0.09	0.08	0.07	0.06	0.05	0.03	0.01

* U.S.P. – Upstream sampling point

† D.S.P. – Downstream sampling point

‡ M.A.C. – Maximum Allowable Concentration in accordance with the Normative of 28 February 2002 on the establishment of limits for the loading of industrial and urban waste water into the natural receptors, NTPA-001/2002 with subsequent modifications and completions

Table 3. Average values of quality indicators from the pollution source of Maleia watercourse

No.	Indicator	Measurement Unit	M.A.C.	Average concentration (2017)
1	pH	-	6.5-8.5	6.1
2	BOD ₅ [mg O ₂ /dm ³]	[mg O ₂ /dm ³]	20	32
3	Sulphates [mg/ dm ³]	[mg/ dm ³]	600	57.6
4	Chloride [mg/ dm ³]	[mg/ dm ³]	500	68.3
5	Magnesium [mg/ dm ³]	[mg/ dm ³]	100	0.03
6	Sodium [mg/ dm ³]	[mg/ dm ³]	-	0.01
7	Potassium [mg/ dm ³]	[mg/ dm ³]	-	0.01
8	NH ₄ ⁺ [mg/ dm ³]	[mg/ dm ³]	2.0	27.1
9	Nitrites [mg/ dm ³]	[mg/ dm ³]	1.0	15.6
10	Nitrates [mg/ dm ³]	[mg/ dm ³]	25.0	75.2
11	Iron [mg/ dm ³]	[mg/ dm ³]	5.0	0.009
12	Phenols [mg/ dm ³]	[mg/ dm ³]	0.3	0.12

To achieve the mathematical model of water movement as well as to measure the local water velocity, it was necessary to insert the input data gathered from the field into the SMS program, respectively: widths of the river sector taken into consideration: 3.58 m; 3.62 m; 3.81 m; depth of water (distance between river bed and water mirror): 0.37 m; 0.43 m; 0.35 m; length of river sector: 60 m; river flow in the interested section: 1.025 m³/s; average flow velocity of the river: 0.73 m/s; estimated time required for the dispersion: 100 seconds; river declivity on the studied sector: 5.41%; isotropic value: 25.

3. Results and discussion

In order to measure the dispersion of polluting species in the aquatic environment of Maleia watercourse, firstly, the segment of river course on which the analysis of pollutants' dispersion performed was delimited. The chosen river segment (Fig. 2) is defined by the following geographical coordinates:

- Lat 45.423432 E (Upstream) Lat 45.423693 E (Downstream);
- Long 23.376615 N (Upstream) Long 23.376896 N (Downstream).

In order to obtain the 2D Mesh (Fig. 3), the Cartesian coordinates were introduced for the selected area from the satellite image. By triangulation the input data (Cartesian coordinates), the quadric triangles and the linear triangles (Fig. 4) were obtained, which were required for the numerical model used by the RMA2 subprogram. In order to increase the processing speed of the subprograms used, the triangles obtained in the previous mesh were merged, to acquire the quadrilateral elements (Fig. 5).

For the purpose of numerical simulation, a sector with a length of 60 m of the Maleia river in the Petrosani city was chosen, which was discretised directly in the SMS system in finite elements by dividing in 23 cross-sections to every 2.6 m, in a total of 520 polygons. Field geometry is shown in Fig. 3.

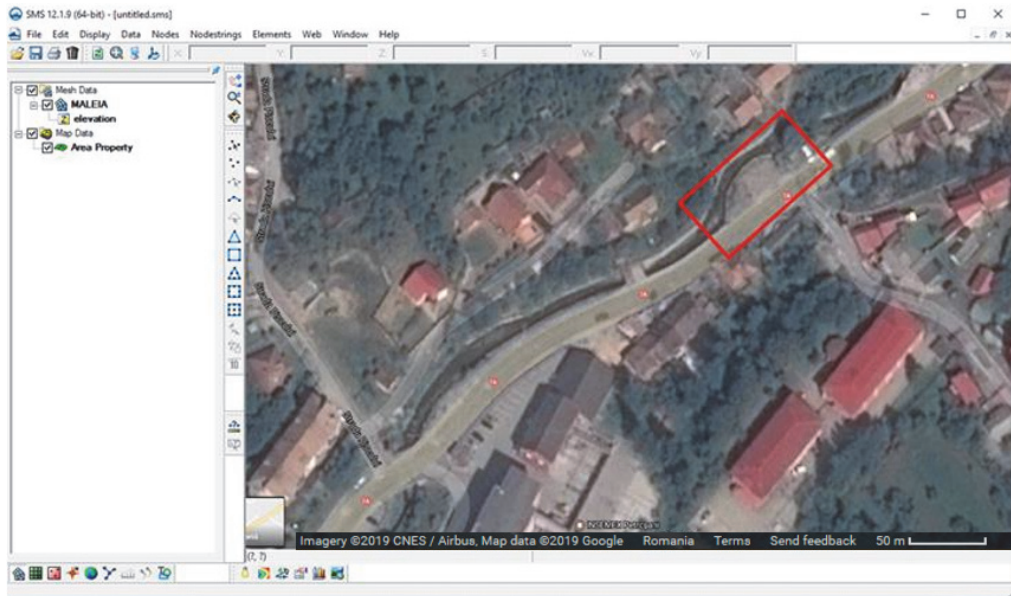


Fig. 2. The satellite image of the river segment taken into study

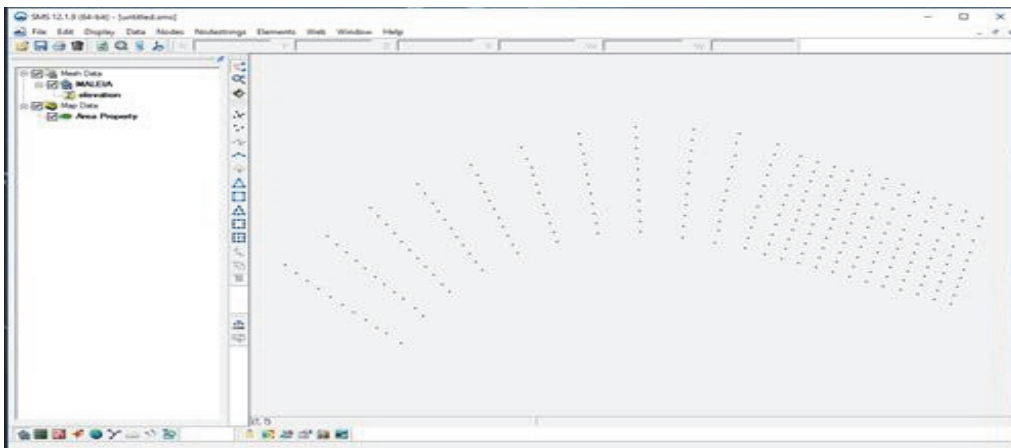


Fig. 3. The 2D mesh for the studied river sector

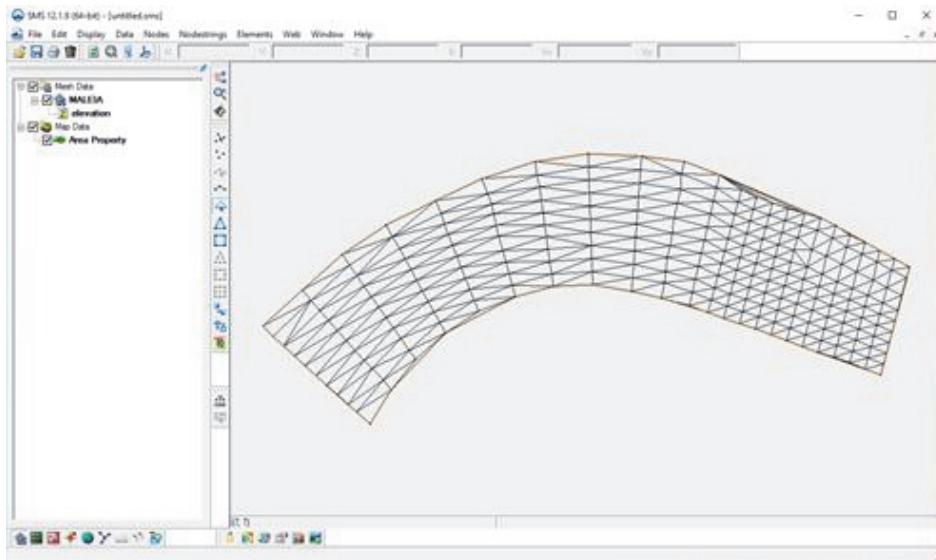


Fig. 4. 2D mesh needed to apply mathematical models

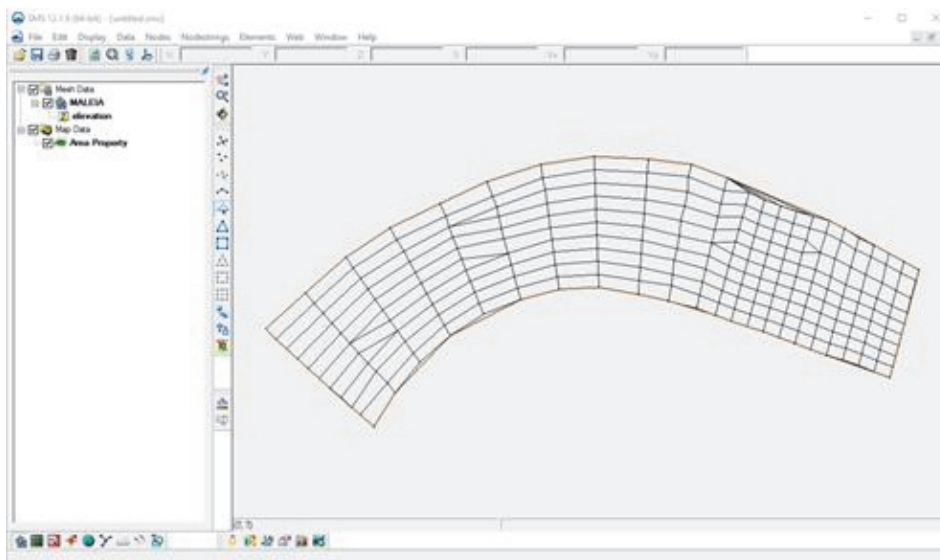


Fig. 5. Mesh 2D obtained with quadrilateral elements

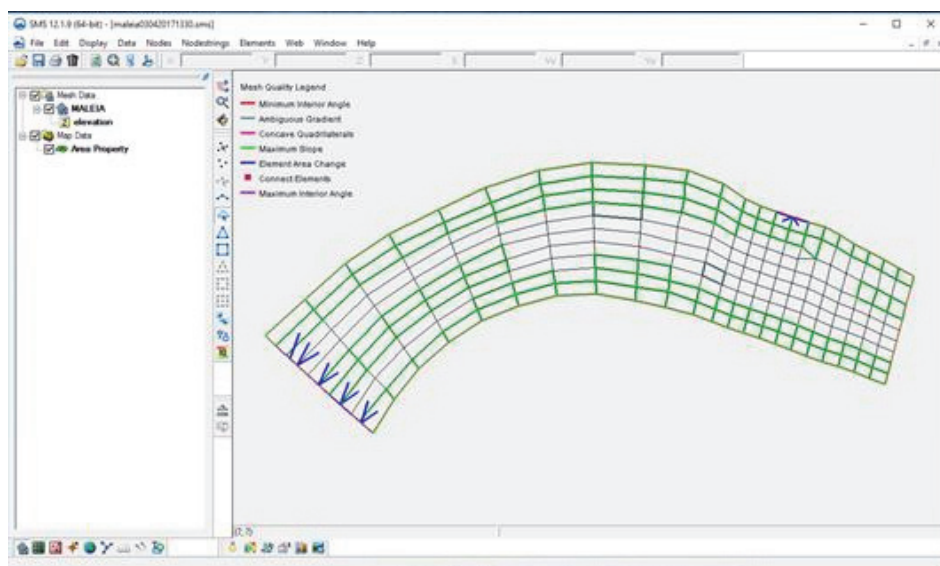


Fig. 6. Running the RMA2 subroutine to verify input data

A model inspection (Fig. 6) was performed in the RMA2 subroutine to check if all simulation items required were correctly inputted to eliminate some inconsistencies between the input data. With the aid of the RMA2 subroutine, the geometry of the studied river sector and the mathematical flow model were achieved (Aquaveo, 2016b). As a result of the execution of the RMA2 program, the hydrodynamics of the studied sector was obtained in all finite elements, especially the speed in the x and y directions, as well as the resulting velocity. Also, the depth of water was determined in all finite elements.

The numerical stability of the RMA2 program has been verified using the Froude number.

For calibrating the model, data collected in 2017 was used. The calibration was performed under the same conditions using the same computing network with the same properties. The model was calibrated by varying the Peclet number within acceptable limits.

A dispersion simulation for ammonia, nitrite and nitrate concentrations as water quality indicators, was performed for Maleia watercourse, because these quality indicators have exceeded the pollution limits.

In order to obtain numerical models regarding the determination of transport and dispersion of pollutants, the RMA4 program in the SMS system was used (Aquaveo, 2016c).

Aiming to achieve the simulations for each pollutant (NH_4^+ , NO_2^- , NO_3^-), the mesh elements were characterized by two coefficients. In this case the roughness coefficient was set to 0.03 (riverbed covered with sand and gravel) and the parameter for turbulence was 0.045. As boundary condition, was applied 27.1 mg/L for NH_4^+ , 15.6 mg/L for NO_2^- and 75.2 mg/L for NO_3^- . For this model, the offshore concentrations were 0.45 mg/L for NH_4^+ , 0.27 mg/L

for NO_2^- and 3.45 mg/L for NO_3^- .

Based on the CFD simulations on the Maleia water sector, it was established:

- after 20 minutes from the time of confluence with the waste water discharge point, the ammonia concentration has become 2.06 mg/L and after 30 minutes it became 1.01 mg/L;

- the ammonium concentration stays pronounced for 20 minutes downstream of the confluent area of the water pollutant;

- after 30 minutes of confluence with watercourse, the value of ammonia concentration has become lower than M.A.C. (2.0 mg/L) across the studied sector.

Based on the CFD simulations on the Maleia water sector, it was established:

- after 20 minutes from the time of confluence with the waste water discharge point, the nitrite concentration has become 1.18 mg/L, and after 30 minutes – 0.53 mg/L;

- the ammonium concentration stays pronounced for 20 minutes downstream of the confluent area of the water pollutant;

- after 30 minutes of confluence with watercourse, the value of nitrite concentration has become lower than M.A.C. (1.0 mg/L) across the studied sector.

Based on the CFD simulations on the Maleia water sector, it was established:

- After 20 minutes from the time of confluence with the waste water discharge point, the nitrate concentration has become 5.72 mg/L, over 30 minutes – 2.83 mg/L;

- after 20 minutes of confluence with watercourse, the value of nitrate concentration has become lower than M.A.C. (25 mg/L) across the studied sector.

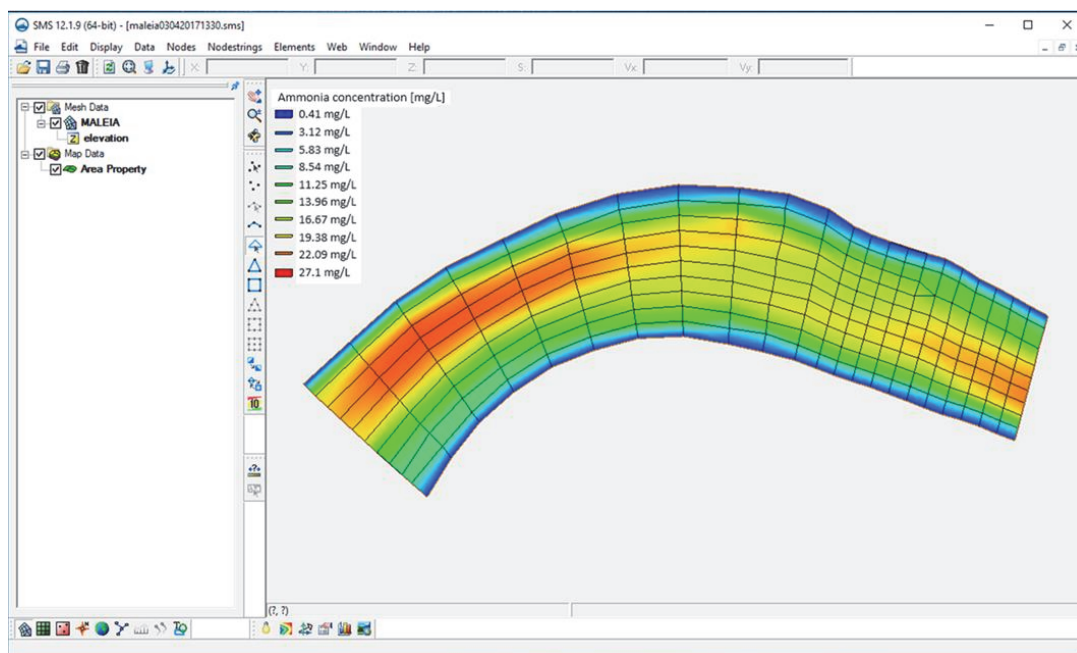


Fig. 7. Simulation of ammonia dispersion

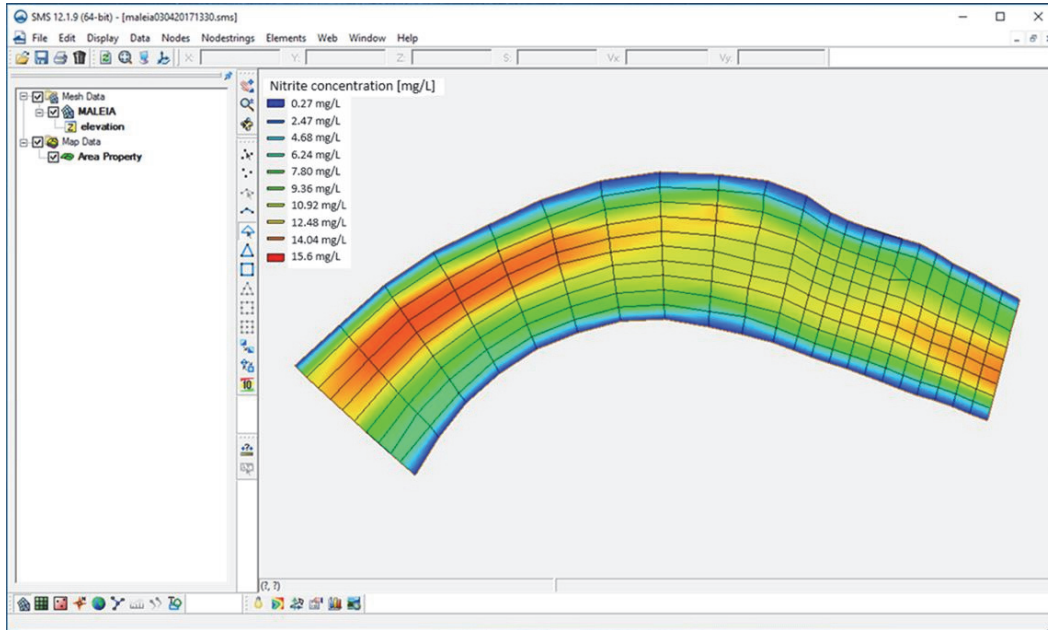


Fig. 8. Simulation of nitrite dispersion

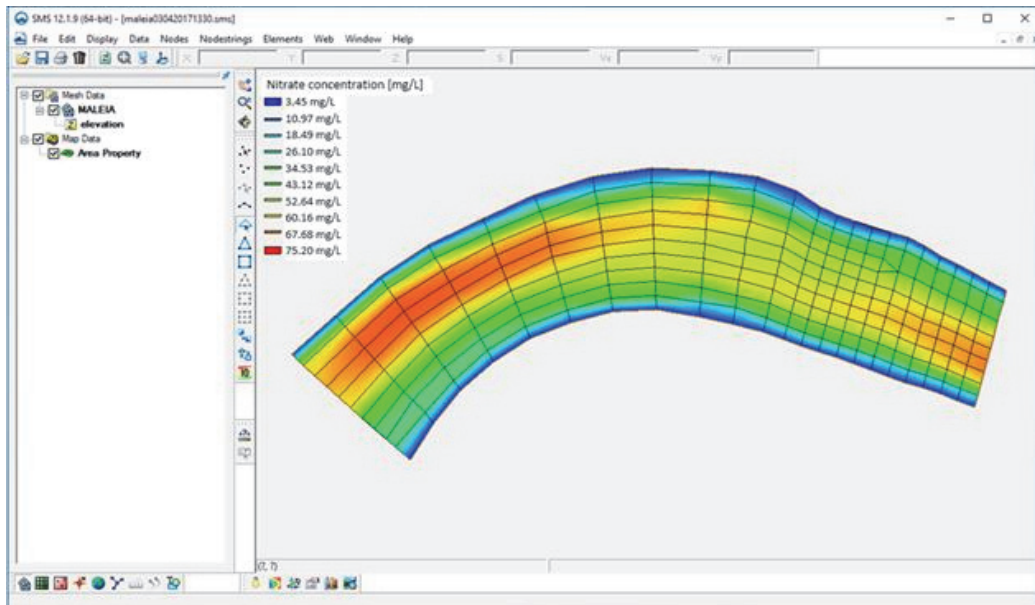


Fig. 9. Simulation of nitrate dispersion

Numerical simulation was performed on a computing network composed of 502 elements, 1181 nodes. Figs. 7, 8 and 9 show the concentration field obtained over 100 seconds at the time of the confluency of the pollutants with water. Also, in Figs. 7, 8 and 9 it is observed that over 100 seconds, the concentration of the pollutant is higher at the right bank, where the confluence of the pollutant occurred with water, and lower at the left bank.

The presence of ammonia in surface water is regarded as a strong indication of recent pollution by wastewater which can be toxic to fish and aquatic life (Jehad et al., 2017).

The distribution of nitrate concentrations depends on the sources of nutrients (agricultural sites) and transport mechanisms.

Nitrites come from the reduction of nitrates in the presence of a reducing flora and a higher temperature (summer) indicating an older pollution.

4. Conclusions

Through the investigation program (monitoring) developed during January 2017 – May 2017, some of the analysed indicators recorded higher values in the monitoring point downstream from household settlements, revealing a local ecological impact on the aquatic environment.

By using the SMS package, in particular the RMA2 and RMA4 modules, the problems of water flow and transport of pollutants in the river systems of Maleia River have been solved. Numerical models

were also generated in order to estimate the space-time evolution of ammonium, nitrite and nitrate dispersion in the studied sector.

Based on the numerical simulation results, it has been established that the numerical models obtained, calibrated and validated can be used on one hand directly for any pollution scenario in the studied sector, and on the other hand in emergency and accidental situations.

The models obtained, allows an estimation of water quality in each finite element of the studied sector, not only in a single sampling point as measured before. The information obtained up to date, allow expanding numerical simulation results of numerical simulation of pollutant transport phenomena for other sectors of the Maleia River, passing through different regions with different flow characteristics.

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