Appliance of Simulation Modelling in Wastewater Treatment

Lovorka Gotal Dmitrović, Mario Lešina, and Hrvoje Selec

Abstract—**A complex adaptive engineering wastewater treatment system for drinking water quality was developed, based on data from two real-world systems. Each component, which is present in the real situation with a water purification system, consists of a series of physical, chemical and / or biological purifiers according to their purpose, i.e. the purification value through the purification process. Developed conceptual model is a computer variables model uses randomly chosen values from the theoretical probability distribution of the variable applied. For the validation of the model, considering that the distributions are asymmetrical non-Gaussian distributions, a non-parametric test was applied. Methodology proposed in the paper is based on the simulation modelling. The design of a complex adaptive engineering system for the purification of communal water on the quality of drinking water is the fundamental outcome of this research, starting from its conceptual level until the realization of the described system at project level.**

Index Terms—**Asymmetrical non-Gaussian distribution, complex adaptive engineering system, simulation modelling, wastewater treatment.**

I. INTRODUCTION

Actual data was collected for a period of 5 years of actual waste water treatment systems on surface water quality (system 1) and surface water treatment systems in drinking water (system 2). The main component of the waste water treatment system is a bioaerating tank, and the surface water treatment system consists of a flocculator and a sand filter. The weekly mean value of the data was calculated, while the Missing data belongs to Missing at random (MAR)), the sample remains representative [1]. For the data processing the recommended deletion method is Listwise deletion, which is only used for the complete rows of table data [2], [3].

Values Missing at random (MAR) is an alternative to data Missing completely at random (MCAR), which occurs when the missing data is relating to a particular variable, like for example an accidentally skipped answer from a questionnaire [4]. The interesting fact is that the Listwise Deletion Method, which is the simplest method, provides very good matching results with the probability distributions [2]. This method, in non-Gaussian probability distribution, closely follows the observed distributions, with the exception of a deviation from the actual value at the peak of the distribution.

For the purposes of this study, the actual, empirical data was collected and used from the non-Gaussian probability distribution of the observed real system. These are asymmetric probability distributions with a tail, as is often the case in modelling complex technical systems [5]. To achieve the authenticity of the model, it is necessary to incorporate the actual system behaviour using the weekly mean concentration values, which were determined from the typical theoretical distribution of probability for every particular event frequency. Using the applications Stat::Fit simulation packages Servicemodel v4.2., the characteristic theoretical distribution of the organic matter concentration, as well as the basic characteristics of descriptive statistics, were obtained at each checkpoint (at the entrance and the exit). These data are shown in Table I.

TABLE I: DESCRIPTIVE STATISTICS AND CHARACTERISTIC THEORETICAL PROBABILITY DISTRIBUTION IN THE CONTROL POINT

	The entrance to the bioaeration tank	Output from to the bioaeration tank	The entrance to the floculator	Output from to the floculator / The entance to the sand filter	Output from to the filter
Theoretical distribution	Log-normal (-207; 6.63; 0.483)	Log-normal (4.68; 3.28; 0.576)	Log-normal (1.83; 0.009; 0.562)	Log-logistic (1.28; 4; 0.697)	Log-logistic (0.904; 5.22; 0.657)
Data points	261	260	258	258	256
Minimum (mgO$_2$/l)	36.1429	9.71429	2.01	1.42	1.164
Maximum (mgO$_2$/l)	1 947.43	146.857	6.275	4.1675	2.892
Mean (mgO$_2$/l)	641.144	36.0885	3.00745	2.05226	1.59937
Median (mgO$_2$/l)	548.429	32	2.806	1.985	1.58
Mode (mgO$_2$/l)	243.786	24.1429	2.63733	2.018	1.647
Standard deviation (mgO$_2$/l)	403.587	19.9632	0.709562	0.392285	0.255514
Variance ((mgO$_2$/l)^2)	162 882	398.529	0.503478	0.153887	0.0652876
Coefficient of variation (mgO$_2$/l)	62.9479	55.3174	23.5934	19.1148	15.9759

After determining the family of curves, an evaluation of the data collection with the selected distribution was determined, with the tests: $\chi 2$ - test, Kolmogorov - Smirnov test and Anderson - Darling test. The results of the data collection with the selected distribution are shown in Table II.

II. DEVELOPMENT OF THE TEAL SYSTEM MODELS

The models of both systems were first designed as conceptual models using the activity cycle diagrams (Fig. 1 and Fig. 2).

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TABLE II: RESULTS OF THE EVALUATION OF DATA COLLECTION WITH THE SELECTED DISTRIBUTION

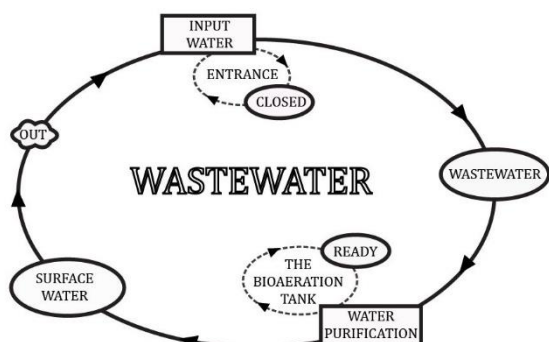|	Distribution	Probability	χ^2		Kolmogorov – Smirnov test		Anderson – Darling test	
			p-value	H_0/H_1	*p*-value	H_0/H_1	*p*-value	H_0/H_1
The entrance to the bioaeration tank	Log-normal (-207; 6,63; 0,483)	0,95	0,739	H_0	0,541	H_0	0,514	H_0
The entrance to the floculator	Log-normal (1,83; 0,00895; 0,562)	0,95	0,889	H_0	0,803	H_0	0,904	H_0
The entance to the sand filter	Log-logistic (1,28; 4; 0,697)	0,95	0,77	H_0	0,988	H_0	0,999	H_0

Fig. 1. ACD system 1.
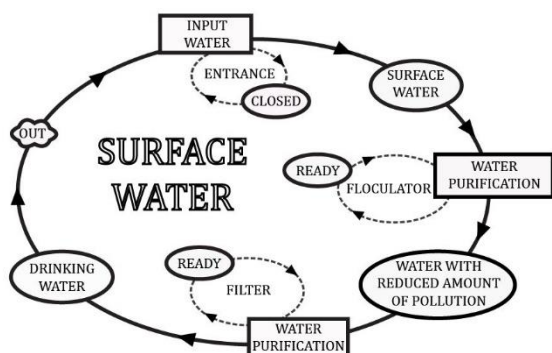
Fig. 2. ACD system 2.

The mathematical model of real system was created, based on the system of differential-difference equations. The Runge-Kutta method was used to solve equations system.

Mathematical modeling framework was applied to develop the model component of water treatment system using differential and difference-differential equations. This occurs for the component according to the following reaction (1) written as differential equation [2].

$$S = (D \cdot (I - S) - dS/dt) / (K + D) \qquad (1)$$

whereas:

I – input concentration in system (mg/l),
S – output concentration in system (mg/l),
dS/dt - changes in water cleanliness (mg/l/h),
K – goodness of purification (1/h),
$1/D$ – time in the water holding in components (h).

The changes in water cleanliness are:

$$dS/dt = D (I-S) - S (K+D) \qquad (2)$$

Initial equation in system component, according to equation (2), is:

$$dS/dt = D \cdot (I - S) - K \cdot S \qquad (3)$$

$$dS/dt = (-D - K) \cdot S + D \cdot I \qquad (4)$$

$$dS/dt + (D + K) \cdot S = D \cdot I \qquad (5)$$

Written in the form of difference equations:

$$S(t+\Delta t) = S(t) + D \cdot (I - S) \cdot \Delta t - K \cdot S \cdot \Delta t \qquad (6)$$

In the component, the difference equation was generated by using the Runge-Kutta method. Assuming that $t(0) = 0$, that is, at time $t(0)$, the output $S(0) = 0$, according to the Runge-Kutta (IV) method, applies:

$$S(t_{i+1}) = S(t_i+\Delta t_i) = S(t_i) + 1/6 \ [K_1^{(i)}+K_2^{(i)}+K_3^{(i)}+K_4^{(i)}] \qquad (7)$$

whereas:

$$K_1^{(i)} = \Delta t_i \cdot F(t_i, S(t_i)) \qquad (8)$$

$$F(t_i, S(t_i)) = D \cdot (I(t_i) - S(t_i) - K(t_i) \cdot S(t_i) \qquad (9)$$

$$K_2^{(i)} = \Delta t_i \cdot F(t_i + \Delta t_i/2, S(t_i) + 1/2 K_1^{(i)}) \qquad (10)$$

$$F(t, S) = (-D - K) \cdot S + D \cdot I \qquad (11)$$

$$F(t_i + \Delta t_i/2, S(t_i) + \tfrac{1}{2} K_1^{(i)}) =$$
$$= (-D - K(t_i + \Delta t_i/2)) \cdot [S(t_i) + 1/2 \ K_1^{(i)} + D \cdot I(t_i+\Delta t_i/2)] \qquad (12)$$

$$K_3^{(i)} = \Delta t_i \cdot F(t_i + \Delta t_i/2, S(t_i) + 1/2 K_2^{(i)}) \qquad (13)$$

$$F(t_i + \Delta t_i/2, S(t_i) + \tfrac{1}{2} K_2^{(i)}) =$$
$$= (-D - K(t_i + \Delta t_i/2)) \cdot [S(t_i) + 1/2 \ K_2^{(i)} + D \cdot I(t_i+\Delta t_i/2) \qquad (14)$$

$$K_4^{(i)} = \Delta t_i \cdot F(t_i + \Delta t_i/2, S(t_i) + K_3^{(i)}) \qquad (15)$$

$$F(t_i + \Delta t_i, S(t_i) + K_3^{(i)}) =$$
$$= (-D - K(t_i + \Delta t_i)) \cdot [S(t_i) + K_3^{(i)} + D \cdot I(t_i+\Delta t_i)] \qquad (16)$$

The goodness of purification isn't constant and it is presented as a theoretical probability distribution:

$$K = f(S)/S = \{[(I-S) \ Đ]-dS/dt\}/S \qquad (17)$$

Retention time (1 / D) is obtained from the expression:

$$1/D=V/Q \qquad (18)$$

whereas:

V - volume component (m^3) and

Q - flow rate of water through a component (m^3 / day).

For the values of goodness (quality) of the purification, using the Stat:Fit application from the Service Model v4.2 simulation package. Characteristic theoretical distribution

and the basic characteristics of descriptive statistics are determined. The data are presented in Table III.

Statistics are determined. The data are presented in Table III.

TABLE III: DESCRIPTIVE STATISTICS AND CHARACTERISTIC THEORETICAL DISTRIBUTION FOR PURIFICATION GOODNESS

	Goodness of purification in the bioaction tank	Goodness of purification in the floculator	Goodness of purification in the filter
Theoretical distribution	Log-normal (-21.3; 3.63; 0.239)	Log-normal (-0.69; 0.131; 0.223)	Log-logistic (-1.75; 21.9; 2.02)
Data points	260	257	255
Minimum	0.856716	-0.141322	-0.0703839
Maximum	55.7228	1.31866	0.875328
Mean	17.504	0.478442	0.287394
Median	15.8148	0.444995	0.272152
Mode	15.1228	0.288617	0.26112
Standard deviation	9.35954	0.265449	0.167315
Variance	87.6011	0.0704631	0.0279944
Coefficient of variation	53.4709	55.4819	58.2182

After determining the family of the curve, the estimation of data collection with the selected distribution was determined, the tests: $\chi2$ - square test, Kolmogorov - Smirnov

test and Anderson - Darling test. The results of the data collection with the selected distribution are shown in Table IV.

TABLE IV: RESULTS OF THE COMPATIBILITY OF PURIFICATION GOODNESS WITH THE SELECTED DISTRIBUTION

	Distribution	Probability	χ^2		Kolmogorov – Smirnov test		Anderson – Darling test	
			p-value	H_0/H_1	p-value	H_0/H_1	p-value	H_0/H_1
Goodness of purification in the bioaeration tank	Log-normal (-21.3; 3.63; 0.239)	0,95	0,0728	H_0	0,675	H_0	0,655	H_0
Goodness of purification in the floculator	Log-normal (-0.69; 0.131; 0.223)	0,95	0,982	H_0	0,991	H_0	0,989	H_0
Goodness of purification in the filter	Log-logistic (-1.746; 21.877; 2,024)	0,95	0,654	H_0	0,949	H_0	0,984	H_0

The computer model was created in Powersim Constructor Version 2.51. The components of real systems where the water is purified from organic matter are: a bioaction tank, a float and filter.

The computer model for each system variable uses randomly selected values from the theoretical probability distribution of that variable (Table I and Table III). According to the expression (2), the Runge-Kutta method calculates a change in water purity (dS / dt), i.e. mass concentration at the output (S).
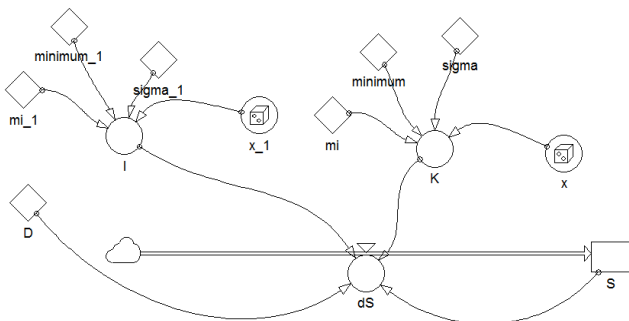

Fig. 3. Computer model for each component of purification system.

By evaluating the simulation model, it is examined whether the simulation model adequately represents the actual system. The actual output values with the output from the model are compared. Since distributions are not included in the Gaussian curve family according to Petz et al., 2012, or that are asymmetric, nonparametric methods are used for the

test (sometimes referred to as "free from distribution") [6]. Since the two independent samples were used, the test sums (Mann-Whitney U-test) were used. The values shown in Table V are obtained. The same table shows the minimum, maximum and mean values for the real mass concentration and the mass concentration obtained by the model.

TABLE V: VALIDATION OF SIMULATION MODELS

		Real value	Model value	Mann-Whitney U test
Floculator	Minimum	1.42	0.66	H_0 Z=1.567208 p=0.117067
	Maximum	4.16	3.5	
	Mean	2.06	2.09	
Filter	Minimum	1.16	1.06	H_0 Z = -1.32451 p= 0.185335
	Maximum	2.89	2.83	
	Mean	1.60	1.64	
Bioaerator	Minimum	9.71	10.09	H_0 Z = -1.62996 p= 0.103106
	Maximum	146.85	135.03	

Test confirmed that there was no statistically significant difference between the range of real values and the range of values obtained by the model.

III. SIMULATION EXPERIMENT

After simulation models of real systems have been developed, the simulated model of the integrated system - an improved model is formed by defining the transition point (waste water in drinking water). The integrated system was

developed by merging the models of both real systems. The activity cycle diagrams of this system is shown in Fig. 4.
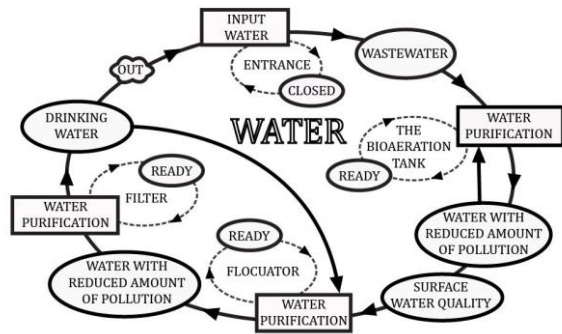

Fig. 4. Integrated system.

There must be at least two control posts for the wastewater treatment system for drinking water. Since the upper limit (UCL) is the prescribed value, control maps are created and certain warning areas and critical events are defined, i.e. a safety and warning band is defined, thus setting the self-regulation of the model. According to the Croatian legislation, the limit value for the concentration of organic matter in surface water discharge are 125 mgO$_2$/L. At another metering point, exit from the purification system, the water quality must correspond to the quality of the drinking water and the limit value is 5.0 mgO$_2$/L. According to these values, checkpoints were created for metering points: measurement point 1 - transition point, metering point 2 - exit from the system. The central line is at x axis, i.e. in y = 0, while the limit is taken from the legal regulation as the upper bound. Control charts are shown in Fig. 5 and Fig. 6.
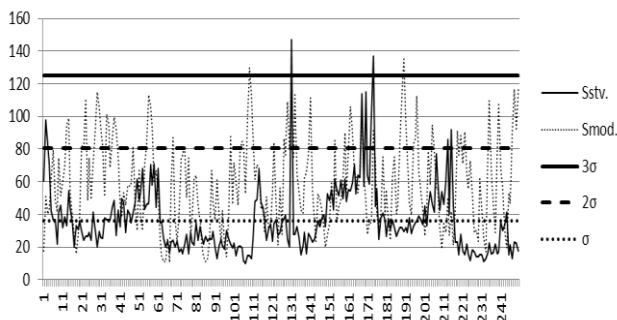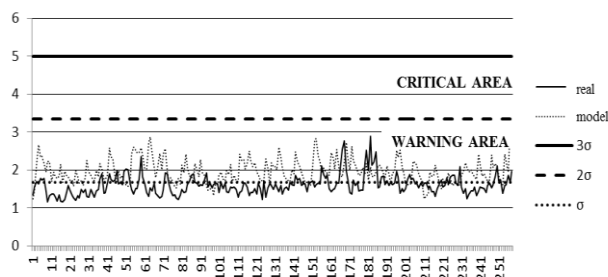

Fig. 5. Control chart of metering point 1.

Fig. 6. Control chart of metering point 2.

IV. THE RESULT AND DISCUSSION

Fig. 5 and 6 show the values of the actual system and the model with the control charts. As visible from the charts at both measuring points, concentration values are occasionally

the critical area. Therefore, a system is proposed in which the water is purified from the organic matter by double passing through a bioaeration tank and double passed through a flocculator and filter (Fig. 7). The double purification results are shown in Fig. 8.
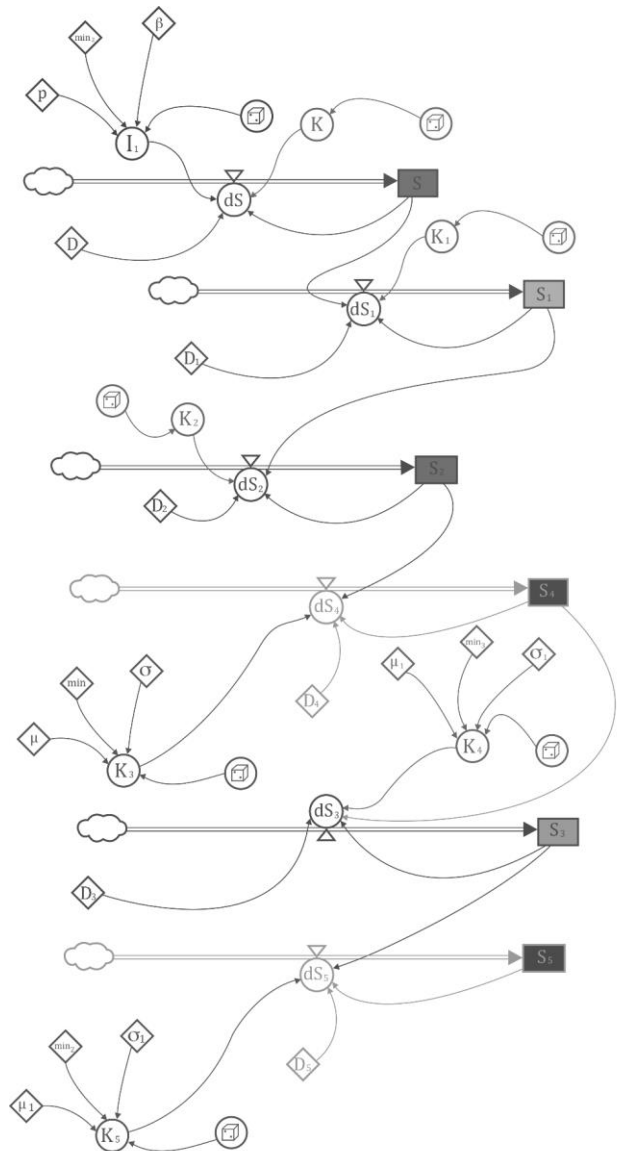

Fig. 7. Wastewater treatment in drinking water.

Fig. 8 shows the values of organic matter concentrations at the output from bioaeration tank 2 (transition point) and filter 2 (system exit).
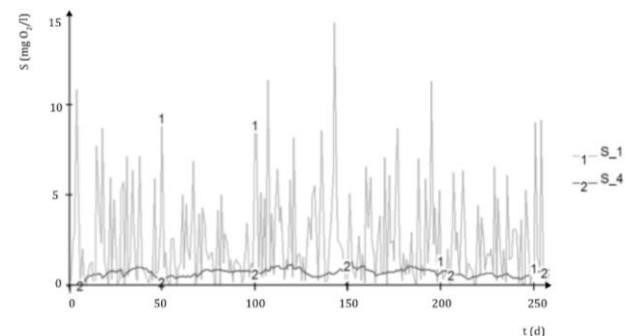

Fig. 8. Comparison of the simulated concentrations of organic matter from bioaeration tank 2 (S_1) and from filter 2 (S_4).

V. Conclusion

The features of the actual systems are transferred to a simulation model under different operating conditions. Adaptive simulation model is created using conceptualisation and parameterization. Adaptive models enable portability in terms of the application of such systems to other locations, i.e. with different values of input concentrations of contamination. Innovative model has been developed to acquire knowledge about wastewater treatment in drinking water on large and inexpensive systems. Simulation modelling methods contribute significantly to the preservation of the environment and human health.

Research goals have been achieved and are:

1) Designed, optimized and validated Conceptual Adaptive Model of the System "Sensitive" to Workplace Changes,
2) A developed and validated model of water purification system that treats municipal waste water on the quality of water for human consumption and
3) Methodology has been established for the research of complex, engineering water purification systems.

Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

Lovorka Gotal Dmitrović conducted the research and developed the mathematical and computer model; developed adaptive model and conducting the experiment; Hrvoje Selec data collection and analysed the data; developed conceptual models; Mario Lešina wrote the paper; all authors had approved the final version.

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