REVISTA eixo
revistaeixo.ifb.edu.br

ISSN 2238-5630
Brasília-DF, v. 15, n. 2, Maio - Agosto de 2026

MATHEMATICAL MODELING OF THE KINETICS OF AEROBIC DECOMPOSITION OF ORGANIC MATTER IN WATER COURSES

MODELAGEM MATEMÁTICA DA CINÉTICA DE DECOMPOSIÇÃO AERÓBIA DA MATÉRIA ORGÂNICA EM CURSOS HÍDRICOS

Leandro Fleck [1]
Maria Hermínia Ferreira Tavares [2]
Eduardo Eyng [3]
Izabel Melz Fleck [4]

ABSTRACT: Mathematical modeling is an important tool to support the management of water resources. This study proposes a mathematical model to simulate self-purification in watercourses. In the study, the temperature of a jar test was adjusted by a water bath in a range of 20 to 28 °C, and the water flow velocity was maintained between 0.29 and 0.87 m s^{-1}, conditions observed in natural watercourses. The kinetic experiments, which treated synthetic wastewater with an initial chemical oxygen demand concentration of 50 mg L^{-1}, were conducted according to a Central Composite Design. From the statistical adjustment of the chemical oxygen demand values, a mathematical equation was generated for each self-purification day. The mathematical model was validated in a self-purification test at 26 °C and 0.38 m s^{-1}, with an initial chemical oxygen demand concentration of 30 mg L^{-1}. The proposed model satisfactorily describes the total variation of responses, with a ratio of 99.46%.
Keywords: flow velocity; self-purification; Streeter-Phelps; temperature.

RESUMO*: A modelagem matemática se apresenta como uma importante ferramenta de apoio à gestão dos recursos hídricos. Este estudo propõe um modelo matemático para simular a autodepuração em cursos hídricos. Para a realização do estudo, utilizou-se um banho-maria acoplado a um jart test, com ajuste de temperatura entre 20 e 28ºC e velocidade de fluxo mantida entre 0,29 e 0,87 m s^{-1}, condições observadas em cursos hídricos naturais. Os experimentos cinéticos, os quais trataram águas residuárias sintéticas com uma concentração inicial de demanda química de oxigênio de 50 mg L^{-1}, foram conduzidos de acordo com um Delineamento Composto Central. A partir do ajuste estatístico dos valores de demanda química de oxigênio, foi gerada uma equação matemática para cada dia de autodepuração. O modelo matemático foi validado em um ensaio de autodepuração conduzido a 26ºC e 0,38 m s^{-1}, com uma concentração inicial de demanda química de oxigênio de 30 mg L^{-1}. O modelo proposto descreve satisfatoriamente a variação total das respostas, com proporção de 99,46%.*
Palavras-chave: velocidade de fluxo; autodepuração; Streeter-Phelps; temperatura.

1.Doutor em Engenharia Agrícola pela Universidade Estadual do Oeste do Paraná (UNIOESTE)
Universidade Estadual de Mato Grosso do Sul (UEMS/Mundo Novo)
E-mail: leandro.fleck@uems.br
Lattes: http://lattes.cnpq.br/2381929054098695
ORCID: https://orcid.org/0000-0001-8763-6404

2. Doutora em Física pela Universidade de São Paulo (USP)
Universidade Estadual do Oeste do Paraná (UNIOESTE/Cascavel)
E-mail: mhstavar@gmail.com
Lattes: http://lattes.cnpq.br/4169267827878056
ORCID: https://orcid.org/0000-0001-8973-4470

3. Doutor em Engenharia Química pela Universidade Estadual de Campinas (UNICAMP)
Universidade Tecnológica Federal do Paraná (UTFPR/Medianeira)
E-mail: eduardoeyng@utfpr.edu.br
Lattes: http://lattes.cnpq.br/1101075438495044
ORCID: https://orcid.org/0000-0001-5190-3339

4. Bióloga pela Universidade Estadual de Mato Grosso do Sul (UEMS)
Universidade Estadual de Mato Grosso do Sul (UEMS/Mundo Novo)
E-mail: izabelmelz.melz@gmail.com
Lattes: http://lattes.cnpq.br/9057842109153802
ORCID: https://orcid.org/0009-0007-0953-768X

Recebido em: 20/05/2025
Aceito em: 13/08/2025

INTRODUCTION

Increasing urbanization and the development of industrial activities, together with inadequate sewage treatment, have contributed to a general deterioration of water quality (SOUZA; SIQUEIRA, 2023). The pollution of watercourses, as mainly observed in developing countries, poses a potential threat to environmental health and human well-being (UDDIN; JEONG, 2021).

Therefore, the monitoring of water quality, which is necessary for water management (SUGAHARA *et al.*, 2023), provides important information about the impacts of human activities on watersheds. In many situations, accurate information is needed for proper management implementation (BAHARDWAJ *et al.*, 2022). In this regard, the use of innovative tools that provide informational support has become indispensable in decision-making processes.

In recent years, major scientific endeavors have been directed to developing a mathematical description of biodegradation processes of the agro-industrial and domestic effluents (FLECK *et al.*, 2019). Different mathematical models have been developed for several types of water bodies (rivers, lakes, reservoirs) (MARTINS *et al.*, 2021). Some of these models included basic indices of water quality, e.g., dissolved oxygen and biochemical oxygen demand (BOD). Sophisticated models include more complex criteria, such as eutrophication levels and toxicity impacts (HADJISOLOMOU *et al.*, 2021).

Thus, mathematical modeling has been consistently used to quantify the transformations of the substances in lotic environments and to investigate the impact of boundary conditions on the aquatic environment (FERREIRA; FERNANDES, 2022). In 1925, the American engineers Streeter and Phelps proposed a simplified model of self-purification of a polluted watercourse (Long, 2020), taking the atmospheric reaeration process into consideration. Among the basic water quality models cited and tested in the literature, the Streeter-Phelps equation is the most popular, due to its simple application (MENDIVIL-GARCÍA *et al.*, 2022). Since the publication of the equations in the Streeter-Phelps model, many researchers have adapted these equations to expand their scope (GOMOLKA *et al.*, 2022). Despite the development of far more complex models, the equations of the Streeter-Phelps model continue to be the basis of modern models (DUC *et al.*, 2021).

Despite the progress over the past decades, the reliability of mathematical modeling as a support tool for water resource management has been questioned, mainly due to the difficulty of reproducing an open system composed of multiple entries. The application of simple models to small rivers is rather difficult (ALOUI *et al.*, 2023), mainly because of the small amount of data available for the calibration procedure, particularly in densely populated areas. The greater the number of cases in which the model was tested, the greater the probability is that the structure and design are appropriate for the observed variable.

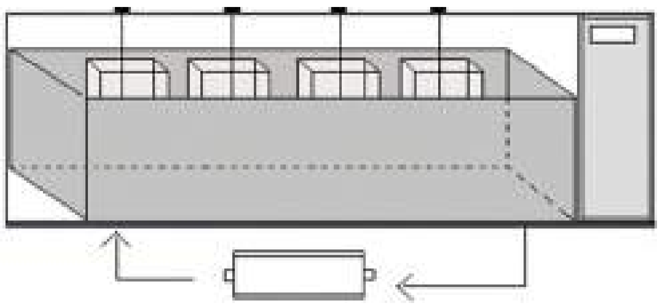
Most current mathematical models of water quality were developed with the purpose of evaluating the capacity of self-purification of watercourses affected by pollutant loads (AMINIRAD *et al.*, 2021); however, the mathematical model used in the simulation of future scenarios must be adjusted to the specific characteristics of a basin, such that the results reflect the impacts on the aquatic environment (FU *et al.*, 2020). This study proposes the creation of a mathematical model of water quality that allows the simulation of the natural process of organic matter aerobic self-purification in a water body.

MATERIAL AND METHODS

Experimental module

For the study a stainless steel water bath (800 mm long, 400 mm high and 200 mm wide), with temperature control in the range of 28 to 120 °C, was coupled to a jar test (Floc Control III, Poli Control). For temperatures below 28 °C, the water inside the bath was returned to a cooling system that was equipped with an adjustable thermostat (see Figure 1).

Figure 1 - Experimental setup used in the kinetic assays of aerobic decomposition of organic matter, consisting of a jar test system immersed in a temperature-controlled water bath, allowing adjustment of mixing speed and maintenance of constant thermal conditions during the experiments.



To reduce convection heat transfer to the environment, polystyrene chips were added to the water bath. Thus, temperatures similar to those under natural conditions were established by the water bath temperature control, and by shaking, the movement during the jar test allowed the simulation of flow velocity levels, as observed under natural conditions.

Synthetic wastewater

The assays were performed using synthetic wastewater with defined concentrations of macro and micronutrients (see Table 1). The synthetic wastewater consisted of proteins, carbohydrates,

ISSN 2238-5630
Brasília-DF, v. 15, n. 2, Maio - Agosto de 2026

lipids, and mineral salts, with its composition defined according to the formulation proposed by Torres (1992). Proteins accounted for 50% of COD and were represented by beef extract. Carbohydrates accounted for 40% of COD and consisted of sucrose, commercial starch and cellulose, contributing 20, 60 and 20%, respectively, of the carbohydrate fraction. The lipids represented 10% of COD, obtained exclusively by the addition of soybean oil. The alkalinity of domestic sewage was simulated by adding 200 mg L^{-1} sodium bicarbonate ($NaHCO_3$). The substrate was also enriched with mineral salt solutions (NaCl, $MgCl_2.6H_2O$ and $CaCl_2.2H_2O$).

Table 1- Synthetic wastewater composition.

Component	% of COD	Source	Concentration for COD of 500 (mg L^{-1})
Proteins	50%	Beef extract 100%	1.17 mL L^{-1}
Carbohydrates	40%	Sucrose 20% Commercial starch 60% Cellulose 20%	36.0 mg L^{-1} 112.0 mg L^{-1} 41.0 mg L^{-1}
Lipids	10%	Soybean oil 100% (emulsified with 3 drops of detergent).	0.056 mL L^{-1}
Mineral salts	-	Solution of 50.0 g L^{-1} NaCl Solution of 1.4 g L^{-1} MgCl2.6H2O Solution of 0.9 g L^{-1} CaCl2.2H2O	5.0 mL L^{-1} 5.0 mL L^{-1} 5.0 mL L^{-1}

Source: Torres (1992).

To simulate the organic matter concentrations found under natural conditions, considering the point of dilution of a liquid effluent in a receiving watercourse for a single point release, the synthetic wastewater was diluted in the ratio of 1:10. Thus, all of the kinetic assays were initiated at a COD concentration of 50 mg L^{-1}. To ensure the same conditions in all of the kinetic assays, fresh synthetic wastewater with the same composition was prepared for each new test. All of the tests were performed in triplicate, with an initial volume of synthetic wastewater of 2 L. The use of synthetic wastewater allowed better control of effluent composition and reduced variability during the kinetic assays, ensuring reproducibility and reliability of the experimental results.

Analytical methods

By controlling the agitation and temperature variables by simulating the flow velocity and temperature observed under natural conditions, respectively, the kinetics of aerobic decomposition of organic matter was evaluated, analyzing the parameter COD using an initial COD concentration of 50 mg L^{-1}. COD was determined by the colorimetric method (Method 5220D), as recommended by APHA (2012).

Experimental design

The effects of the flow velocity and temperature on the aerobic organic matter decomposition kinetics were evaluated using a central composite design (CCD), i.e., a factorial arrangement of 2^2 treatments, including four factorial tests and three replications at the center point, resulting in a total of seven tests. Table 2 shows the treatment design matrix with real and coded values of the studied factors.

Table 2 - Treatment designs matrix.

Test	Temperature (°C)	Flow velocity (m s^{-1})
1	+1 (28.0)	-1 (0.29)
2	-1 (20.0)	-1 (0.29)
3	+1 (28.0)	+1 (0.87)
4	-1 (20.0)	+1 (0.87)
5	0 (24.0)	0 (0.58)
6	0 (24.0)	0 (0.58)
7	0 (24.0)	0 (0.58)

A central composite design (CCD) without rotatability was adopted to ensure that the experimental domain remained constrained to environmentally realistic conditions, thereby focusing the analysis on the region of practical interest. This design enabled reliable estimation of linear and interaction effects while avoiding extrapolation beyond ranges representative of natural watercourses, which could reduce the interpretability of the kinetic parameters.

The real temperature and flow velocity values were defined based on the waters from the Rio Alegria, located in the urban area of the municipality of Medianeira, Paraná, Brazil, which represents a typical urban watercourse subjected to organic load inputs. These data were used as a realistic environmental reference to define the experimental conditions, without restricting the applicability of the proposed kinetic model to a single river system.

The climate in the municipality of Medianeira is humid subtropical, with hot summers and an annual average temperature of 21 °C. To determine the temperature values, the watercourse temperature was measured at different points and times of the day. To determine the medium flow velocity values, the flow velocity was measured at two different points of the same watercourse (high and low flow velocity). The flow velocity was then converted to an angular velocity to obtain the turbulence that would be observed in the field in the laboratory.

Kinetic experiments and generation of the proposed mathematical model

All of the kinetic assays lasted 15 days. To determine the kinetics of the process for each CCD test, aliquots were withdrawn daily with sufficient volume (2.5 mL) to determine the COD. Prior to sampling, the volume of each system was filled daily to the initial volume of 2 L with distilled water to offset the loss caused by natural evaporation and by sampling.

According to the main objective of the study, that is, to model the kinetics of aerobic decomposition of organic matter, the mathematical model that was dependent on temperature and flow velocity was related to time. As the COD analysis was performed daily, a mathematical equation was generated for each self-purification time (1, 2, 3, … , 15 days). Thus, by the statistical adjustment of the seven COD values per day of self-purification (one representative value of each condition of the temperature and flow rate of the main design) with the program Statistica (version 7.0), it was possible to obtain of coefficients of the encoded mathematical model given by Eq. 1:

$$COD = a_1 + a_2T + a_3V + a_4TV$$

Eq. (1)
where:
a: adjusted coefficients of the experimental data;
T: encoded value of the river temperature;
V: encoded value of the river flow velocity.

The significance of the equations representing each day of self-purification was evaluated by Analysis of Variance (ANOVA) at a confidence interval of 90%, which was chosen because of the large variability that is characteristic of the process of microbial wastewater treatment (RODRIGUES; IEMMA, 2009). Thus, the final model that evaluates the kinetics of aerobic decomposition of organic matter is a matrix, consisting of 15 self-purification equations.

To avoid the influence of the initial concentration of organic matter (COD) on the efficiency of the model in describing the decomposition kinetics, the proposed model was applied using relative COD values based on the initial concentration that was generated (50 mg L^{-1}). The relative COD is calculated according to Eq. 2:

$$\left(\frac{\overset{15}{(COD)}}{\underset{n=1}{(COD)_0}}\right) = 1 + \left[\frac{(COD)_1 - (COD)_0}{50}\right] + \ldots + \left[\frac{(COD)_{15} - (COD)_{14}}{50}\right] * C_0$$

Eq. (2)
where:
$COD_{0\text{-}15}$: concentration of remaining COD on each day of self-purification (mg L^{-1}).
C_0: Initial concentration of COD (mg L^{-1}).

Proposed mathematical model validation

The mathematical model was validated based on a self-purification kinetic assay performed at 26 °C and 0.38 m s^{-1}, which corresponds to 120 rpm at the jar test. The kinetic assay started with an organic matter concentration of 30 mg L^{-1}, value different from the initial COD concentration in which the mathematical model was generated, as a way to test the applicability and reliability of the same for different concentrations of organic matter.

The COD was analyzed daily (Method 5220D, APHA 2012). The reliability of the proposed model was determined by the comparison of the COD concentration values obtained under real conditions to the simulated values. The experimental data were subjected to variance analysis for the proposed mathematical model and to normality analysis (Shapiro-Wilk test) and homoscedasticity at the 0.05 significance level.

Performance analysis of the mathematical model

When correlating the estimated values with the measured values, the following statistical indicators were considered: precision (correlation coefficient "r"); accuracy (Willmott index "d"); and confidence or performance ("c"). Precision is given by the correlation coefficient, which indicates the random error. Accuracy corresponds to the discrepancy between the estimated and observed values, given by the concordance index, and is represented by the letter "d". The closer to 1 the obtained values are, the higher the correlation. Index "d" is given by Eq. 3:

$$d = 1 - \left[\sum (Pi - Oi)^2 / \sum \left(|Pi - O| + |Oi - O|\right)\right]$$

Eq. (3)
where:
Pi: estimated values;
Oi: observed values;
O: mean of the observed values.

From the combined indices of precision and accuracy, a new index "c" is generated (CAMARGO; SENTELHAS, 1997), expressed by Eq. 4:

$$c = r * d$$

Eq. (4)
where:
r: correlation coefficient;
d: concordance index.

The criterion used to interpret the performance of the models by index "c" is shown in Table 3 (CAMARGO; SENTELHAS, 1997).

ISSN 2238-5630
Brasília-DF, v. 15, n. 2, Maio - Agosto de 2026

Table 3 - Interpreting criteria for the index "c".

"c" value	Performance
> 0.85	Excellent
0.76 to 0.85	Very good
0.66 to 0.75	Good
0.61 to 0.65	Average
0.51 to 0.60	Below average
0.41 to 0.50	Poor
≤ 0.40	Very poor

RESULTS AND DISCUSSION

Analysis of variance for the 15 self-purification equations

Table 4 shows the remaining COD concentration for all trials of the treatment designs in a 15-day self-purification period. It is observed that at the conditions of 28 ° C and 0.87 m s^{-1}, the final remaining COD was 5.11 mg L^{-1}, which is the maximum efficiency of removal of organic load obtained from all the tests performed (89.78%).

Table 4 - Remaining COD (mg L^{-1}) in all trials of the treatment design.

Day	28 °C 0.29 m s^{-1}	20 °C 0.29 m s^{-1}	28 °C 0.87 m s^{-1}	20 °C 0.87 m s^{-1}	24 °C 0.58 m s^{-1}	24 °C 0.58 m s^{-1}	24 °C 0.58 m s^{-1}
0	50.00	50.00	50.00	50.00	50.00	50.00	50.00
1	37.18	47.12	41.51	49.81	47.31	43.21	47.17
2	35.59	43.40	31.76	31.16	42.23	43.21	38.47
3	28.54	33.36	25.43	29.51	37.44	37.54	39.92
4	25.69	28.82	24.64	28.56	29.16	29.25	28.20
5	22.80	24.14	23.85	28.39	23.87	22.55	23.05
6	19.94	24.14	17.32	27.36	18.89	18.89	18.78
7	15.66	23.86	14.24	27.11	17.48	16.91	16.02
8	10.08	20.03	11.18	25.60	17.08	16.49	15.44
9	9.91	19.32	9.45	21.92	15.62	16.33	15.01
10	9.67	18.61	9.01	20.45	15.49	16.73	14.72
11	7.97	18.04	8.23	16.70	13.10	15.95	14.52
12	7.69	18.45	7.45	14.08	11.10	11.73	13.25
13	7.55	18.71	5.18	13.47	10.51	10.41	12.22
14	7.56	18.04	5.11	12.72	10.70	10.01	11.95
15	7.35	17.33	5.11	11.58	10.71	10.05	11.32

Multiple linear regression and hypothesis tests for the parameters of the model, e.g., the F test, are useful to verify the suitability and applicability of the generated mathematical model. The test for regression significance determines whether there is a linear relationship between the response variable (COD reduction) and any of the regression variables (temperature and flow velocity) (NADAL *et al.*, 2003).

The mathematical equations representing the 1st and 7th to 15th day of self-purification were statistically significant, with a confidence interval of 90%. All of the statistically significant equations fit well to the experimental data, describing the total variation of the responses with a ratio greater than 84% ($R^2 > 0.84$) (see Table 5). However, in order to increase the proportion of the total response variability explained by the regression model, no significant mathematical equations were kept in the representative mathematical model of the process.

Ledesmo *et al.* (2013) evaluated the temporal and spatial variations of water quality parameters of the Rio Tercero (Córdoba, Argentina), correlating experimental data with satellite images. To this end, models of simple and multiple linear regression were generated to determine the chlorophyll-a concentration in this watercourse, and the resulting mathematical models showed coefficients of determination (R^2) of 0.68 and 0.76, respectively, i.e., 76% of the total variation in the chlorophyll-a concentration was explained by the linear regression model. The coefficients adjusted to the experimental data were statistically significant, at the 0.05 significance level. According to the results, the studied river waters are considered excellent for irrigation and unfit for animal consumption, due to the low salt concentrations.

Table 5 - F test for the 15 days of self-purification.

Day	Source of variation	Sum of squares	Degree of freedom	Mean square	Calculated F	Chart F	p-value	R^2
1st	Regression	96.16	3	32.05	5.45	5.39	0.09*	0.84
	Error	17.64	3	5.88				
	Total	113.80	6					
2nd	Regression	95.23	3	31.74	1.35	5.39	0.40	0.57
	Error	70.71	3	23.57				
	Total	165.94	6					
3rd	Regression	31.04	3	10.35	0.21	5.39	0.88	0.18
	Error	145.59	3	48.53				
	Total	176.64	6					
4th	Regression	13.01	3	4.34	1.82	5.39	0.31	0.65
	Error	7.14	3	2.38				
	Total	20.16	6					
5th	Regression	18.22	3	6.07	3.32	5.39	0.17	0.77
	Error	5.49	3	1.83				
	Total	23.72	6					
6th	Regression	59.31	3	19.77	3.17	5.39	0.18	0.76
	Error	19.09	3	6.36				
	Total	78.40	6					
7th	Regression	117.28	3	39.09	5.57	5.39	0.09*	0.85
	Error	21.07	3	7.02				
	Total	138.35	6					

ISSN 2238-5630
Brasília-DF, v. 15, n. 2, Maio - Agosto de 2026

Day	Source of variation	Sum of squares	Degree of freedom	Mean square	Calculated F	Chart F	p-value	R^2
8th	Regression	164.58	3	54.86	100.35	5.39	0.001*	0.99
	Error	1.64	3	0.55				
	Total	166.23	6					
9th	Regression	123.16	3	41.05	94.01	5.39	0.001*	0.99
	Error	1.31	3	0.44				
	Total	124.47	6					
10th	Regression	105.75	3	35.25	23.14	5.39	0.01*	0.96
	Error	4.57	3	1.52				
	Total	110.32	6					
11th	Regression	86.86	3	28.95	9.11	5.39	0.05*	0.90
	Error	9.54	3	3.18				
	Total	96.40	6					
12th	Regression	85.17	3	28.39	34.62	5.39	0.007*	0.97
	Error	2.46	3	0.82				
	Total	87.63	6					
13th	Regression	111.11	3	37.04	52.17	5.39	0.004*	0.98
	Error	2.13	3	0.71				
	Total	113.24	6					
14th	Regression	98.96	3	32.99	51.01	5.39	0.004*	0.98
	Error	1.94	3	0.65				
	Total	100.9	6					
15th	Regression	86.69	3	28.89	84.99	5.39	0.002*	0.99
	Error	1.02	3	0.34				
	Total	87.71	6					

*significant at the 0.1 significance level.

Proposed mathematical model

The proposed mathematical model, which determines the organic matter aerobic decomposition kinetics within the given ranges of temperature (20 to 28 °C) and flow velocity (0.29 to 0.87 m s^{-1}) is presented below:

$$COD = \begin{bmatrix} COD_1 = 44.76 - 4.56T + 1.76V + 0.41TV \\ COD_2 = 37.97 - 1.80T - 4.02V + 2.10TV \\ COD_3 = 33.11 - 2.23T - 1.74V + 0.19TV \\ COD_4 = 27.76 - 1.76T - 0.33V - 0.20TV \\ COD_5 = 24.09 - 1.47T + 1.32V - 0.80TV \\ COD_6 = 20.76 - 3.56T + 0.15V - 1.46TV \\ COD_7 = 18.75 - 5.26T + 0.45V - 1.17TV \\ COD_8 = 16.56 - 6.09T + 1.67V - 1.12TV \\ COD_9 = 15.37 - 5.47T + 0.54V - 0.77TV \\ COD_{10} = 14.95 - 5.09T + 0.30V - 0.63TV \\ COD_{11} = 13.50 - 4.64T - 0.27V + 0.40TV \\ COD_{12} = 11.96 - 4.35T - 1.15V + 1.03TV \\ COD_{13} = 11.15 - 4.86T - 1.90V + 0.72TV \\ COD_{14} = 10.87 - 4.52T - 1.97V + 0.72TV \\ COD_{15} = 10.49 - 4.11T - 1.99V + 0.88TV \end{bmatrix}$$

where:
COD1-15: representative equations of the first to the fifteenth day of self-depuration;
T: encoded value of the river temperature;
V: encoded value of the river flow velocity.

The encoding of the temperature and flow velocity values, measured in natural conditions, for application in the representative equations of the self-purification process was done using the Eqs. 5 and 6:

Eq. (5) $$T = \frac{Tm - 24}{4}$$

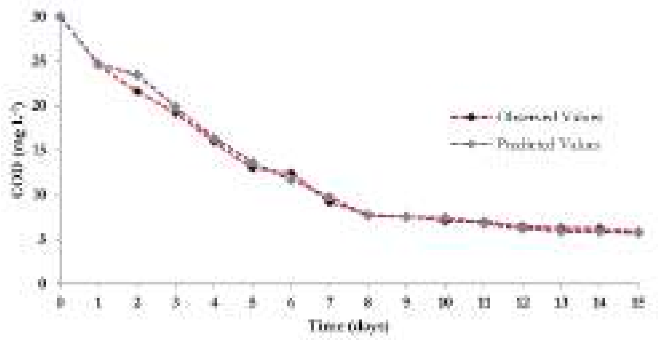
Eq. (6) $$V = \frac{Vm - 0{,}58}{0{,}29}$$

where:
T: encoded temperature value;
Tm: temperature measured under natural conditions;
V: encoded flow velocity value;
Vm: flow velocity measured under natural conditions.

Proposed mathematical model validation

Validation procedures are used to ensure that the values generated by a model are consistent with those generated by the real system (ZONGO *et al.*, 2024). The proposed mathematical model, including the equations that were not statistically significant, satisfactorily described the organic matter aerobic decomposition kinetics from an initial COD concentration of 30 mg L^{-1}, at a temperature and flow rate of 26 °C and 0.38 m s^{-1}, respectively. The observed values were close to those predicted by the mathematical model, with a maximum error of 1.91 mg L^{-1} (Figure 2).

Figure 2 - Observed and predicted COD using the proposed model.



The pattern observed in Figure 2 was expected because according to Von Sperling (2007), after being affected by a pollutant load, the watercourse (represented by the system that was used) has the ability to restore the conditions prior to an external influence (effluent discharge) through the natural process of self-purification. Thus, parallel to the reduction of the remaining COD, the dissolved oxygen concentration increases gradually, with a tendency to reach saturation levels after organic matter stabilization.

Variance analysis for the proposed mathematical model

The proposed linear regression model, composed of 15 self-purification equations, is statistically significant (Table 6), with a p-value (2.49x10-17) below the adopted significance level (5%). The mathematical model described the total variation of responses (COD concentration values observed at the validation test) with a ratio of 99.46%, proving its ability to predict the kinetics of the self-purification process in natural watercourses. Thus, the mathematical model is considered valid within the ranges of temperature and flow velocity for which it was created.

Table 6 - Analysis of variance for the values simulated by the mathematical model.

Source of variation	Sum of squares	Degree of freedom	Mean square	p-value	R^2
Predicted values	866.21	1	866.21	2.49x10-17*	0.9946
Error	4.62	14	0.33		
Total	870.83	15			

* Significant at the 0.05 significance level.

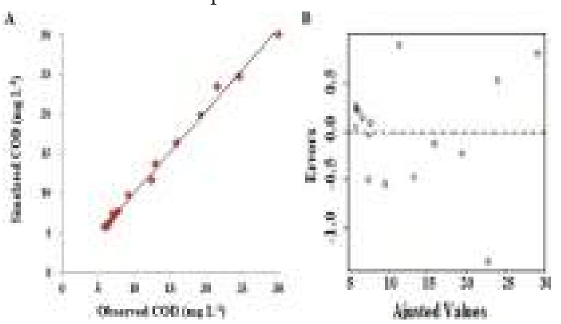
Error analysis

The Shapiro-Wilk normality test showed that the errors are normally distributed, with a p-value of 0.58, i.e., higher than the significance level (5%). Thus, the modeled results were considered reliable.

The good fit of the proposed model to the experimental data was confirmed by the points of COD concentration approximation (simulated COD x observed COD) along of the straight, representing the perfect fit (Fig. 3a). The residues are randomly distributed around the zero mean, with no behavior pattern or trend, i.e., the variance of the dependent variable is not just focused on a limited field of independent values. Thus, there is no evidence to reject the hypothesis of error homoscedasticity. There is a linear relationship between the explanatory variables (temperature and flow velocity) and the response variable (COD concentration) (Fig. 3b).

During the rainy season (March) and dry season (August), Gonçalves *et al.* (2011) evaluated and simulated the electrical conductivity and concentration of dissolved oxygen, chloride, ammonia, nitrate, and biochemical oxygen demand (BOD) at Rio Jaú, in the urban area of the city of Jaú (SP - Brazil). Similar to the results obtained in the present study, a good fit of the mathematical model to the field data was observed, indicating that it may be used in studies simulating future scenarios to predict the self-purification capacity of watercourses or to quantify the impacts of specific actions.

Figure 3 - Mathematical model reliability analysis to describe the experimental data.



Performance analysis

There was a strong positive correlation between the simulated and measured values (0.997) with little discrepancy between them, as proved by the Willmott index (0.969). The performance of the mathematical model in describing the experimental data was excellent, with a performance index over 0.85 (0.966), as described by Camargo and Sentelhas (1997).

CONCLUSIONS

1. The equations that were not statistically significant (i.e., for the second, third, fourth, fifth and sixth days of self-purification) satisfactorily described the aerobic decomposition of organic matter kinetics in the validation test, justifying their inclusion in the final mathematical model.

2. The mathematical model satisfactorily described the process of self-purification of natural watercourses within the limits of temperature and flow velocity for which it was created.

3. The proposed mathematical model can be used to simulate the kinetics of the aerobic decomposition of organic matter in watercourses from the launch of industrial effluents, considering the conditions of temperature and flow velocity in which it was generated.

ACKNOWLEDGMENTS

We would like to thank the Federal University of Technology – Paraná, for making the laboratories available for the analysis and to the CAPES for the granted scholarship.

REFERENCES

AKASHEDEEP, B.; DAGAR, V.; KHAN, M. O.; AGGARWAL, A.; ALVARADO, R. KUMAR, M.; IRFAN, M.; PROSHAD, R. Smart IoT and machine learning-based framework for water quality assessment and device component monitoring. **Environmental Science and Pollution Research**, v.29, p. 46018-46036, 2022. *Disponível em:* https://doi.org/10.1007/s11356-022-19014-3. *Acesso em:* 04 de jul. 2024.

ALOUI, S.; MAZZONI, A.; ELOMRI, A.; AOUISSI, J.; BOUFEKANE, A.; ZGHIBI, A. A review of Soil and Water Assessment Tool (SWAT) studies of Mediterranean catchments: Applications, feasibility, and future directions. **Journal of Environmental Management,** v. 326, p. 1-20, 2023. *Disponível em:* https://doi.org/10.1016/j.jenvman.2022.116799. *Acesso em:* 22 de fev. 2024.

APHA. **Standard Methods for the Examination of Water and Wastewater**. 22th ed. Washinton, DC – EUA: Ed. American Public Health Association, American Water Works Association, Water Environment Federation, 2012.

AMINIRAD, H.; ABESSI, O.; KOOTENAEI, F. G.; MIRREZAEI, M. A.; TAGHIZADEH, T.; SAEIDI, P.; DARVISHI, G. Investigation of self-purification capacity and water quality of Haraz river during dry and wet season. **Journal of Applied Research in Water and Wastewater**, v.8, n.1, p. 21-27, 2021. *Disponível em:* https://doi.org/10.22126/arww.2021.6175.1201. *Acesso em:* 19 de fev. 2024.

CAMARGO, A. P.; SENTELHAS, P C. *Avaliação do desempenho de diferentes métodos de estimativa da evapotranspiração potencial no estado de São Paulo, Brasil.* ***Revista Brasileira de Agrometereologia,*** v.5, n.1, p. 89-97, 1997. *Disponível em:* https://www.researchgate.net/publication/284194031_Avaliacao_do_desempenho_de_diferentes_metodos_de_estimativa_da_evapotranspiracao_potencial_no_Estado_de_Sao_Paulo_Brasil. *Acesso em:* 8 de jun. 2024.

DUC, N. H.; AVTAR, R.; KUMAR, P.; LAN, P. P. Scenario-based numerical simulation to predict future water quality for developing robust water management plan: a case study from the Hau River, Vietnam. **Mitigation and Adaptation Strategies for Global Change,** v.26, n.7, p. 26-33, 2021. *Disponível em:* https://doi.org/10.1007/s11027-021-09969-y. *Acesso em:* 8 de jun. 2024.

FERREIRA, D. M.; FERNANDES, C. V. S. Integrated water quality modeling in a river-reservoir system to support watershed management. **Journal of Environmental Management**, v.324, p. 1-11, 2022. *Disponível em:* https://doi.org/10.1016/j.jenvman.2022.11644. *Acesso em:* 14 de jul. 2024.

FLECK, L.; TAVARES, M. H. F.; EYNG, E.; ORSSATTO, F. Optimization of the nitrification process of wastewater resulting from cassava starch production. **Environmental Technology, v.** 40, n.25, p. 3318-3327, 2019. *Disponível em:* https://doi.org/10.1080/09593330.2018.1472300. *Acesso em:* 13 de jul. 2024.

FU, B.; HORSBURGH, J. S.; JAKEMAN, A. J.; GUALTIERI, C.; ARNOLD, T.; MARSHALL, L.; GREEN, T. R.; QUINN, N. W. T.; VOLK, M.; HUNT, R. J.; VEZARRO, H. L.; CROKE, B. F. W.; JAKEMAN, J. D.; SNOW, V.; RASHLEIGH, B. Modeling Water Quality in Watersheds: From Here to the Next Generation. **Water Resources Research**, v.56, p. 1-28, 2020. *Disponível em:* https://doi.org/10.1029/2020WR027721. *Acesso em:* 14 de jul. 2024.

GONÇALVES, J. C. S. I.; SARDINHA, D. S.; BOESSO, F. F. *Modelo numérico para simulação da qualidade da água do trecho urbano do Rio Jaú, município de Jaú* (SP). ***Revista de Estudos Ambientais***, v.13, n.2, p.44-56, 2011. *Disponível em:* https://doi.org/10.7867/1983-1501.2011v13n2p44-56. *Acesso em:* 15 de mar. 2024.

GOMOLKA, Z.; TWAROG, B.; ZELAWSKA, E. State Analysis of the Water Quality in Rivers in Consideration of Diffusion Phenomenon. **Applied Sciences**, v.12, n.3, p.1-21, 2022. *Disponível em:* https://doi.org/10.3390/app12031549. *Acesso em:* 14 de maio 2024.

GRONEWOLD, A. D., QIAN, S. S., WOLPERT, R. L.; RECKHOW, K. H. Calibrating and validating bacterial water quality models: A Bayesian approach. **Water Research**, v.43, n.10, p. 2688-2698, 2009. *Disponível em:* https://doi.org/10.1016/j.watres.2009.02.034. *Acesso em:* 12 de abr. 2024.

HADJISOLOMOU, E.; STEFANIDIS, K.; K.; HERODOTOU, H.; MICHAELIDES, M.; PAPATHEODOROU, G.; PAPASTERGIADOU. Modelling freshwater eutrophication with limited limnological data using Artificial Neural Networks. **Water**, v.13, p. 1-15, 2021. *Disponível em:* https://doi.org/10.3390/w13111590. *Acesso em:* 25 de mar. 2024.

LONG, B. T. Inverse algorithm for Streeter–Phelps equation in water pollution control problem. **Mathematics and Computers in Simulation,** v.171, p. 119-126, 2020. *Disponível em:* https://doi.org/10.1016/j.matcom.2019.12.005. *Acesso em:* 25 de fev. 2024.

MARTINS, G. M. F.; COUTO, E. A.; MARQUES, G. M. *Modelagem matemática como suporte à gestão dos recursos hídricos na bacia hidrográfica do rio Araçuaí* (MG). ***Revista Ibero-Americana de Ciências Ambientais***, v.12, n.11, p. 335-348, 2021. *Disponível em:* http://doi.org/10.6008/CBPC2179-6858.2021.011.0027. *Acesso em:* 13 de fev. 2024.

MENDIVIL-GARCÍA, K.; AMABILIS-SOSA, L. E. A.; SALINAS-JUÁREZ, M. G.; PAT-ESPADAS, A.; RODRÍGUES-MATA, A. E.; FIGUEROA-PÉREZ, M. G.; ROÉ-SOSA, A. Climate change impact assessment on a tropical river resilience using the Streeter-Phelps dissolved oxygen model. **Frontiers in Environmental Science,** v.26, p. 1-15, 2022. *Disponível em:* https://doi.org/10.3389/fenvs.2022.903046. *Acesso em:* 14 de maio de 2024.

NADAL, C. A.; JULIANO, K. A.; RATTON, E. *Testes Estatísticos utilizados para validação de regressões múltiplas aplicadas na avaliação de imóveis urbanos.* ***Boletim de Ciências Geodésicas,*** v.9, n.2, p. 243-262, 2003.

RODRIGUES, M. R.; IEMMA, A. F. ***Planejamento de Experimentos e Otimização de Processos***. 2. ed. São Paulo: Cárita, 2009.

SOUZA, C. J.; SIQUEIRA, G. W. *Os impactos ambientais de efluentes industriais: Ocaso do Frigorífico São Francisco em Redenção-PA*. ***Research, Society and Development***, v.12, n.1, p. 1-19, 2023. *Disponível em:* http://dx.doi.org/10.33448/rsd-v12i1.39375. *Acesso em:* 13 de jun. 2024.

SUGAHARA, C. R.; FERREIRA, D. H. L.; MENDES, J. P. *Análise de indicadores de sustentabilidade para a gestão da segurança hídrica nas bacias hidrográficas dos rios Piracicaba, Capivari e Jundiaí.* ***Revista Gestão e Sustentabilidade Ambiental,*** [s. l.], v.12, n.1, p.1-22, 2023. *Disponível em:* https://doi.org/10.59306/rgsa.v12e12023e12164. *Acesso em:* 5 de jul. 2024.

TORRES, P. ***Desempenho de um reator anaeróbio de manta de lodo (UASB) de bancada no tratamento de substrato sintético simulando esgotos sanitários.*** 1992. *Dissertação (Mestrado em Engenharia Hidráulica e Saneamento) – Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos*, 1992.

UDDIIN, M. J.; JEONG, Y. Urban river pollution in Bangladesh during last 40 years: potential public health and ecological risk, present policy, and future prospects toward smart water management. **Heliyon**, v. 7, p. 1-23, 2021. *Disponível em:* https://www.cell.com/heliyon/pdf/S2405-8440(21)00212-7.pdf. *Acesso em:* 3 de maio 2024.

VON SPERLING, M. ***Estudos e Modelagem da Qualidade da Água***. 1. ed. *Departamento de Engenharia Sanitária e Ambiental. Minas Gerais*: 2007.

ZONGO, J.; ZABSONRE, J. D. D.; ROAMBA, B. Formal derivation of a new sediment transport model using a multiscale procedure: Numerical Validation. **Partial Differential Equations in Applied Mathematics,** v. 9, p. 1-21, 2024. *Disponível em:* https://doi.org/10.1016/j.padiff.2023.100606. *Acesso em:* 7 de maio 2024.