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(RESEARCH ARTICLE)

Pollutant dispersion modeling in lakes interconnected by channels: A solution using the Bulirsch-Stoer method

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Abstract

This article presents a mathematical model for predicting the entry of pollutants into lakes interconnected through channels. Modeling the dynamics of pollutant dispersion in lakes was performed using three different input functions. The resulting model was solved by the Bulirsch-Stoer method, implemented to solve the system of ordinary differential equations that describe the problem, and the results were compared with data available in the literature. Practically, no differences were found between the model results and the reference data, in the simulations carried out under the same conditions. Therefore, the Bulirsch-Stoer Method can be safely used to solve this type of problem, as long as the initial conditions and the size of the integration step are adequate.

Keywords: Pollution; Modeling; Simulation; Numerical Method; Bulirsh-Stoer

1. Introduction

Protecting the environment and keeping water pollution-free is a global responsibility. Although several wastewater treatment plants are established to deal with water pollution, most wastewater is discharged directly into rivers or lakes. Therefore, it is important to understand the mechanism of a natural purification system to develop predictive models to represent the system and predict the rate of change in the amount of pollutants discharged into this system [1].

Pollution of water sources occurs through contamination by physical, chemical and biological elements, which can be harmful to organisms, plants and human activity, and is a very serious problem, as water is essential for life, food production, energy and industries of various types [2].

More than 3/4 of the Earth's surface is covered with water, but approximately 97.3% of this water is found in the oceans and therefore cannot be used for the aforementioned tasks. There remains, then, 2.7% of fresh water, of which 2.4% are located in places of difficult access, in underground regions and in glaciers, leaving only 0.3% of the planet's water for use. Brazil holds 13% of the available freshwater in the world, with approximately 73% located in the Amazon basin [2].

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A worrying factor related to water pollution is that groundwater, lakes, rivers, seas and oceans are the final destination of any and all water-soluble pollutants released into the air or soil. Thus, in addition to the pollutants that are released directly into the reservoirs, the water networks still receive pollution from the atmosphere and the lithosphere.

The largest group of lakes in terms of total area and the second largest in the world by volume of water is located in North America, between the United States and Canada, east of North America, whose names are: Superior, Michigan, Huron, Erie and Ontario. This group of lakes occupies a surface of 244,106 km^2 and contains 21% of the freshwater on Earth, with a volume of 22,671 km^3, forming the largest connected area of freshwater on the planet [3].

Due to the importance and peculiar characteristics of these lakes, this system has been the target of several pollution dynamics studies, whose results can be adapted for application in other systems. Among the various methods found in the literature to solve this problem, the Differential Transformation Method is frequently cited, having been tested with some modifications by several authors. The method is based on the flow balance between interconnected lakes [8, 10, 12, 18], resulting in a system of ordinary differential equations.

The solutions presented by several authors, using the different mentioned methods, involve complex mathematical development and, in addition to providing the same results, require advanced computer programming skills. For this reason, in this work the flow balance principle is used to develop the mathematical model, but the solution is performed numerically using the Bulirsch-Stoer method [4, 5, 6].

Therefore, the objective of this work is to discuss the dynamics of pollution flows in a system of lakes interconnected by channels, to present a solution of the model using the Bulirsch-Stoer numerical technique, and to compare the results with data available in the literature.

2. Material and methods

2.1 Model of pollution dynamics in lakes

Mixing problems refer to a variety of different problems where two or more substances are mixed at various rates. The mixtures problems cover from mixing chemicals in a tank to diffusing cigarette smoke through the air in a room. In this article, the modeling of the mixture of pollutants in lakes is presented [7].

2.1.1 The mixing equation

The rate of change of the polluting mixture is the difference between the amount of polluting mixture entering the system and the amount leaving it, defined by the following equation:

$$\frac{dM}{dt} = C_{in}(t) \cdot Q_{in}(t) - C_{out}(t) \cdot Q_{out}(t) \tag{1}$$

2.1.2 Pollutant generation rate and the dynamics of pollution in the lake

Pollutants have various chemical properties and some of them are non-polar and do not react with water. So this pollutant can only leave the system through the outflow. Some pollutants are polar and react with water, which can generate more or less pollutants. The variable $k(t)$ represents the pollutant generation rate and can be defined as:

$$\begin{cases} \text{k(t)} = 0;\ \text{No reaction.} \\ \text{k(t)} > 0;\ \text{No contaminat generation} \end{cases} \tag{2}$$

The variable $k(t)$ is also used in chemistry and determines the order of the reaction (in this case, reactions of order 0 or 1). Then, another term is added to the model of Equation (1):

$$\frac{dM}{dt} = [C_{in}(t) \cdot Q_{in}(t) - C_{out}(t) \cdot Q_{out}(t)] - k(t) \cdot C(t) \cdot V(t) \tag{3}$$

2.1.3. Modified model

To make the model easier to apply, without significantly affecting its accuracy, the following assumptions were made:

(1) The volume of the lake remains constant;
(2) The flow rate remains constant;
(3) The reaction rate remains constant;
(4) The water and the pollutant in the lake are well mixed.

The volume of lakes generally does not fluctuate in a short period, so the first assumption seems plausible. Assuming that the volume is constant, the flow rate must also remain constant. Therefore, the second assumption is also plausible. The third assumption is made to make the model easier to use, but it is limited to zero-order and first-order reactions. Assuming that the lake is well mixed means that the concentration of the pollutant inside the lake is equal to the concentration of the outflow. This assumption makes the model easier to manage and is also of limited use. Using premises 1 to 4, the model expressed by Equation (3) is rewritten as:

$$\frac{dM}{dt} = Q \cdot C_{in}(t) - Q \cdot C(t) - k \cdot C(t) \cdot V \tag{4}$$

Multiplying and, at the same time, dividing Equation (4) by the volume, it is obtained the following robust equation:

$$\frac{dC(t)}{dt} = \frac{Q}{V} \cdot C_{in}(t) - \frac{Q}{V} \cdot C(t) - k \cdot C(t) \tag{5}$$

The time it would take to fill the lake if there were no outflow, and how long it would take to drain the lake if there were only outflow, can be determined by rewriting Equation (5), defining the residence time of the pollutant in the lake as $Q/V = \theta_r$ to obtain:

$$\frac{dC(t)}{dt} = \frac{1}{\theta_r} \cdot C_{in}(t) - \frac{1}{\theta_r} \cdot C(t) - k \cdot C(t) \tag{6}$$

2.2 Pollutant input models

Three types of models were used to simulate the entry of pollutants into lakes and to predict the rate of change in the concentration of these pollutants in lakes. These input models are: impulse, step, and sine functions.

2.2.1 Impulse input model

The impulse model is used for pollutants that are released into the lake immediately. Impulse input functions have a peak, and at all other points the function is zero.

$$C(t) = \begin{cases} C_{in}, t \geq 0 \\ 0, t < 0 \end{cases} \tag{7}$$

2.2.2 Step input model

The step model is used for pollutants that enter the lake at constant concentration and constant rate, and continue in the same way indefinitely. The pollutant enters the system at time zero and the concentration before this time is zero.

$$C(t) = \begin{cases} 0, t \leq 0 \\ C_{in}, t > 0 \end{cases} \tag{8}$$

2.2.3. Sinusoidal input model

The sinusoidal model is used for pollutants that are introduced into the lake periodically. Pollution enters the system at an average concentration and periodically varies around this average. The sinusoidal input changes the input concentration making the model more useful.

$$C_{in}(t) = C_m \left[1 + a \cdot sen\left(\frac{2\pi}{T} \cdot t\right)\right] \tag{9}$$

2.3 Pollution dispersion model in lakes

The model of pollutant dynamics in interconnected lakes discussed here is well supported in the literature by several authors and has been solved using several methods. The system used as a reference in this work is represented by a set of three lakes, interconnected by channels, through which pollutants flow [8, 11,. 18], as illustrated in Figure 1

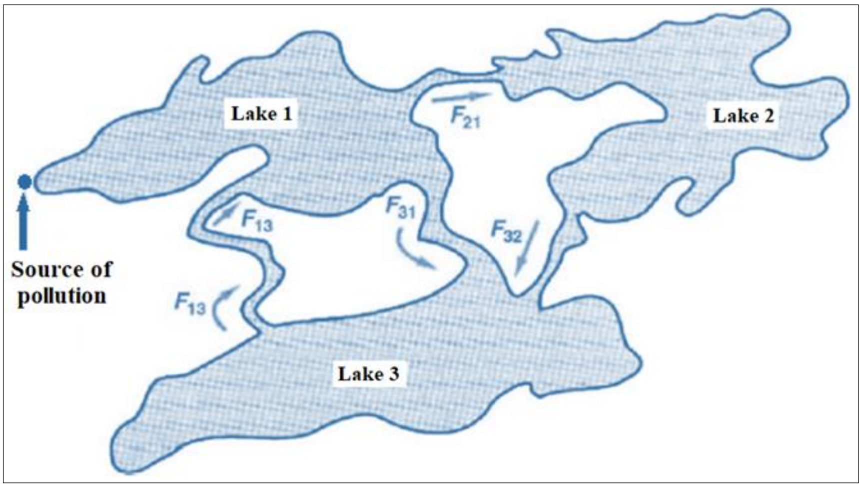


Figure 1 System of lakes with interconnecting channels

2.3.1 Mathematical formulation

The modeling was developed considering the lake system represented in Figure 1, each of them considered a large compartment, and the interconnection channels considered as tubes between the compartments [8, 9]. The arrows in Figure 1 indicate the direction of flow in the channels or pipes. A pollutant is introduced into the first lake at a rate $p(t)$, which can be constant or variable with time.

The level of pollution of each lake at any time can be determined by defining $x_i(t)$ as the amount of pollution in lake i, at any time, $t \geq 0$, where $i = 1, 2, 3$, assuming that the pollutant in each lake must be evenly distributed across the lake by some mixing process, and the volume of water V_i in lake i remains constant for each of the lakes. Furthermore, it is assumed that the pollutant is of the persistent type and does not degrade to other forms. Therefore, the concentration of the pollutant in lake i is given by:

$$c_i(t) = \frac{x_i(t)}{V_i} \tag{10}$$

Each lake is initially considered free of any contaminant, so $x_i(0) = 0$ for each of them, $i = 1, 2, 3$. The dynamic behavior of the lake system can be modeled by defining the constant F_{ji} to represent the flow rate from lake i to lake j. Therefore, the pollutant flow from lake i to lake j at any instant is defined by $r_{ji}(t)$:

$$r_{ji}(t) = F_{ji}\, c_i(t) = \frac{F_{ji}}{V_i} x_i(t) \tag{11}$$

The rate of change in the concentration of pollutants in lake i, $r_{ji}(t)$, flowing into lake j at time t is defined by the difference between the rate in and the rate out:

$$r_{ji}(t) = r_{ji}^{in}(t) - r_{ji}^{out}(t) \tag{12}$$

The flow rate in each lake must balance the outflow from the lake, so that the volume of each lake remains constant. Then, according to Figure 1, we have the following balances:

$$For\ Lake\ 1: F_{13} = F_{21} + F_{31} \tag{13}$$

$$For\ Lake\ 2: F_{21} = F_{32} \tag{14}$$

$$For\ Lake\ 3: F_{31} = F_{32} + F_{13} \tag{15}$$

Applying the principle expressed by Equation (12) for each lake, combined with Equations (13), (14) and (15), results in the following system of first-order ordinary differential equations that describe the flow rates of pollutants in the system of lakes represented in Figure 1:

$$\begin{cases} \dfrac{dx_1}{dt} = -\left[\left(\dfrac{F_{31}}{V_1}\right) + \left(\dfrac{F_{21}}{V_1}\right)\right] \cdot x_1(t) + \left(\dfrac{F_{13}}{V_3}\right) \cdot x_3(t) + p(t) \\ \dfrac{dx_2}{dt} = \left(\dfrac{F_{21}}{V_1}\right) \cdot x_1(t) - \left(\dfrac{F_{32}}{V_2}\right) \cdot x_2(t) \\ \dfrac{dx_3}{dt} = \left(\dfrac{F_{31}}{V_1}\right) \cdot x_1(t) + \left(\dfrac{F_{32}}{V_2}\right) \cdot x_2(t) - \left(\dfrac{F_{13}}{V_3}\right) \cdot x_3(t) \end{cases} \tag{16}$$

2.3.2 Model Solution

Solutions of the system of Equations (16) using various methods can be found in the literature, for example, differential transformation techniques [8, 10, 12, 18], method of variational iteration [13], revised Adomian decomposition method [9], and analytical methods [14, 15, 16].

In this work, the solution of the system of Equations (16) was performed by the Bulirsch-Stoer method [4, 5, 6]. This method was chosen due to its proven efficiency [17], ease of implementation in any programming language according to the researcher's choice, and for being an open source and public domain algorithm.

The results of lake pollution simulations were compared with literature data under the same conditions [8, 18], but any other conditions can be used to predict the dynamics of pollutants in lakes. The data referring to the volume of water in the lakes and the flows between them used in Equations (16) are organized in Table 1.

Table 1 Volume of water in the lakes, and flows between them, used to test the pollution model [8]

Lakes	Water volume in the lakes		
	$[\mathbf{mi^3}]$	$[\mathbf{km^3}]$	$[\ \mathbf{m^3}]$
1	1200	5002	5.002×10^{12}
2	1050	4377	4.377×10^{12}
3	850	3543	3.543×10^{12}
Flows F_{ji}	**Pollutant flows between lakes**		
	$[\mathbf{mi^3/day}]$	$[\mathbf{km^3/day}]$	$[\mathbf{m^3/day}]$
F_{21}	68	283.44	2.834×10^{11}
F_{31}	105	437.66	4.377×10^{11}
F_{13}	85	354.30	3.543×10^{11}
F_{32}	96	400.15	4.001×10^{11}

3. Results

3.1 Validation of the lake pollution model

In the validation of the model described by the system of Equations (16), the lake system presented in Figure 1, and the conditions in Table 1 [8], were used with an impulse-type input function of pollutant, with a constant load of 100 kg/year. The results for the three lakes are shown in Tables 2, 3 and 4, respectively.

Results of Biazar and Rahimi [8] were obtained by solving the model by the differential transformation method for a short period of time (36.5 days). The three types of pollutant input functions discussed earlier were tested. In this work, the model was solved by the Bulirsch-Stoer method using these same contaminant entry models and the same conditions used by Biazar and Rahimi [8].

It can be seen in Tables 2, 3 and 4 that the results of the two methods, with impulse input function, are practically identical, with a maximum relative error of approximately 0.03526 %, in absolute value, for lake 3. The initial input rate of pollutant was a pulse of 100 kg/year, and therefore, after 0.1 year (36.5 days) approximately 10 kg of pollutants will be dispersed in Lake 1.

The pollutant dispersion dynamics in Lakes 2 and 3 depends on the interaction between the lakes through the flows between them, since they do not receive pollutants directly. Although the reference results used in the model validation were for a short period, they are sufficient to validate the model solution by the Bulirsch-Stoer method.

The step and sinusoidal pollutant input models were also tested but, when compared with the results from Biazar and Rahimi [8], no differences were observed. Therefore, the results were practically identical for the three input models tested, and the model solution by the Bulirsch-Stoer method was considered validated.

Table 2 Simulated results using the impulse pollutant input model compared with data obtained from Biazar and Rahimi [8] for Lake 1

Step	**Time**		**Amount of Pollutant in Lake 1** [**kg**]		
	[**year**]	[**day**]	**This Work**	**Biazar and Rahimi [8]**	**Error** [%]
0	0.00	0.00	0	0	0
1	0.01	3.65	0.999934489	0.999934489	0.000000000
2	0.02	7.30	1.999737984	1.999737984	0.000000000
3	0.03	10.95	2.999410522	2.999410522	0.000000000
4	0.04	14.60	3.998952144	3.998952144	0.000000000
5	0.05	18.25	4.998362889	4.998362889	0.000000000
6	0.06	21.90	5.997642796	5.997642796	0.000000000
7	0.07	25.55	6.996791905	6.996791905	0.000000000
8	0.08	29.20	7.995810255	7.995810255	0.000000000
9	0.09	32.85	8.994697884	8.994697885	-0.000000011
10	0.10	36.50	9.993454834	9.993454834	0.000000000

Table 3 Simulated results using the impulse pollutant input model compared with data obtained from Biazar and Rahimi [8] for Lake 2

Step	**Time**		**Amount of Pollutant in Lake 2** [**kg**]		
	[**year**]	[**day**]	**This Work**	**Biazar and Rahimi [8]**	**Error** [%]
0	0.00	0.00	0	0	0
1	0.01	3.65	0.000031031	0.000031031	0.000031031
2	0.02	7.30	0.000124110	0.000124110	0.000000000
3	0.03	10.95	0.000279215	0.000279215	0.000000000
4	0.04	14.60	0.000496325	0.000496325	0.000000000
5	0.05	18.25	0.000775419	0.000775419	0.000000000

6	0.06	21.90	0.001116476	0.001116476	0.000000000
7	0.07	25.55	0.001519474	0.001519474	0.000000000
8	0.08	29.20	0.001984392	0.001984392	0.000000000
9	0.09	32.85	0.002511210	0.002511210	0.000000000
10	0.10	36.50	0.003099905	0.003099905	0.000000000

Table 4 Simulated results using the impulse pollutant input model compared with data obtained from Biazar and Rahimi [8] for Lake 3

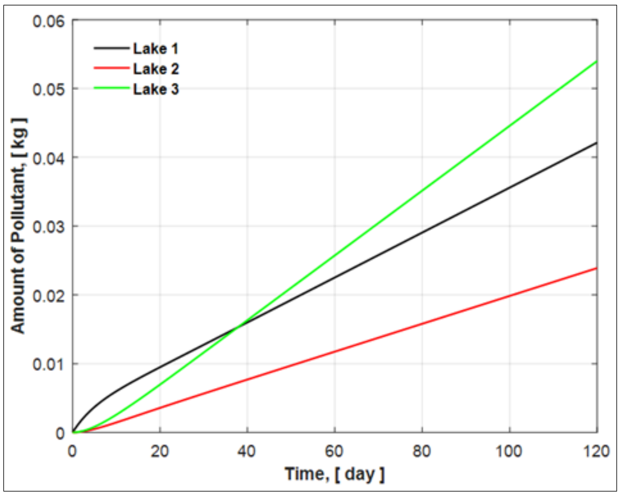
Step	Time		Amount of Pollutant in Lake 3 [kg]		
	[year]	[day]	This Work	Biazar and Rahimi [8]	Error [%]
0	0.00	0.00	0	0	0
1	0.01	3.65	0.000034478	0.000034480	0.001450179
2	0.02	7.30	0.000137897	0.000137907	-0.007251264
3	0.03	10.95	0.000310231	0.000310263	-0.010313831
4	0.04	14.60	0.000551453	0.000551531	-0.014142451
5	0.05	18.25	0.000861540	0.000861692	-0.017639713
6	0.06	21.90	0.001240465	0.001240728	-0.021197233
7	0.07	25.55	0.001688204	0.001688621	-0.024694707
8	0.08	29.20	0.002204730	0.002205353	-0.028249446
9	0.09	32.85	0.002790019	0.002790905	-0.031745975
10	0.10	36.50	0.003444046	0.003445261	-0.035265833

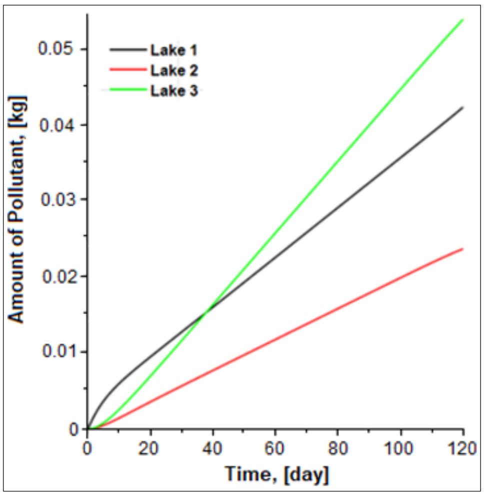
3.2 Numerical application

In addition to Biazar and Rahimi [8], several researchers have solved this same problem using different methods, including Biazar and Zarei [18], who used the fractional differential transformation method. Most of these methods are complicated and difficult to solve, in addition to not providing an improvement in the solution of the problem discussed in this work, when compared to the Bulirsch-Stoer method. Examples of applications are presented below, using data from Biazar and Zarei [18] as a reference.

3.2.1 Application 1 - Impulse-type pollutant input function

Simulated results using an input impulse $p(t) = 10^{-3}$ kg/day for a period equal to 120 days, and integration step equal 0.01 day for Bulirsch-Stoer method (Figure 2a), compared to the results from Biazar and Zarei [18] using the fractional differential transformation method (Figure 2b).



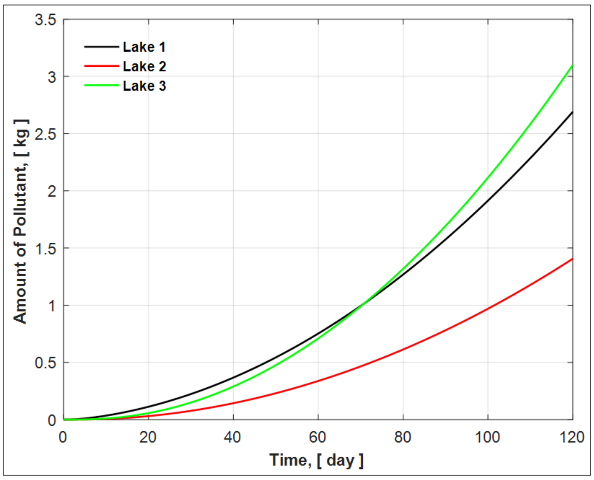


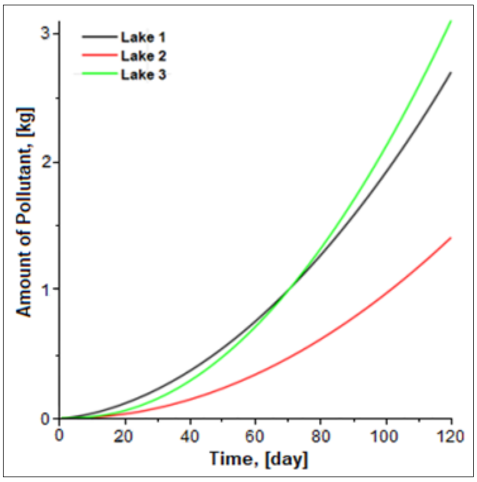
(a) Present work **(b) Biazar and Zarei [18]**

Figure 2 Simulated amount of pollutant in Lakes 1, 2, and 3, with an impulse input rate of 10^{-3} kg/day for a period of 120 days: (a) Bulirsch-Stoer method, and (b) Biazar and Zarei [18] 100 terms polynomial

3.2.2 Application 2 – Time-dependent pollutant input function

Simulated results using an input function $p(t) = 10^{-3} \cdot t$ kg/day for a period equal to 120 days, and integration step equal 0.01 day for Bulirsch-Stoer method (Figure 3).



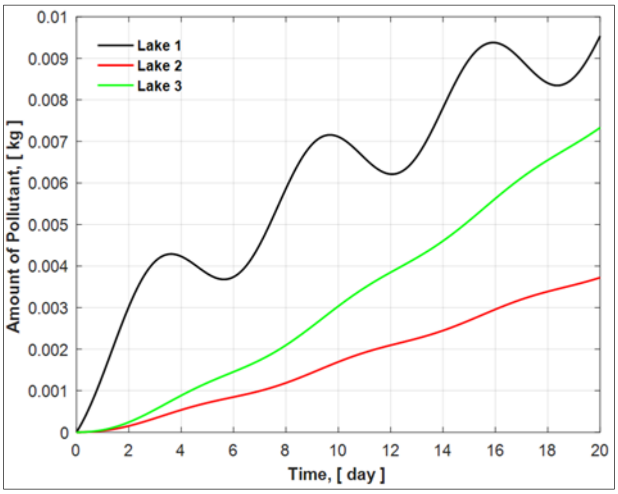


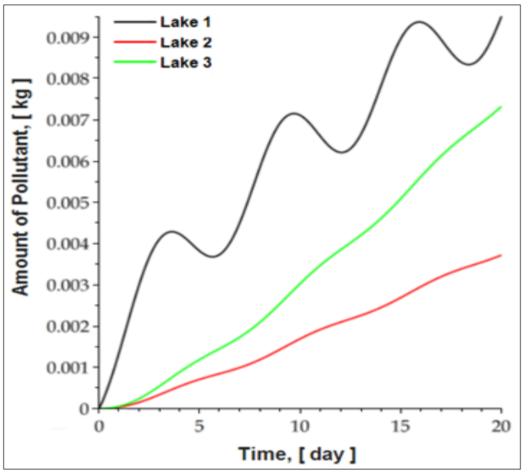
(a) Present work **(b) Biazar and Zarei [18]**

Figure 3 Simulated amount of pollutant in Lakes 1, 2, and 3, with an input rate of $10^{-3} \cdot t$ kg/day for a period of 120 days: (a) Bulirsch-Stoer method, and (b) Biazar and Zarei [18] 100 terms polynomial

3.2.3 Application 3 – Sinusoidal pollutant input function

Simulated results using an input function $p(t) = 10^{-3} \cdot (1 + \sin(t))$ kg/day for a period equal to 20 days, and integration step equal 0.01 day for Bulirsch-Stoer method (Figure 4).



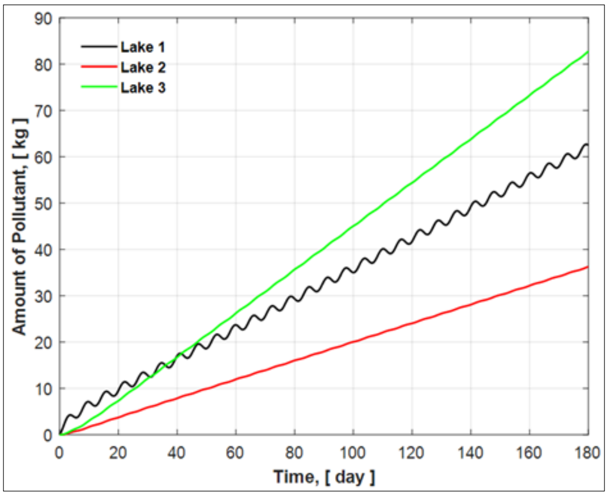


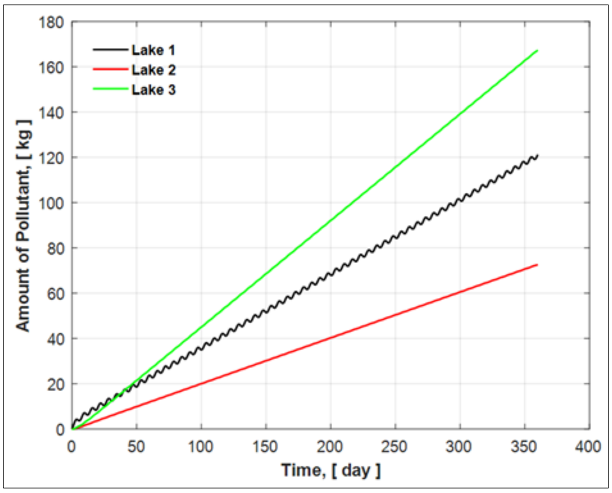
(a) Present work **(b) Biazar and Zarei [18]**

Figure 4 Simulated amount of pollutant in Lakes 1, 2, and 3, with an input rate of $10^{-3} \cdot (1 + \sin(t))$ kg/day for a period of 20 days: (a) Bulirsch-Stoer method, and (b) Biazar and Zarei [18] 100 terms polynomial

3.2.4 Application 4 - Industrial waste

An example of a factory that dumps waste into the lake is presented, producing more during the day than at night due to operating hours, characterizing a periodic entry of contaminants. The pollutant concentration in the lake eventually converges to the average inlet concentration of the contaminant. In this case, an input model $p(t) = 1 + \sin(t)$ kg/day and the parameter values presented in Table 1 were assumed (Figure 5).





(a) **(b)**

Figure 5 Simulated amount of pollutant in Lakes 1, 2, and 3, with input function $p(t) = 1 + \sin(t)$, for (a) 180 days, and (b) 360 days periods

4. Discussion

The modeling of a system of three lakes with interconnecting channels was performed by a system of three coupled ordinary differential equations. The Bulirsch-Stoer method was tested, using as a reference results obtained in the literature [8], and applied to solve four application examples [18]. There are no differences between the results of this work and those presented by these researchers. However, it is important to point out that the Bulirsch-Stoer method is easier to implement.

In Application 1, pollution starts at the first lake at a constant rate. It is observed that the amount of pollutant in lake 1, $x_1(t)$, increases with the input model at the instant when the pollutant load enters the lake, but when the pollutant enters other lakes through interconnected channels, the pollution in lake 2, $x_2(t)$, and in lake 3, $x_3(t)$, increases. Then the pollutant enters the first lake again and this fact prevents the decrease in the amount of pollution in the first lake.

In Application 2, pollution starts in the first lake at any time, but when the pollutant enters the second and third lakes, the pollutant enters the first lake again, so the amount of pollutant in lake 1, $x_1(t)$, increases further than usual.

In Application 3, pollution starts from the first lake with the sinusoidal inlet model. In this input model, when the pollutant release reaches its peak, the amount of pollutant in lake 1, $x_1(t)$, increases, and when the pollution release reaches its minimum, $x_1(t)$ decreases.

In Application 4, the analysis is similar to that of Application 3, but there are no fluctuations in the amount of pollutant in lakes 2 and 3, possibly because there has been enough time for the pollutant dispersion rate to converge to the mean, due to the longer simulated residence time.

Nomenclature

Symbol	**Description****	**Unit**
M	Mass of contaminant	kg
C_{in}	Input concentration of contaminant	$kg\ m^{-3}$
C_{out}	Output concentration of contaminant	$kg\ m^{-3}$
Q_{in}	Volumetric flow into the lake	$m^3\ s^{-1}$
Q_{out}	Volumetric flow out of the lake	$m^3\ s^{-1}$
t	Time	s
θ_r	Residence time	s
k	Pollutant generation rate	s^{-1}
V	Water volume in the lake	m^3
a	Normalized amplitude of sine function	$-$
T	Period of fluctuations in concentration	s
$c_i(t)$	Average pollutant concentration in lake i at time t	$kg\ m^{-3}$
$x_i(t)$	Amount of pollutant in lake i at time t	kg
V_i	Volume of lake i at time t	m^3
$r_{ji}(t)$	Pollutant flow from lake i to lake j, at time t	$kg\ s^{-1}$
F_{ji}	Liquid flow from lake i to lake j, at time t	$m^3\ s^{-1}$

** Units are given in SI, and converted appropriately whenever necessary.

5. Conclusion

The solutions of the pollution dispersion problem in lakes, using the Bulirsch-Stoer method, did not show differences in relation to the Adomian Differential Decomposition Method, nor to the Fractional Differential Transformation method under the same conditions. However, it was not possible to compare the computational efficiency among the methods, because computational times were not available. On the other hand, it can be said that the Bulirsch-Stoer method is efficient in solving initial value problems described by ordinary differential equations.

The pollution problem in lakes was solved by assuming that they are not being depolluted (or drained), which allows monitoring the level of pollution over time. It is important to emphasize that the control of the pollution levels in the water sources allows minimizing its harmful effects to the life. Therefore, studies to model the dynamics of depollution in lakes and other sources are recommended, in order to implement measures to control the level of pollution and establish strategies to maintain the sustainability of these vital natural resources.

Compliance with ethical standards

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Disclosure of conflict of interest

There is no conflict of interest on this article.

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