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A Computational Approach in Estimating the Amount of Pond Pollution and Determining the Long Time Behavioural Representation of Pond Pollution Model

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Abstract

This paper specifically develops a computational approach in estimating the amount of pond pollution and determining the long time(every 48 hours) behavioural representation of the pond pollution model.This approach, which can be considered as an extension of the block predictor-corrector methods in form of implicit block multistep method has many computational advantages usingvariable step size technique. Moreover, it possesses some important advantages of designing a suitable step size, stopping criteria(prescribed tolerance level) and error control/minimization as well. This makes the new approach specifically efficient for solving systems of first-order ordinary differentialequations. Analysis of some theoretical properties of the method is carried out to ascertain the extent of performance of the method. Again, numerical results are given to display the performance and efficiency of this new method on system first-order ordinary differential equations.

Keywords and phrase: Computational approach • Variable step size technique • Implicit block multistep method • Pond pollution • Stopping criteria

1 Introduction

As presented in Chaurasia and Pandey [4], Nag and Gupta [17], water is an elixir of life. It controls the evolutions and works of universe on the earth hence it is mother of all living world. Again, water can be described as one of the most abundant compounds in earth approximately covering three-fourth of the earth's surface. Majority of water usable on earth is saline in existence; only a small quantity exists as fresh water. Fresh water has become a scarce commodity because of over exploitation and pollution (See Refs. [7], [8], [19], and [20]). Industrial, sewage and municipal wastes are being endlessly added to the water reservoirs impacting the physico-chemical quality of water making it unsuitableas reported byDwivedi and Pandey [5]. Unrestrained discharge of domestic waste water into the ponds has ensuedin eutrophication of ponds as introduced by Pandey and Pandey[18]. Physico-chemical properties (pH, conductivity, free CO2, COD, alkalinity, chlorinity-salinity, ions such as Na+ and K+) of water in any aquatic system are largely ruled by the existing meteorological condition, and are important for determining the structural and functional status of natural water. Hydrological condition of water affects the aquaculture activities, fish productivity and species composition of aqua fauna, eutrophication and overall loss of biodiversity that leads to degradation of pond ecosystem. The magnitude and dynamics of oxidation-reduction reaction by different elements present in water plays a vital role in governing most of the chemical, biochemical and microbial behaviours in the pond water, and also maintaining congenial environment condition as discussed in Nag and Gupta [17].

The ever-increasing development in electronic computer has modified many scientists and engineers to employ numerical methods using parallel computation to solve mathematical models arising from real life application. The computational solution of large ODEs systems needs large amount of computing power. Experts of parallel computing tend to be those with large mathematical problems tends to evaluate with the desire to obtain faster and more precise results as in Majidand Suleiman[13].

This study is interested with the development of a computational approach in form ofimplicit block multistep method using variable step size technique for solving system of non-stiff first order ordinary differential equations of the form as seen in Majid and Suleiman[14].

$$y' = f(x, y(x)), \; f: R^m \to R^m, \; y(x_0) = y_0,$$
$$x \in [a,b]. \tag{1}$$

The solution is generally written as

$$\sum_{i=1}^{j} \alpha_i y_{n+ii} = h \sum_{i=1}^{j} \beta_i f_{n+i} \tag{2}$$

where h is the step size $\alpha_j = 1, \alpha_i, \; i = 1, \ldots j, \; \beta_j$ are unknown constants which are uniquely determined such that the formula is of order j as discussed in Akinfenwa et al. [2].

We assume that $f \in R$ is sufficiently differentiable on $x \in [a,b]$ and satisfies a global Lipchitz condition, i.e., there is a constant $L \geq 0$ such that

$$\left|f(x,y)-f\left(x,\overline{y}\right)\right|\le L\left|y-\overline{y}\right|,\ \forall y,\overline{y}\in R.$$

Under this presumption, equation (1) assured the existence and uniqueness defined on $x\in[a,b]$ as discussed in Xie and Tian [22].

Equation (1) can solved by many existing methods but those methods will estimate the computational solutions at one point consecutively. Thus we demand a quicker method that can generate quicker solution to the problem. Block methods for the numerical solution of first order ODEs have been proposed by several researchers. Among them, numerous one-block and multi-block methods have been suggested for the computational solution of ODEs. Block methods further the numerical solution by a block of more than one new solution values at a time and enjoy high accuracy, good stability and efficiency in parallel computing (See Refs. [2], [3], [12], [13], [15] and [22])

Definition 1.1 According to Akinfenwa et al. [2]. A block-by-block method is a method for computing vectors $Y_0, Y_1, \ldots$ in sequence. Let the r-vector (r is the number of points within the block) Y_μ, F_μ, and G_μ, for n=mr, m=0, 1,... be given as $Y_w=(y_{n+1},\ldots,y_{n+r})^T, F_w=(f_{n+1},\ldots,f_{n+r})^T$, then the l-block r-point methods for (1) are given by

$$Y_w=\sum_{i=1}^{j}A^{(i)}Y_{w-i}+h\sum_{i=1}^{j}B^{(i)}F_{w-i}$$

where $A^{(i)}$, $B^{(i)}$, $i=0,\ldots,j$ are r by r matrices as introduced by Fatunla [6].

Thus, from the above definition a block method has the advantage that in each application, the solution is approximated at more than one point simultaneously. The number of points depends on the structure of the block method. Therefore applying these methods can give quicker and faster solutions to the problem which can be managed to produce a desired accuracy. See Majid and Suleiman [12], Mehrkanoon et al. [15].

The block algorithm proposed in this paper is based on interpolation and collocation. The continuous representation of the algorithm generates a main discrete collocation method to render the approximate solution Y_{n+i} to the solution of (1) at points $x_{n+i}, i=1,\ldots k$ as discussed in Akinfenwa et al. [2].The main aim of this paper is to introduce a computational approach in form of implicit block multistep method for estimating the amount of pond pollution and determining the long time behavioural representation of the pond pollution model.

The residualof this paper is discussed as follows: in Section 2 the introductory idea behind the computational method is discussed and a continuous representation $Y(x)$ for the exact solution $y(x)$ which is used to generate a main discrete block method for solving (1) is derived. In Section 3 the order of accuracy of the methods is introduced. In Section 4 the stability regions of the block predictor-corrector methods are discussed. In Section 5 we show the accuracy of the methods with the pond pollution problem. In conclusion, Section 6 gives presents some final remarks.

2 Derivation of the Method

Following [2] in this section, the aim is to derive the principal block method of the form (2). We move forward by seeking an approximation of the exact solution $y(x)$ by assuming a continuous solution $Y(x)$ of the form

$$Y(x)=\sum_{i=0}^{q+k-1} m_i \vartheta_i(x) \tag{3}$$

such that $x\in[a,b]$, m_i are unknown coefficients and $\vartheta_i(x)$ are polynomial basis functions of degree $q+k-1$, where q is the number of interpolation point and the collocation points k are respectively chosen to satisfy $q=j$ and $k\geq 1$. The integer $j\geq 1$ denotes the step number of the method. We thus construct a j-step block method block method with $\vartheta_i(x)=\left(\frac{x-x_i}{h}\right)^i$ by imposing the following conditions

$$\sum_{i=0}^{q} m_i\left(\frac{x-x_i}{h}\right)^i = y_{n+1},\ i=0,\dots,q-1 \tag{4}$$

$$\sum_{i=0}^{q} m_i i\left(\frac{x-x_i}{h}\right)^{i-1} = f_{n-i},\ i=0,\dots,j, \tag{5}$$

where y_{n+i} is he approximation for the exact solution $y(x_{n+i})$, $f_{n+i}=f(x_{n+i},y_{n+i})$, n is the grid index and $x_{n+i}=x_n+ih$. It should be noted that equations (4) and (5) leads to a system of $q+1$ equations of the AX=B where

$$A=\begin{bmatrix} x_n^0 & x_n & x_n^2 & \cdots & x_n^j \\ x_{n-2}^0 & x_{n-2} & x_{n-2}^2 & \cdots & x_{n-2}^j \\ x_{n+1}^0 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^j \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ x_{n+j-1}^0 & x_{n+j-1} & x_{n+j-1}^2 & \cdots & x_{j-1}^j \\ 0 & 1 & 2x_{n+j} & \cdots & jx_{n+j}^{j-1} \end{bmatrix}$$

$$X=\left[a_0,a_1,a_2,\dots,a_k\right]^T$$
$$U=\left[f_n,f_{n+1},f_{n+2},\dots,f_{n+k\text{-}1},y_{n\text{-}k}\right]^T \tag{6}$$

Solving equation (6) using Mathematica, we get the coefficients of m_i and substituting the values of m_i into (4) and after some algebraic computation, the implicit block multistep method is obtain as

$$\sum_{i=0}^{q-1}\alpha_i y_{n+i} = h\sum_{i=0}^{q-1}\beta_i f_{n+i} \tag{7}$$

where α_i and β_i are continuous coefficients.

3 Investigation of Some Theoretical properties

3.1 Order of Accuracy

Adopting Lambert(1973) and Akinfenwa et al. (2013), we define the associated linear multistep method (7))and the difference operator

$$L[y(x);h] = \sum_{i=0}^{j}\left[\alpha_i y(x+ih) - h\beta_i y'(x+ih)\right]. \tag{8}$$

Assuming that $y(x)$ is sufficiently differentiable, we can write the terms in (8) as a Taylor series expression of $y(x_{n+i})$ and $f(x_{n+i}) \equiv y'(x_{n+i})$ as

$$y(x_{n+i}) = \sum_{k=0}^{\infty}\frac{(ih)}{k!}y^{(k)}(x_n) \text{ and } y'(x_{n+i}) = \sum_{k=0}^{\infty}\frac{(ih)}{k!}y^{(k+1)}(x_n). \tag{9}$$

Substituting (8) and (9) into (7) we obtain the following expression

$$L[y(x);h] = c_0 y(x) + c_1 h y^{(1)}(x) + \ldots + c_p h^p y^{(p)}(x) + \ldots, \tag{10}$$

From Lambert, Akinfenwa et al. (2013), we observed that the implicit block multistep method of (7) has order p, if $c_p,\ p = 0,1,2,\ldots,i = 1,2,\ldots,j$, are given as follows:

$$c_0 = \alpha_0 + \alpha_1 + \alpha_2 + \cdots + \alpha_k,$$

$$c_1 = \alpha_0 + \alpha_1 + \alpha_2 + \ldots + k\alpha_k - (\beta_0 + \beta_1 + \beta_2 + \ldots + \beta_k),$$

$$c_q = \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + \cdots + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_0 + 2^{q-1}\beta_1 + \beta_2 + \cdots + k^{q-1}\beta_k),$$

$q = 2,3\ldots$

Thus, the method (7) has order p=4 and error constants given by the vector,

$$C_5 = \left[-\frac{77}{360}, -\frac{8}{45}, -\frac{9}{40}\right]^T$$

Agreeing with Lambert [11], we say that the method (2) has order p if

$$L[y(x);h] = O(h^{p+1}),\ C_0 = C_1 = \ldots = C_p = 0,\ C_{p+1} \neq 0. \tag{11}$$

Therefore, C_{p+1} is the error constant and $C_{p+1}h^{p+1}y^{(p+1)}(x_n)$ is the principal local truncation error at the point x_n.

3.2 Stability Analysis

In order to analyze the method for stability, (7) is normalize and written as a block method given by the matrix finite difference equations as in[2] and [10].

$$A^{(0)}Y_m = A^{(1)}Y_{m-1} + h(B^{(0)}F_m + B^{(1)}F_{m-1}), \qquad (12)$$

where

$$Y_m = \begin{bmatrix} y_{n+1} \\ y_{n+1} \\ . \\ . \\ . \\ y_{n+r} \end{bmatrix}, \; Y_{m-1} = \begin{bmatrix} y_{n-r+1} \\ y_{n-r+2} \\ . \\ . \\ . \\ y_n \end{bmatrix}, \; F_m = \begin{bmatrix} f_{n+1} \\ f_{n+1} \\ . \\ . \\ . \\ f_{n+r} \end{bmatrix}, \; F_{m-1} = \begin{bmatrix} f_{n-r+1} \\ f_{n-r+2} \\ . \\ . \\ . \\ f_n \end{bmatrix}.$$

The matrices $A^{(0)}, A^{(1)}, B^{(0)}, B^{(1)}$ are r by r matrices with real entries while $Y_m, Y_{m-1}, F_m, F_{m-1}$ are r-vectors specified above.

Following Ken et al.[10], we adopted the boundary locus method to determine the region of absolute stability of the block method and to obtain the roots of absolute stability. Substituting the test equation $y' = -\lambda y$ and $h' = h\lambda$ into the block (12) to obtain

$$\rho(r) = \det\left[r\left(A^{(0)} + B^{(0)}h\lambda\right) - \left(A^{(1)} - B^{(1)}h\lambda\right)\right] = 0 \qquad (13)$$

Substituting $h = 0$ in (13), we obtain all the roots of the derived equation to be equal to be less than or equal to 1. Hence, according to Lambert [11], theblockmethod is absolutely stable.

As discussed byAdesanya et al. [2], the boundary of the region of absolute stability can be obtained by substituting (7) into

$$\bar{h}(r) = \frac{\rho(r)}{\sigma(r)} \qquad (14)$$

and let $r = e^{i\theta} = \cos\theta + i\sin\theta$ then after simplification together with evaluating (1.14) at 30^0 within $[0^0, 180^0]$, which gives the region ofabsolute stability to be $[-5.983, 0]$ after evaluation at interval of $\bar{h}(\theta)$. The stability region is shown in Fig. 1.

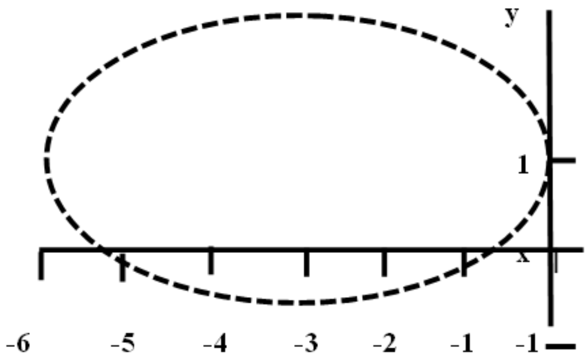

Fig. 1 Showing region of absolute stability of the block method.

4Implementation of the Method

According to Lambert [11], Milne's device proposes that it possible to estimate the principal local truncation error of the predictor-corrector method without estimating higher derivatives of $y(x)$. Assume that $p = p^*$, where p^* and p represents the order of the predictor and corrector method with the same order. Now for a method of order p, the principal local truncation errors can be written as

$$C^*_{p+1} h^{p+1} y^{(p+1)}(x_n) = y(x_{n+j}) - W_{n+j} + O(h^{p+2}) \tag{15}$$

Also,

$$C_{p+1} h^{p+1} y^{(p+1)}(x_n) = y(x_{n+j}) - C_{n+j} + O(h^{p+2}) \tag{16}$$

where W_{n+j} and C_{n+j} are called the predicted and corrected approximations given by method of order p while C^*_{p+1} and C_{p+1} are independent of h.

Neglecting terms of degree $p+2$ and above, it is easy to make estimates of the principal local truncation error of the method as

$$C_{p+1} h^{p+1} y^{(p+1)}(x_n) \cong \frac{C_{p+1}}{C^*_{p+1} - C_{p+1}} \left| W_{n+j} - C_{n+j} \right| \tag{17}$$

Noting the fact that $C_{p+1} \neq C^*_{p+1}$ and $W_{n+j} \neq C_{n+j}$.

Moreover, the estimate of the principal local truncation error (17) is used to decide whether to accept the results of the current step or to redo the step with a smaller step size. The step is accepted based on a test as described by (17) as in Uri and Linda (1998). Equation (17) is the convergence test otherwise called Milne's estimate for correcting to convergence

Furthermore, equation (17) guarantees the convergence criterion of the method during the test evaluation.

5 Numerical Experiment

The performance of the implicit block multistep method was carried out on non-stiff problem as discussed below.

Experiment 5.1 Pond Pollution

Consider three ponds connected by streams, as in Fig. 2. The first pond has a pollution source, which spreads via connecting streams to the other ponds. The plan is to construct a computational approach in estimating the amount of pond pollution and determine the long time behavioural representation of pond pollution model [9].

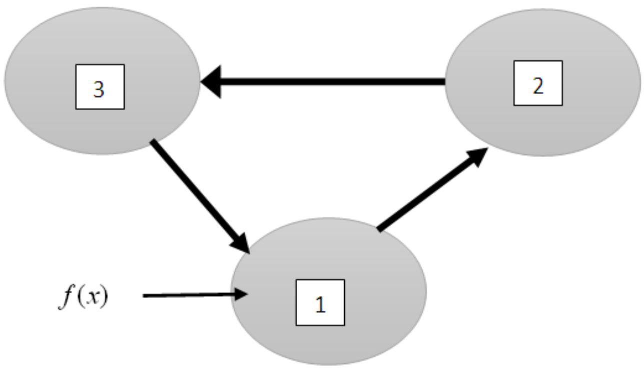

Fig. 2 Three ponds 1, 2, 3 of volumes V_1, V_2, V_3 connected by streams.

The pollution source $f(x)$ is in pond 1. (http://www.math.utah.edu/~gustafso/2250systems-de.pdf.)

Assume the following.

- Symbol $f(x)$ is the pollutant flow rate into pond 1 (Ib/min).
- Symbol $f_1(x), f_2(x), f_3(x)$ denote the pollutant flow rates out of ponds 1, 2, 3, respectively (gal/min). It is assumed that the pollutant is well-mixed in each pond.
- The three ponds have volumes V_1, V_2, V_3 (gal), which remain constant.
- Symbols $y_1(x), y_2(x), y_3(x)$ denote the amount (Ibs) of pollutant in ponds 1, 2, 3, respectively.

5.2 Model formulation

The pollutant flux is the flow rate times the pollutant concentration, e.g., pond 1 is emptied with flux f_1 times $y_1(x)/V_1$. A compartment analysis is summarized in the following diagram.

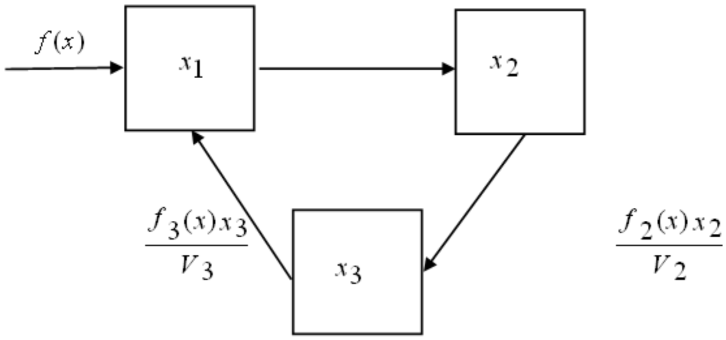

Fig. 3 Pond diagram. The compartment diagram represents the three-pond pollution problem of Fig. **2.**

The diagram plus compartment analysis gives the differential

$$y_1^{'}(x) = \frac{f_3(x)}{V_3^{'}} y_3(x) - \frac{f_1(x)}{V_1^{'}(x)} y_1(x) + f(x)$$

$$y_2^{'}(x) = \frac{f_1(x)}{V_1^{'}} y_1(x) - \frac{f_2(x)}{V_2^{'}(x)} y_2(x)$$

$$y_3^{'}(x) = \frac{f_2(x)}{V_2^{'}} y_2(x) - \frac{f_3(x)}{V_3^{'}(x)} y_3(x)$$

For a specific numerical example, we take $\frac{f_i}{V_i} = 0.001,\ 1 \le i \le 3,$ and let $f(x) = 0.125 Ib/\min$ for the first 48 hours (2880 minutes), thereafter $f(x) = 0$. We expect due to uniform mixing that after a long time there will be $(0.125)(2880) = 360$ pounds of pollutant uniformly deposited, which is 120 pounds per pond.
Initially, $x_1(0) = x_2(0) = x_3(0) = 0$, if the ponds were pristine. The specialized problem for the first 48 hours is

$$y_1^{'}(x) = 0.001 y_3(x) - 0.001 y_1(x) + 0.125$$

$$y_2^{'}(x) = 0.001 y_1(x) - 0.001 y_2(x)$$

$$y_3^{'}(x) = 0.001 y_2(x) - 0.001 y_3(x)$$

The solution to this system is

$$y_1(x) = e^{-\frac{3x}{2000}} \left(\frac{125\sqrt{3}}{9} \sin\left(\frac{\sqrt{3}x}{2000}\right) - \frac{125}{3} \cos\left(\frac{\sqrt{3}x}{2000}\right) \right) + \frac{125}{3} + \frac{x}{24},$$

$$y_2(x) = -\frac{250\sqrt{3}}{9}e^{-\frac{3x}{2000}}\sin\left(\frac{\sqrt{3}x}{2000}\right) + \frac{x}{24},$$

$$y_3(x) = e^{-\frac{3x}{2000}}\left(\frac{125}{3}\cos\left(\frac{\sqrt{3}x}{2000}\right) + \frac{125\sqrt{3}}{9}\sin\left(\frac{\sqrt{3}x}{2000}\right)\right) + \frac{x}{24} - \frac{125}{3}$$

After 48 hours elapse, the approximate pollutant amounts in pounds are

$y_1(2880) = 162.30,\ y_2(2880) = 119.61,\ y_3(2880) = 78.08.$

It should be remarked that the system above is altered by replacing 0.125 by zero, in order to predict the state of the ponds after 48 hours. The corresponding homogeneous system has an equilibrium solution $y_1(x) = y_2(x) = y_3(x) = 120$. This constant solution is the limit at infinity of the solution to the homogeneous system, using the initial values $y_1(2880) \approx 162.30,\ y_2(2880) \approx 119.61,\ y_3(2880) \approx 78.08.$

Table 1 Computational Estimates on the Amount of Pond Pollution Model After Every 48 Hours and Their Exact Results.

FPP Estimates	FP Exact Results	SPP Estimates	SP Exact Results	TPP Estimates	TP Exact Results
153.261	162.302	116.522	119.614	90.2176	78.0843
272.991	281.661	237.184	240.008	209.825	198.331
392.986	401.667	357.184	360	329.83	318.333
512.79	521.667	476.844	480	450.366	438.333
632.986	641.667	597.183	600	569.831	558.333
752.986	761.667	717.183	720	689.831	678.333
872.79	881.667	836.844	840	810.366	798.333

The following notational system are used in the table.

FPP Estimates	Defines the Computational FirstPond Pollutant Estimates of the Systems of Differential Equations.
SPP Estimates	Defines the Computational SecondPond Pollutant Estimates of the Systems of Differential Equations.
TPP Estimates	Defines the Computational ThirdPond Pollutant Estimates of the Systems of Differential Equations.
FP Exact Results	Defines the First Pond Pollutant Exact Results.
SP Exact Results	Defines the Second Pond Pollutant Exact Results.
TP Exact Results	Defines the Third Pond Pollutant Exact Results.

Note. Figs. 1, 2 and 3 are free hand drawing.

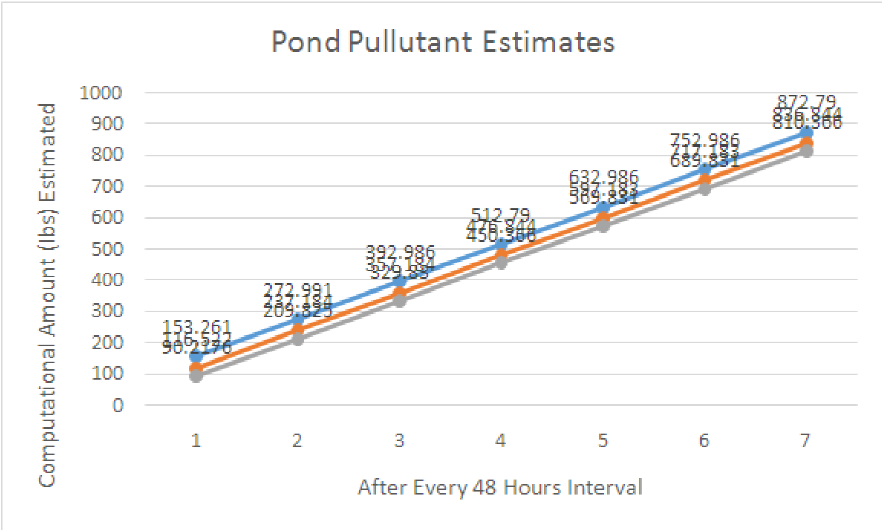

Fig.4 Describes the growing trend together with the amount (Ibs) of pond pollution model after every 48 hours of ponds 1, 2, 3, respectively.

Note Fig. 4 was executed using Microsoft Excel.

6 Conclusions

Table 1 displays the Computational estimates on the amount of pond pollution model after every 48 hours and their exact results. From the first pond pollutant estimates and second pond pollutant estimates, both results yield a good approximation after every forty eight hours (48 hrs.) when compared with their exact results. Again, the results of the third pond pollutant estimates were all greater than their exact results. This is also very good when compared with the results of the first and second pond pollutant estimates. Hence, we have been able to develop a computational approach in form of implicit block multistep method to estimate the amount of pond pollution after a long time (every 48 hours).

Fig.2 describes the pollutant flow rate into pond 1 (1b/min). Since it is observed that the pollutant spreads via the connecting streams to the other ponds.Fig. 4 shows the graphical picture of the growing trend together with amount (Ibs)of pond pollution after every 48 hours of ponds 1, 2, 3, respectively.

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