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Lotka-Volterra Model of Wastewater Treatment in Bioreactor System using 4th Order Runge-Kutta Method

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ABSTRACT

Wastewater treatment is essential to preserve the ecosystem and to ensure water resources are uncontaminated. This paper presents the Lotka-Volterra model of nonlinear ordinary differential equations of the interaction between predator-prey and substrate. The dimensionless ordinary differential equations of the model are solved using the 4th Order Runge-Kutta method (RK4) in MATLAB®. This study discusses the behaviour parameters of predators, prey and substrate. The results are shown graphically for different values of each parameter. Hence, the biological reaction of clean water from the interaction of predator-prey and substrate in wastewater treatment is identified. The higher the concentration of prey, the faster the concentration of substrate reaches 0 with and without the natural death of prey. The clean water will be produced whenever the concentration of prey and the concentration of predator are in balance regardless of the natural death rate. Stability analysis using the Jacobian matrix at the equilibrium point is also performed to determine the stability of the system.

Keywords: *Lotka-Volterra, predator-prey, stability, substrate, wastewater treatment*

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INTRODUCTION

A bioreactor system is a vessel where a chemical process involving active organisms takes place [1]. Organisms, namely bacteria which are directly responsible for converting supplied substrate into non-toxic products, become a basis of a food chain [2]. The biological reactions in bioreactor subsume the predator (P) feeds the prey (X) and the prey (X) consumes the substrate (S) to flourish its concentration respectively. The predator-prey-substrate model is applied to investigate the biological interaction in wastewater treatment. The model states the process of purification which is prey and predator in a substrate must be present to break down solid particles and remove them from the substrate [3].

The wastewater treatment process is to remove contaminants (prey) from wastewater to become effluent liquid [4]. The wastewater treatment is necessary to keep our water sources clean. Hence, it can be safely used for daily activities. The wastewater treatment is made possible with the concept of the predator-prey relationship.

The basic Lotka-Volterra model was proposed in the late 1920s by [5] and [6] where it predicts the oscillatory behaviour in the predator-prey interactions. It involves a pair of differential equations and focuses on predicting predator-prey behaviour in two cultures using experimental and mathematical modelling. They also considered three differential equations of substrate inhibiting predator-specific growth rate models. Furthermore, the Lotka-Volterra model has been explored extensively to study the dynamic behaviour of the model by considering time delay and spatial diffusion [7,8,9]. The model of predator-prey can be solved using various numerical techniques such as the Runge Kutta method [10,11], finite element method [12] and nonstandard finite difference methods [13].

This study highlights the analytical expressions of the model using the RK4. Constant step size is employed in the RK4, and it is very stable in terms of the results. This paper investigates the biological reaction of the prey-predator-substrate interaction in a bioreactor that focuses on the predator, prey and substrate behaviour and analyses the simulation results of predator and prey with various concentrations. Several assumptions have been made to maintain the simplicity of the model. The first assumption is that the bioreactor is adequately well stirred to achieve complete mixing. Next, the pH and temperature are kept constant and the flow of the substrate through the reactor is sufficiently fast to avoid cell growth that occurs on the walls of the reactor [14].

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MATHEMATICAL FORMULATION

The Lotka-Volterra model of predator-prey-substrate equations is defined by Sadikin et al. [1] as in the following Equations 1 until 3:

The concentration of substrate:

$$V\frac{dS}{dt} = F(S_0 - S) - \frac{1}{\alpha_s}\cdot\frac{\mu_x SXV}{K_s + S} \tag{1}$$

The concentration of prey:

$$V\frac{dX}{dt} = -F(X_0 - X) + \frac{\mu_x SXV}{K_s + S} - \frac{1}{\alpha_x}\cdot\frac{\mu_p XPV}{K_x + X} - k_x XV \tag{2}$$

The concentration of predator:

$$V\frac{dP}{dt} = -F(P_0 - P) + \frac{\mu_p XPV}{K_x + X} - k_p PV \tag{3}$$

where V is the volume of the bioreactor, F is the flow rate through the bioreactor, and residence time $\tau = \frac{V}{F}$. The parameters $K_s, K_x, \alpha_s, \alpha_x, \mu_p, \mu_x$ are all positive and S_0, X_0, P_0 are more than or equal to 0 with S is the substrate concentration, X is the prey concentration and P is the of predator concentration. K_s is the Monod constant for prey-substrate interaction, K_x is the Monod constant for predator-prey interaction, α_s is the substrate yield factor or the rate of prey produced versus substrate consumption. α_x is the prey yield factor or the rate of predator produced versus prey consumption, μ_p is the maximum specific growth rate of predator upon prey and μ_x is the maximum specific growth rate of prey upon predators which are constants. The k_x and k_p are the death coefficients of prey and predator, respectively.

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By introducing dimensionless variables for the substrate concentration $\left(S^* = S / K_s\right)$, the prey concentration $\left(X^* = X / (\alpha_s K_s)\right)$, the predator concentration $\left(P^* = P / (\alpha_x \alpha_s K_s)\right)$ and the time $\left(t^* = \mu_x t\right)$ [1]. The system of differential equations 1 until 3 can be written in the dimensionless form as in the following Equations 4 until 6:

$$\frac{d(S^*)}{d(t^*)} = \frac{1}{\tau^*}(S_0^* - S^*) - \frac{S^* \cdot K_s^*}{1+S^*} \tag{4}$$

$$\frac{d(X^*)}{d(t^*)} = -\frac{1}{\tau^*}(X_0^* - X^*) + \frac{S^* \cdot X^*}{1+S^*} - \frac{\mu_p^* \cdot X^* \cdot P^*}{K_x^* + X^*} - k_x^* \cdot X^* \tag{5}$$

$$\frac{d(P^*)}{d(t^*)} = -\frac{1}{\tau^*}(P_0^* - P^*) + \frac{\mu_p^* \cdot X^* \cdot P^*}{K_x^* + X^*} - k_p^* \cdot P^* \tag{6}$$

The parameters used are the dimensionless saturation constant for the prey $\left(K_x^* = K_x / \alpha_s K_s\right)$, the feed concentration $\left(S_0^* = S_0 / K_s\right)$, the dimensionless death coefficient parameters $\left(k_i^* = k_i / \mu_x\right)$, the dimensionless maximum specific growth rate of the predator $\left(\mu_p^* = \mu_p / \mu_x\right)$and the dimensionless residence time $\left(\tau^* = \mu_x \tau\right)$. The values of parameters are $S_0^* = 1000$, $K_x^* = 264$ and $\mu_p^* = 0.96$ with $k_x^* = k_p^*$ [1].

The RK4 method in this paper is written as below [15]:

$$w_{i+1} = w_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$
$$w_i\left(t_0\right) = w_0, \text{ where } i = 1, 2, \ldots, n$$

h is defined as the step-size and $t_i = t_0 + ih$ with the formula
$k_1 = hf\left(t_i, w_i\right)$, $k_2 = hf\left(t_i + \frac{h}{2}, w_i + \frac{k_1}{2}\right)$, $k_3 = hf\left(t_i + \frac{h}{2}, w_i + \frac{k_2}{2}\right)$ and $k_4 = hf\left(t_i + h, w_i + k_3\right)$.

The initial value problem of the equations with the RK4 method is solved using MATLAB®.

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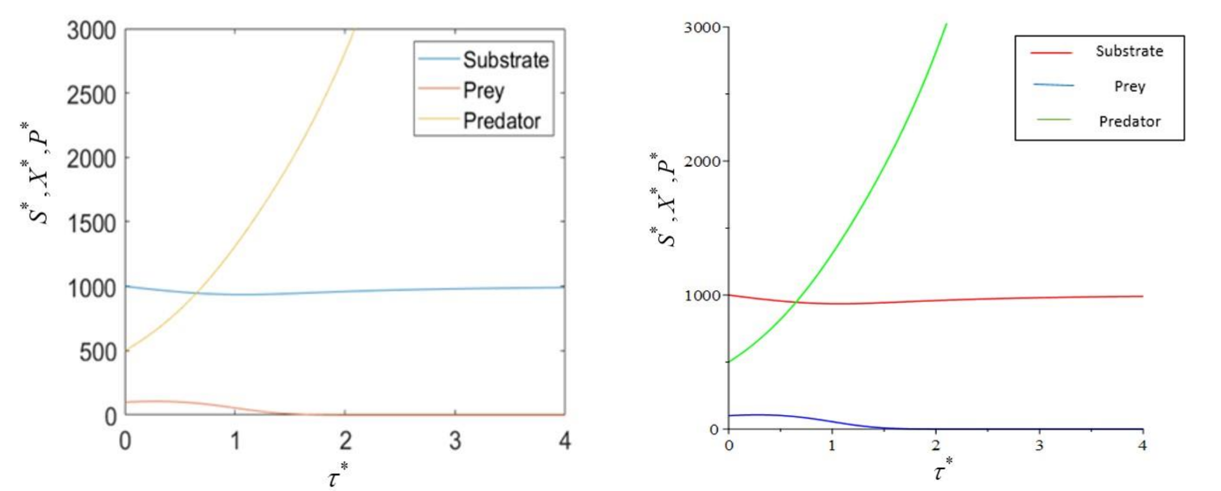
RESULTS AND DISCUSSION

Comparative study for the predator-prey-substrate model with the numerical results of RK4 method using the built-in function in MAPLE software is performed to prove and validate the numerical results obtained using MATLAB® by comparing the concentration pattern on the dimensionless substrate (S^*), prey (X^*) and predator (P^*) against dimensionless residence time (τ^*).



a) MATLAB®

b) MAPLE software

Figure 1: The graphical comparison using (a) MATLAB® and (b) MAPLE software for steady-state predator-prey co-existence solution with no death $\left(k_x = k_p = 0\right)$

Figures 1(a) and 1(b) show the graphical comparison of the RK4 method using MATLAB® and built-in function in MAPLE software respectively. The identical results verify both methods are in agreement with one another. Hence, the numerical results obtained are considered reliable and valid.

Table 1 depicts the steady-state predator washout model with no death is stable when τ^* is in between 1.001 and 1.311. Next, the steady-state predator washout model with natural death present is stable when τ^* is in between 1.111 to 1.581. Lastly, the steady-state predator-prey co-existence model with natural death present is stable when τ^* is in between 1.581 to 1.862 [1].

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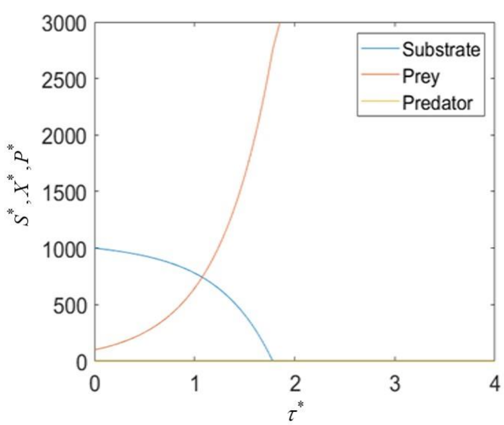
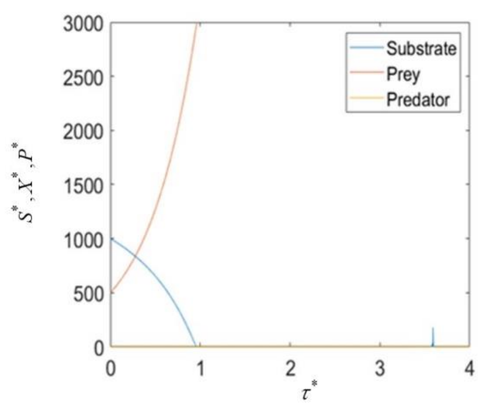
Table 1: The different types of simulation with the value of τ^* and the values of S^*, X^* and P^*

Simulation of the steady-state system	τ^*	Concentration of S^*, X^*, P^*
Predator washout with no natural death	1.156	$S_0^* = 1000, X_0^* = (100, 500), P_0^* = 0$
Predator washout with natural death present	1.346	$S_0^* = 1000, X_0^* = (100, 500), P_0^* = 0$
Predator-prey co-existence with natural death present	1.7215	$S_0^* = 1000, X_0^* = 700, P_0^* = 500$ $S_0^* = 1000, X_0^* = 500, P_0^* = 500$ $S_0^* = 1000, X_0^* = 500, P_0^* = 700$



a) $X^* = 100$ and $P^* = 0$



b) $X^* = 500$ and $P^* = 0$

Figure 2: Steady-state predator washout without death, $k_i^* = 0$ diagrams show the relationship between variation of substrate, predator and prey concentration $\left(S^* = 1000, X^*, P^*\right)$ and residence time $\left(\tau^*\right)$ in a bioreactor

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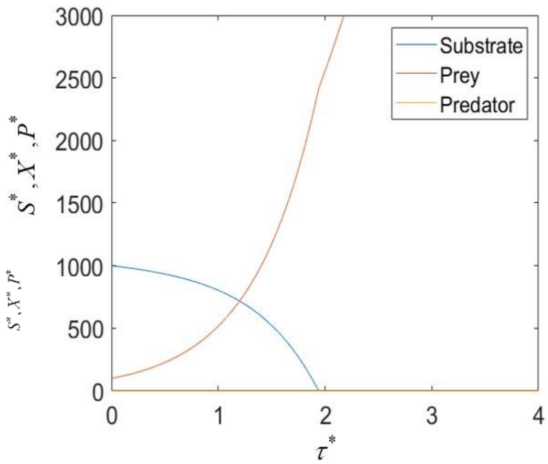
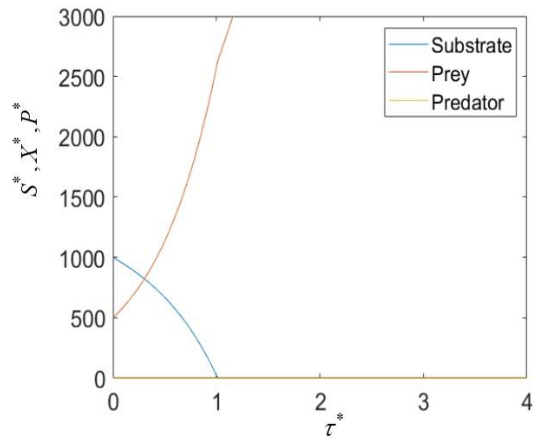


a) $X^* = 100$ and $P^* = 0$



b) $X^* = 500$ and $P^* = 0$

Figure 3: Steady-state predator washout with death, $k_i^* = 0.1$ diagrams show the relationship between variation of substrate, predator and prey $\left(S^* = 1000, X^*, P^*\right)$ and residence time $\left(\tau^*\right)$ in a bioreactor

The results in Figure 2 illustrate the substrate concentration (S^*) decreases as the concentration of prey (X^*) increases over residence time (τ^*). The higher the concentration of prey (X^*), the faster the concentration of substrate (S^*) reaches 0. The prey (X^*) consumes the substrate (S^*) in order to grow and without the predator (P^*) present, the concentration of prey (X^*) will keep increasing over residence time (τ^*). Similar observation occurs to predator washout with the death coefficient of concentration of prey (X^*) is 0.1 as shown in Figure 3. The residence time (τ^*) taken for the substrate concentration (S^*) to reach 0 in Figure 3 is slightly longer because natural death exists for the prey (X^*). No clean water will be present at the end.

As shown in Figure 4, when the concentration of prey (X^*) is 700 and predator (P^*) is 500, the concentration of substrate (S^*) will reach 0 at $0.5 < \tau^* < 1.5$. It is not the best result as there is no substrate (S^*) present at some point in the timeline. When the concentration of prey (X^*) and predator (P^*) both are 500, it gives out the best result because the concentration of substrate (S^*) is always present. Hence, the concentration of prey (X^*) reaches 0 at $1.5 < \tau^* < 2.5$, and the concentration of substrate (S^*) will attain normal over time. When the concentration of

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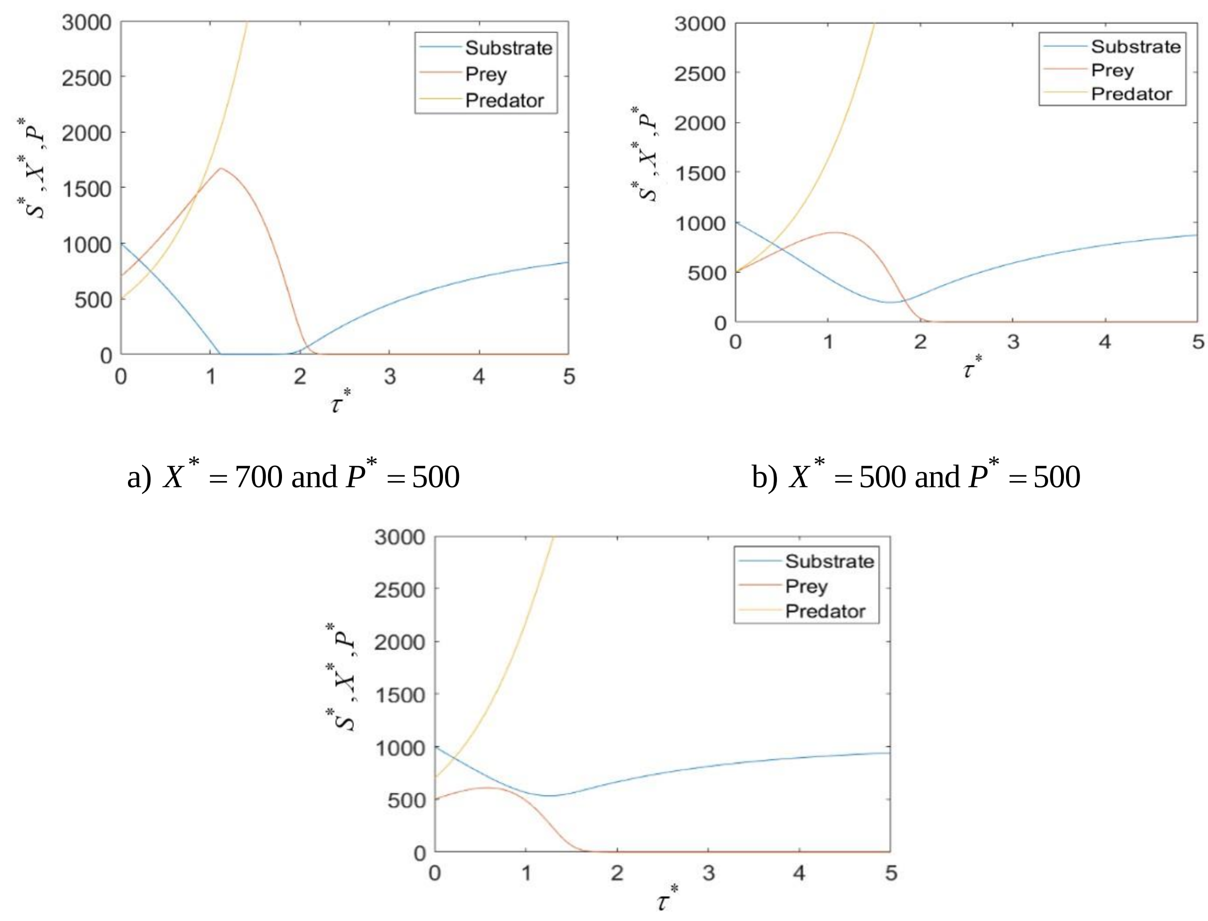
prey (X^*) is 500 and predator (P^*) is 700, it gives out the best result because the concentration of substrate (S^*) always exists. Hence, the concentration of prey (X^*) reaches 0 at 1.0 < τ^* < 2.5, the concentration of substrate (S^*) will attain normal over time. Similar observations were obtained for predator-prey co-existence without death.



a) $X^* = 700$ and $P^* = 500$

b) $X^* = 500$ and $P^* = 500$

c) $X^* = 500$ and $P^* = 700$

Figure 4: Steady-state predator-prey co-existence with death diagram shows the relationship between variation of substrate, predator and prey $\left(S^* = 1000, X^*, P^*\right)$ and residence time $\left(\tau^*\right)$ in a bioreactor

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Analysis of Stability

Finding stability of a controlled system is significant to determine whether the system is stable or unstable. The Jacobian matrix *J* at the equilibrium point of the dimensionless ordinary differential equations 4 until 6 is presented as:

$$J = \begin{pmatrix} \sigma_4 - \dfrac{X^*}{S^*+1} - \dfrac{2000}{3443} & -\dfrac{S^*}{S^*+1} & 0 \\ \dfrac{X^*}{S^*+1} - \sigma_4 & \dfrac{S^*}{S^*+1} - \sigma_3 + \sigma_1 + \dfrac{2000}{3443} & -\sigma_2 \\ 0 & \sigma_3 - \sigma_1 & \sigma_2 + \dfrac{2000}{3443} \end{pmatrix}$$

where $\sigma_1 = \dfrac{24P^* X^*}{25\left(X^*+264\right)^2}$, $\sigma_2 = \dfrac{24X^*}{25\left(X^*+264\right)}$, $\sigma_3 = \dfrac{24P^*}{25\left(X^*+264\right)}$ and $\sigma_4 = \dfrac{S^* X^*}{\left(S^*+1\right)^2}$.

The stability of the system is discussed based on the result of the Jacobian matrix and the eigenvalues, λ, are obtained using MATLAB®. The stability analysis of the equilibrium point is defined according to [16] as described in Table 2.

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Table 2: Stability of equilibrium point

Eigenvalue type	Stability
All Real and positive	Unstable
All Real and negative	Stable
All Real and mixed positive & negative	Unstable
Complex with positive real (+a + b*i*)	Unstable
Complex with negative real (-a + b*i*)	Stable
Complex with imaginary only (0 + b*i*)	Unstable

Table 3 shows the eigenvalues are real numbers with mixed positive and negative. The system is unstable as indicated in Table 2, where having mixed positive and negative real eigenvalues is an essential and sufficient condition of an unstable system. The steady-state equilibrium of the system exists at τ^*.

Table 3: The summary of the stability

System	τ^*	Eigenvalues, λ
Predator washout with no death ($k_x^* = k_p^* = 0$)	1.156	-0.8651, 0.8651, 0.8651
Predator washout with death ($k_x^* = k_p^* = 0.1$)	1.346	-0.7429, 0.6429, 0.6429
Predator-prey co-existence with death ($k_x^* = k_p^* = 0.1$)	1.7215	-0.5809, 0.4809, 0.4809

CONCLUSION

In conclusion, this paper describes the three-level food chain in a bioreactor. The bioreactor contains predator, prey, and substrate with the substrate being the least superior out of all. The parameters' behaviour is observed in different conditions and calculated using the RK4 method. The biological reaction of each variable can be observed on the graph shown. Our findings can be summarised as follows:

- The higher the concentration of prey, the faster the concentration of substrate reaches 0 with and without the natural death of prey.

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- The clean water will be produced when the concentration of prey is maintained at 500, while the concentration of predator is 500 and above regardless of the natural death rate.
- The stability analysis indicates there exists instability in the system.

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AUTHOR'S CONTRIBUTION

Zaileha Md Ali, Ezmir Faiz Mohd Puard and Muhamad Hariz Sudin carried out the research, wrote, provided the theoretical framework and revised the article. Nur Aziean Mohd Idris designed the research, supervised research progress, anchored the review, revisions and approved the article submission.

CONFLICT OF INTEREST STATEMENT

The authors agree that this research was conducted in the absence of any self-benefits, commercial or financial conflicts and declare absence of conflicting interests with the funders.

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