BIODEGRADATION MODEL OF A TOXIC SUBSTANCE

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INTRODUCTION

Industrialization has brought humankind a modern way of living with a lot of comforts. However, industrialization has also brought with it problems such as generation of toxic substances from manufacturing [1]. When not handled properly, toxic substances can spill into the environment leading to contamination.

One of the methods to clean up contamination is through microbial-based processes i.e. biodegradation [1]. However, biodegradation rates vary and thus affect cleanup efforts, remediation, and long-term management [2]. Thus, there is a need to study the rate of contaminant biodegradation.

Classical first-order reaction kinetic equations can be applied in models to simulate sequential degradation reactions of various substances such as radionuclides and of interest in this project, contaminants such as pesticides, chlorinated solvents, and nitrogen species in water [2]. For a toxic substance, the kinetics of its degradation can thus be described by:

$$\frac{dX}{dt} = -kX \qquad [Eq. 1]$$

where X is the concentration (in mg/L) of the toxic substance at any time t and k is the rate constant (positive, in day^{-1}). The rate constant k is usually dependent on temperature T through the Arrhenius equation, but can alternatively be computed as follows:

$$k = -\frac{(T-a)^2}{b} + c \qquad [Eq. 2]$$

where a, b, and c are constants.

In this project, the biodegradation kinetics of a certain toxic substance with $a = 21$, $b = 100$, and $c = 0.81$ is modeled in Python. Specifically, biodegradation was evaluated considering two temperatures: (1) constant and optimal temperature and (2) daily temperature fluctuations from 13 to 30 ºC.

METHODOLOGY

Optimal Temperature for Most Rapid Degradation (File: optimal_temperature.py)

The temperature for most rapid degradation T_{opt} is the temperature at which $Eq. 1$ or the rate of decrease of the toxic substance concentration dX/dt is minimum (or maximum absolute value). To find T_{opt} numerically using Python, k and then dX/dt where computed for various T and X (Figure 1). A graph of dX/dt vs T was then created to verify the existence of a minimum. Finally, T_{opt} was extracted as the T where dX/dt is a minimum.

```
# Create an array of concentrations at 1, 2, and 3 mg/L
X = [1, 2, 3] # mg/L

# Create an array of temperatures from 0 to 50 oC
T = np.linspace(0, 50, 1000)

# Calculate k and dXdt
dXdt = dict()
for Xi in X: # Calculate dXdt for each concentration and temperature
   k = - ((T - a) ** 2) / b + c # Rate constant in 1/day
   dXdt[Xi] = -k * Xi # Rate of degradation of toxic substance, mg/L*day
```

Figure 1. Code snippet for numerical determination of T_{opt}.

The numerical result was compared to the analytical result, which can be obtained by taking the temperature derivative of $Eq. 1$ and setting it to zero (note $dX/dT = 0$ and $X \neq 0$):

$$0 = -k\frac{dX}{dT} - X\frac{dk}{dT} \Rightarrow 0 = -\frac{2}{b}\left(T_{opt} - a\right) \Rightarrow T_{opt} = a \qquad [Eq. 3]$$

Degradation Model at Constant and Optimal Temperature (File: model_constant_Topt.py)

The degradation model ($Eq. 1$ and $Eq. 2$) at the constant optimal temperature T_{opt} was programmed in Python (Figure 2a). The model (a differential equation) was then solved numerically using Scipy Module's "odeint" function (Figure 2b). Lastly, a plot of X vs t was created using the Matplotlib module.

```python
# Model
def model(X, t):
    k = -((T - a) ** 2) / b + c # Compute for the kinetic constant
    dXdt = -k * X # Compute for derivative

    return dXdt
```

(a)

```python
# Solve ODE numerically
# Initial conditions
X0 = 1 # mg/L

# Integration limits
start = 0 # days
end = 7 # days
t = np.linspace(start, end, 1000)

# Get solution
X = scipy.integrate.odeint(model, X0, t)
```

(b)

Figure 2. Code snippets of (a) model creation and (b) numerical integration.

Degradation Model with Daily Temperature Fluctuations (File: model_variableT.py)

The degradation model with daily temperature fluctuations was similar to the previous model, except for an additional equation that models T as a function of time t (Figure 3, function "temp (t)"). This equation was modeled as a sinusoidal function with a period of 1 day, maximum temperature of 30 ºC and minimum temperature of 13 ºC spaced 0.5 days apart (i.e. assumes 30 ºC at 12:00 and 13 ºC at 00:00), and $T = T_{opt}$ at $t = 0$ (ensures similar initial conditions as the first model). An equation that models such a trend is:

$$T = \frac{30 - 13}{2}\sin\big(2\pi(t - \delta)\big) + \frac{30 - 13}{2} + 13 \qquad [Eq. 5]$$

$$\delta = -\arcsin\left(\frac{T_{opt} - 21.5}{1} \cdot \frac{2}{30 - 13}\right)/(2\pi) \qquad [Eq. 6]$$

Similar to the previous model, this model (a differential equation) was then solved numerically using Scipy Module's "odeint" function. Lastly, a plot of X vs t was created using the Matplotlib module.

```python
# model for temperature at time t
def temp(t):
    delta = -np.arcsin((T_opt - 21.5) * 2 / (30 - 13)) / (2 * np.pi)  # Compute for delta, Eq. 6
    T = ((30 - 13) / 2) * np.sin(2 * np.pi * (t - delta)) + (30 - 13) / 2 + 13  # Compute for temperature, Eq. 5

    return T

# Model
def model(X, t):
    T = temp(t) # Compute for the temperature at time t
    k = -((T - a) ** 2) / b + c # Compute for the kinetic constant
    dXdt = -k * X # Compute for derivative

    return dXdt
```

Figure 3. Code snippet of model creation with temperature fluctuations.

RESULTS AND DISCUSSION

Optimal Temperature for Most Rapid Degradation

The result for T_{opt} using the numerical method (Figure 4) via Python is $T_{opt} = 21.02^oC$. This agrees well with the analytical method ($Eq. 3$) at $T_{opt} = a = 21^oC$.

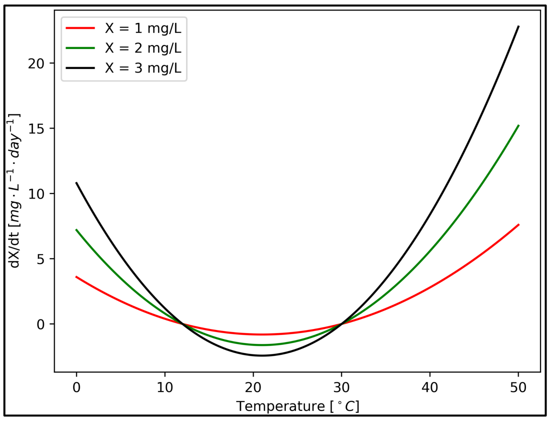


Figure 4. Numerical method for T_{opt} using Python.

Degradation Model at Constant and Optimal Temperature

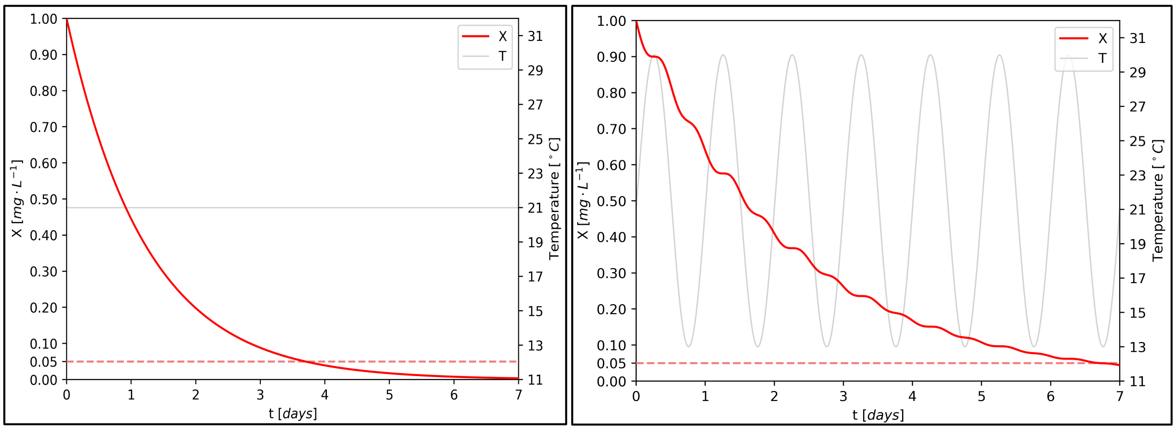
Figure 5a below shows X vs t at a constant temperature of $T_{opt} = 21°C$. The plot resembles an exponential (decay) function, which is the solution of a first-order differential equation. This confirms that proper modelling in Python was performed.

Considering that temperature is constant at T_{opt}, rapid biodegradation of the toxic substance was observed. At approximately $t = 3.8\ days$, 95% of the toxic substance has already biodegraded. Further, at $t = 7\ days$, almost all of the toxic substance has biodegraded.

Degradation Model with Daily Temperature Fluctuations

Figure 5b below shows X vs t with daily temperature fluctuations. The plot slightly resembles an exponential (decay) function with some sinusoidal parts. Initially, rapid biodegradation is observed until around $t = 0.4\ days$ since initially, the temperature was at T_{opt}. However, as the day progresses, biodegradation rate slows down as temperature moves away from T_{opt}. This cycle then continues and repeats each day.

Compared to the model at constant and optimal temperature, biodegradation is slower in this model. 95% of the toxic substance was biodegraded after approximately $t = 6.5\ days$ only vs $t = 3.8\ days$ in the previous model. Further, at $t = 7\ days$, approximately 4% of the toxic substance was still remaining vs almost complete biodegradation in the previous model.



(a) (b)

Figure 5. X vs t at (a) constant $T = T_{opt} = 21°C$ and (b) fluctuating daily T.

CONCLUSIONS

Industrialization has brought with it problems such as generation of toxic substances from manufacturing. When not handled properly, toxic substances can contaminate the environment. One of the methods to clean up this contamination is through microbial-based processes i.e. biodegradation [1]. However, biodegradation rates vary and thus affect cleanup efforts, remediation, and long-term management [2]. Thus, there is a need to study the rate of contaminant biodegradation. In this project, the biodegradation kinetics of a certain toxic substance was evaluated in Python considering two temperatures: (1) constant and optimal temperature and (2) daily temperature fluctuations from 13 to 30 ºC. Results showed that the optimal temperature is at 21ºC. Further, the model with daily temperature fluctuations showed slower biodegradation kinetics compared to the model at the constant optimal temperature. The large discrepancy between the two models highlights the need to use the more complex but more realistic model with daily temperature fluctuations for better decisions/plans for cleanup of toxic substances.

REFERENCES

[1] K. Dubey, K. Pant, A. Pandey and M. Sanroman, Biodegradation of Toxic and Hazardous Chemicals, Boca Raton: CRC Press, 2024.

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[3] Onya Magazine, "Top Water Contamination Disasters That Shook The World," Onya Magazine, 19 April 2023. [Online]. Available: https://www.onyamagazine.com/australian-affairs/top-water-contamination-disasters-that-shook-the-world/. [Accessed 16 May 2025].