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## Study of Dieldrin in Coralville Reservoir

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## Study of Dieldrin in Coralville Reservoir

### Abstract

Using existing experimental data taken over a period of roughly 12 years that documents the concentrations of dieldrin levels in the environment and fatty tissue of the fish, we construct a model of the total dieldrin concentration decline. Comparisons between the experimental data and speculative data can be made using calculus and elements of statistics in order to better understand the movement of dieldrin in the reservoir. Because of the potentially harmful exposure effects of dieldrin to humans as well as the environment, it is important to be able to predict when stability has been restored to the ecosystem.

### Keywords

Dieldrin, Coralville Reservoir, Environmental Pollution

## PROBLEM STATEMENT

Fit a model to the existing data on the concentration of dieldrin in water, sediment, and fish in the Coralville reservoir and analyze its predictions.

## MOTIVATION

Dieldrin is an insecticide originally produced in the late 1940s as an alternative to the infamous DDT. Because of its effectiveness, it was used enthusiastically from the 1950s to the early 1970s. However, it was later observed to pose a significant risk to the ecosystems exposed to it (Kegley, Hill and Orme) and has been linked to the acceleration of the onset of Parkinson's disease in humans (Kanthasamy, Kitazawa and Kanthasamy; Fackelmann). Dieldrin molecules were shown to be exceedingly resilient in the natural biodegradation process (Cooke); moreover, the distribution of the chemical could be magnified by the food chain of a given environment, making it particularly threatening and is now banned throughout most of the world (World Health Organization).

In the 1970s, the concentration of dieldrin in the Coralville Reservoir reached “actionable levels” and commercial fishing was banned. It is important to determine when the natural processes of evaporation, biodegradation, and outflow have successfully restored the reservoir ecosystem back to its natural state so that commercial activities could be resumed. Because there are so many biological variables in the mix of things of this nature, the decline of dieldrin concentrations is not steadily, declining curve and, thus, must be approximated using calculus and elements of statistics.

## MATHEMATICAL DESCRIPTION AND SOLUTION APPROACH

For this project, we assume that the concentration of dieldrin in water  $C_2$  (in  $\mu\text{g/L}$ ) follows the dynamic model given by the differential equation:

$$\frac{dC_2}{dt} = B(A - C_2) \quad (1)$$

where  $A$  and  $B$  are constants. When integrated, equation (1) yields

$$\ln(A - C_2) + C = -B t$$

with  $C$  being an integration constant, which can be further rewritten as:

$$C_2 = -e^{-(Bt+C)} + A \quad (2)$$

giving the concentration as a function of time.

$t$ (yrs)	0	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5	11.5
$C_T$ ( $\mu\text{g/L}$ ) <i>Experimental</i>	.026	.023	.019	.016	.012	.008	.007	.007	.008	.005	.003
$C_T$ ( $\mu\text{g/L}$ ) <i>Predicted</i>	.026	.022	.020	.018	.016	.014	.011	.009	.007	.005	.003

**Table 1:** Total (water plus sediment) concentrations of dieldrin in the Coralville reservoir as a function of time: known experimental values (Schnoor) in row 2 and values predicted by the model in row 3.

The data for the total concentration of dieldrin,  $C_T$ , in the Coralville reservoir (Schnoor) is shown in Row 2 of Table 1 (labeled “experimental”): this is its concentration in water and sediment together;  $C_2$  is some fraction of  $C_T$ . For this reservoir, it is known that  $C_2 = \frac{2}{3}C_T$ . Therefore, Equation 2 can be converted to represent the total concentration as a function of time as follows:

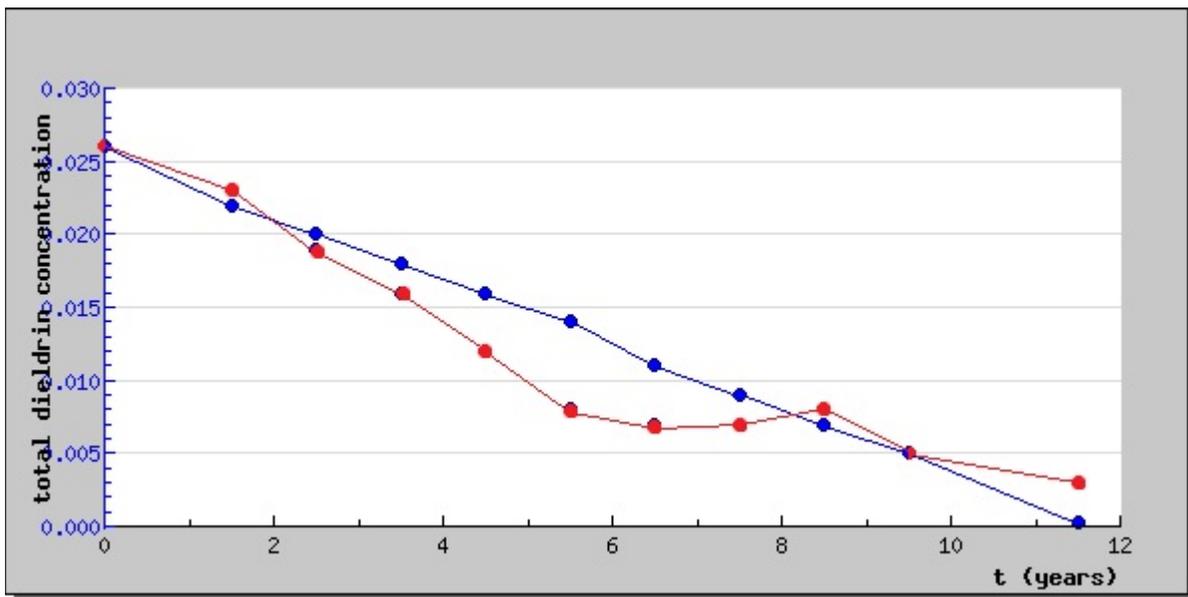
$$C_T = \frac{3}{2}[-e^{-(Bt+C)} + A] \quad (3)$$

and the values of the constants  $A$ ,  $B$ , and  $C$  can be set to best fit the experimental data.

For simplicity of analysis, we let  $C = 0$  and determine the value of  $A$  by using the concentration at  $t = 0$  and the value of  $B$  by using the concentration at  $t = 11.5$  (in order to make sure the prediction fits the data at both the beginning and the end of the given interval). We find that  $A = 1.0173$  and  $B = -0.00145$ . Equation 3 then becomes

$$C_T = \frac{3}{2}[-e^{0.00145t} + 1.0173] \quad (4)$$

and we can use it to predict total concentration values at other points in time. These predictions are shown in Row 3 of Table 1 and a graph comparing the given experimental values with the values predicted by the model is shown in Figure 1 below.



**Figure 1:** A comparison of experimental (red) and predicted (blue) values of  $C_T$  vs. time based on data in Table 1.

For our model, we also assume that the dieldrin concentrations are in equilibrium among the water, sediment, and fish in the reservoir. Thus, its concentration in the fish can be related to its concentrations in the water by the equilibrium relationship:

$$C_F = K_{FW}C_2 \quad (4)$$

where  $C_F$  is in  $\mu\text{g}/\text{kg}$ ,  $C_2$  is in  $\mu\text{g}/\text{L}$ , and  $K_{FW}$  is a fish-water partition coefficient, often taken to be equal to the octanol-water partition coefficient  $K_{OW}$  because octanol is a model compound for fatty tissue.  $K_{OW}$  for dieldrin takes on values ranging from  $\log_{10} K_{OW} = 4.8$  to  $\log_{10} K_{OW} = 5.4$ .

Using Equation 4 with Equation 2, which describes the concentration of dieldrin in water, we find that

$$C_F = K_{FW}[-e^{-(Bt+C)} + A]$$

and furthermore assuming the equivalence of  $K_{FW}$  and  $K_{OW}$  and using the values we found earlier for  $A$  and  $B$  (assuming for simplicity still that  $C = 0$ ), we can obtain two equations representing the high and low extreme estimates for  $C_F$  as follows:

$$C_{F(\text{low})} = 10^{4.8}[-e^{0.00145t} + 1.0173]$$

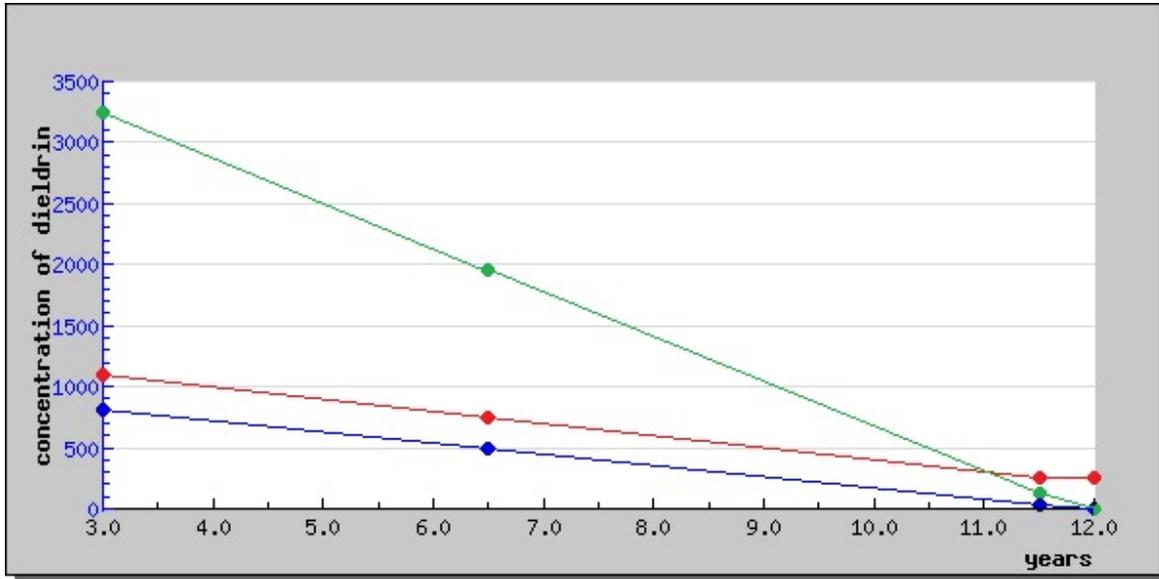
$$C_{F(\text{high})} = 10^{5.4}[-e^{0.00145t} + 1.0173]$$

and use these to predict the concentration of dieldrin in fish for an arbitrary time value.

$t$ (yrs)	3	6.5	11.5	12
$C_F$ ( $\mu\text{g}/\text{kg}$ ) <i>Experimental</i>	1100	750	250	260
$C_F$ ( $\mu\text{g}/\text{kg}$ ) <i>Low Prediction</i>	814	492	31	0
$C_F$ ( $\mu\text{g}/\text{kg}$ ) <i>High Prediction</i>	3240	1959	123	0

**Table 2:** Experimental values for the concentration of dieldrin in fish in the Coralville reservoir along with the high and low predictions from the model.

The known experimental values for  $C_F$  along with the predicted high and low estimates are shown in Table 2 and compared in Figure 2.



**Figure 2:** A comparison of experimental values (red) of  $C_F$  and the low and high extreme values (blue and green, respectively) vs. time based on data in Table 2.

## DISCUSSION

From Figure 1, we see that the experimental values for the total concentration of dieldrin in water and sediment seem to be following the pattern of an inverse exponential curve. The best-fit model, on the other hand, is almost linear along the points considered. This noticeable difference between the experimental and the predicted values can at least partly be attributed to the fact that the integration constant  $C$  in Equation 3 was set to 0. It may be possible to approximate the data more accurately with this model if the constant  $C$  is chosen differently (and the constants  $A$  and  $B$  are adjusted accordingly).

The graph in Figure 2 that shows the concentration of dieldrin in fish supports the idea that the parameter  $C$  needs to be chosen more carefully. We see that while the lower approximation aligns well with the experimental results, being off by an almost constant value at each point, the higher approximation very obviously misses the mark. One would expect the experimental value to lie somewhere between the lower and the higher approximations if these approximations were accurate, but we see that this is not the case for half of the data points: there, the higher approximation dives below the experimental values.

## CONCLUSION AND RECOMMENDATIONS

Overall, it is apparent that the given model with the chosen constants is not a good representation of the experimental data. At any rate, it is clear that setting  $C$  equal to 0 to simplify the model *over*-simplified the model. The shapes of the prediction curves, however, do follow the general shape of the experimental curves, leaving hope that the model may still prove to be accurate with a more appropriate choice of constants.

Thus, a natural extension of this project would be to optimize the constant values for this model and to see how closely it is possible to approximate the data without changing any of the other assumptions. One possible way to do this would be to use one of the middle points in the experimental data for  $C_T$  in addition to the initial and the last point. A more complex solution would be to perform a (non-linear) least squares analysis of the given data assuming the solution has the form of Equation 3 and to optimize the values with an iterative algorithm. Only after comparing the results of such an analysis with the experimental data set would it be possible to determine whether or not an exponential (plus constant) solution is capable of adequately modeling the given data.

## NOMENCLATURE

Symbol	Description	Units
$t$	Time	years
$C_2$	Concentration of dieldrin in the water	$\mu\text{g/L}$
$C_T$	Total concentration of dieldrin in the environment	$\mu\text{g/L}$
$C_F$	Concentration of dieldrin in the fatty tissue of fish	$\mu\text{g/kg}$
$K_{FW}$	Fish-water partition coefficient	
$K_{OW}$	Octanol-water partition coefficient	

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