MATHEMATICAL MODELLING OF RESIDUAL EFFECTS OF DISTILLERY EFFLUENTS APPLICATION BY FINITE DIFFERENCE METHOD

Jyoti U. Devkota¹, Sabita Aryal²

¹ Assistant Professor, Department of Mathematical Sciences, ²Lecturer, Department of Environmental Science and Engineering, School of Science, Kathmandu University, Dhulikhel, Kavre, P.O. Box: 6250, Kathmandu, Nepal.

¹Corresponding Author E-Mail : drjdevkota@ku.edu.np

ABSTRACT

Mathematical Modelling has immense applications in various fields ranging from biomedical sciences to environmental sciences. Here, mathematical modelling has been applied to an environmental pollution, in particular soil pollution problem. Finite difference method has been successfully used to predict the residual effect of potassium (K), an important component of poly-methanated effluents. Further various parameters of the soil such as electro conductivity, pH etc. have been analysed mathematically. Their inter-relationships have also been studied.

KEY WORDS

Finite difference method, Curve fitting, Distillery Effluents, Ordinary Differential Equations, Partial Differential Equations.

INTRODUCTION

Nepal has agriculture-based economy. Sugarcane is used in producing sugar, which is of great commercial importance. In the process of sugar production, molasses, an industrial byproduct is also produced. Alcohol is further produced from this Molasses. Methane and Post Methanated Effluent (PME) are its by-products. 12-15 litres of liquid effluent is produced from each litre of alcohol. Alcohol and Methane gas has commercial use but the P.M.E, which in liquid form has no commercial demand. This wastewater, with high organic and salt load, when mixed with natural water sources without further treatment, poses a serious threat to the aquatic ecosystem. Not only is the cost involved in the treatment of the effluent very high but also the storage and management of the PME can also be very expensive. But it has been seen that PME contains organic matter and nutrients like potassium, nitrogen, and calcium, which are useful as fertilizers (Aryal Sabita, 1998). So it is applied directly to the land as irrigation water as it helps in restoring and maintaining soil fertility, aids to increase soil micro flora, helps improvement in physical and chemical properties of the soil, facilitates increase in the water retaining capacity of the soil and is ideal for sugarcane, maize, wheat and rapeseed production. But higher salt load in PME can affect the production functions of such an agro ecosystem, which may not give sustained yield after a long period of continuous application of effluents. High use of PME increases the K– potassium in the soil.

Motivation

The data of K and other components of the soil are obtained as a result experiment on distillery effluent use in agriculture started at Indian Agricultural Research Institute in 1993 and continued till 1997. In these experiments PME was applied on maize and wheat crops

grown on 5 X 4 plot, five effluent doses (0, 10, 20, 30, 40%) in four replications (Aryal Sabita, 1998). The experiment was conducted in a randomised block design (RBD). In total of 28 applications of PME over a span of three and half years the data on K is noted. In all there were 7 experiments each lasting of six months in which wheat and maize crops were harvested after different concentrations of PME and needed doses of N and P only. In the last six months the land was irrigated with plain water and normal doses of N and P. Thus in the last half year the PME application was discontinued and wheat crop was grown with the application of recommended level of N, P to see the residual effects of accumulated salts in plots previously treated with different levels of PME. The soil previously treated with PME had an excess of K. The experiment lasted for four years. According to (Aryal Sabita, 1998) the data are the results of the experiment conducted on soil of test farm belonging to Mehrauli series classified as sandy loam, non acidic and mixed hyperthermic type of ustochrept. It is well drained, deep and yellowish in colour. The water table is generally deeper than two metres. The percentage of sand, silt and clay in the profile ranged from 46.1-56.8, 29.9-35.6, and 13.3-18.3 respectively. The bulk density varied between 1.459-1.156 g/cc. Percent volumetric moisture retained at field capacity and permanent wilting point ranged from 17.8 –25.8 and 6.6-10.4 respectively. The pH, electrical conductivity (ds/m) and organic carbon (%) ranged from 8.0-8.4, .25-.35 and 0.13-0.45 respectively. Available N, P_2O_5 and K_2O ranged from 138.8-168.2, 5.9-11.9 and 160.3-190.3 kg/ha, respectively in various soil layers.

Problem Description

Figure 1: Sketch of Poly Methanated Effluents generation process.

Objectives

- 1. To Study how the various parameters are linked to one another.
- 2. To analyse statistically various factors influencing K.

3. To apply finite difference method for predicting the values of K.

The data were analysed keeping these objectives in mind. The relationships were looked at mathematically and they confirmed their biological properties. In addition, the interesting properties of the soil and of K, which were normally revealed in the laboratory, were discovered while analysing the data. Thus after some replications of the experiment the results can be obtained by data analysis and modelling which in turn saves time and money, which would have to be spent in the laboratory and field to get the same level of information.

Materials and Methods

Modelling:

Assumptions

Let P.M.E treatment be fixed. Let t denote the time, $t = 1, 2, 3, 4$. Let the ground depth be denoted by d, $d = 1, 2, \ldots, 6$. Let K (t, d) denote the concentration of K at time t and depth d. The change in K depends on the following

- P.M.E concentration in water (control, 10% , 20% , 30% , 40%).
- Time t.
- Depth d.
- The crops (wheat or maize).

Keeping the crop and concentration fixed we find $K = K(t,d)$.

Various parameters of surface and profile of the soil are analysed. The correlation table 1 gives the extent of interrelationships between the Electro conductivity (EC), pH, K of surface and profile of the soil.

Table 1: Karl Pearson's Coefficient of Correlation Between EC, pH and K of Surface and Profile.

From Table 1 we can verify mathematically biological relations between the various parameters.

- 1. EC Surface, Profile and K Surface, Profile is very highly positive correlated. This implies that if K surface increases then the EC Surface, EC Profile, K Profile also increase and visa versa.
- 2. There is a mediocre negative correlation between pH and K for both surface and profile. Thus if one increases the other decreases and visa versa.

Mathematical Model

In order to convert this problem to a finite difference problem intensive data analysis had to be done. K $(t+1, d)$ -K (t, d) $t = 1, 2, ...4$ and $d = 1, 2...6$ that is the change in K for a unit change in time was analysed and showed a very good cubic fit with respect to depth with $.92 < R^2 < 99$, where R^2 *100 is the percentage of variance explained by the model. This can be seen in Figure 3. The closer the R^2 to 1, the more efficient the model.

Or,
$$
\frac{\partial K(t, d)}{\partial t}\Big|_{t \text{ fixed}} = C_1(t) * d^3 + C_2(t) * d^2 + C_3(t) * d + C_4
$$
...(1)

Similarly the data analysis revealed that K $(t + 1, d)$ -K (t, d) is linear with respect to time for fixed depth.

Or,
$$
\frac{\partial K(t, d)}{\partial t}\Big|_{d \text{ fixed}} = \lambda(d)^* t + c \dots
$$
 (2)
Differentiating (2) w. r. t d we get,

$$
\frac{\partial^2 K(t, d)}{\partial d^* \partial t} = \lambda'(d)^* t
$$
.................(3)
Differentiating (1) w. r. t d

3* () ² * () * () * (,) 2 3 2 1 *C t d C t d C t t d ^K ^t ^d* ⁼ ⁺ ⁺ ∂ ∂ [∂] ………………………….(4)

The data analysis revealed that $C_1(t)$, $C_2(t)$, $C_3(t)$, is linear with respect to t with R^2 as high as $R^2 = .99$. Thus $C_1(t) = a_1 * t$, $C_2(t) = a_2 * t$, $C_3(t) = a_3 * t$. Substituting in (4) we get

$$
\frac{\partial^2 K(t,d)}{\partial t^* \partial d} = (a_1 * d^2 + a_2 * d + a_3)t = \lambda'(d)^* t = \frac{\partial^2 K(t,d)}{\partial d^* \partial t}
$$

So, Now the Finite Difference Method can be applied.

We apply central difference operator.

 The idea of finite difference method is to replace the continuous differential operator by a discrete difference operator that is defined on the grid points, Applying Taylor's expansion [2]

$$
u(x+h) = u(x) + hu'(x) + \frac{h^2u''(x)}{2} + \frac{h^3u'''(x)}{6} + O(h^4)
$$

$$
u(x-h) = u(x) - hu'(x) + \frac{h^2u''(x)}{2} - \frac{h^3u'''(x)}{6} + O(h^4)
$$

We obtain the following approximations

- Forward Difference Operator: $\frac{u(x+h)-u(x)}{h}$ + O(h), *h* $\frac{u(x+h)-u(x)}{h}$ + $O(h)$, $u \in C^2$
- Backward Difference Operator: $\frac{u(x) u(x h)}{h} + O(h)$ *h* $\frac{u(x) - u(x-h)}{h} + O(h), u \in C^2$
- Central Difference Operator: $\frac{u(x+h)-u(x-h)}{h}+O(h^2), u\in C^3$ *h* $\frac{u(x+h)-u(x-h)}{h}+O(h^2), u \in$
- Second Difference Operator: $\frac{u(x+h) 2u(x) + u(x+h)}{h^2} + O(h^2)$ $\frac{u(x+h)-2u(x)+u(x+h)}{h}+O(h^2), u \in C^3$

The data of K is analysed with respect of change in time and change in depth.

The figures below show the change in K with change in depth and also the change in K($t + 1$, d)-K(t , d) with respect to depth. Curve fitting has revealed cubic polynomial to be the curve of best fit with .95 $\langle R^2 \times 0.99$, where $R^2 * 100$ is the percentage of variance explained by the model. The closer the R^2 to 1, the more efficient the model.

Figure 2: Change in K with respect to change in depths after different harvests of Maize.

Figure3: Change in K over time with respect to change in depths after different harvests of Maize.

So, taking the data analysis into consideration(we have observed the change in K for a

forward shift in time and change in K for change in depth), we apply the forward central

difference operator. For example for $t = 2$ and $d = 3$ K_t , $d = \frac{\partial K(t, d)}{\partial t} = \frac{K(3, 3) - K(2, 3)}{\Delta t}$ for discrete case. The second derivative is central with respect to depth.

$$
\frac{\partial^2 K(t,d)}{\partial t \partial d} = \frac{K(3,4) - K(3,2) - (K(2,4) - K(2,2))}{2\Delta t \Delta d} = \frac{K(3,4) - K(3,2) - K(2,4) + K(2,2)}{2\Delta t \Delta d}
$$

Applying forward central stencil to the vector K= [K₁₁, K₂₁, K₃₁, K₄₁, K₁₂, K₂₂, K₃₂, K₄₂,

 K_{13} , K_{23} , K_{33} , K_{43} , K_{14} , K_{24} , K_{34} , K_{44}] we get the following

Figure 4: An example of forward central finite difference stencil for time $t = 1, 2, 3, 4$ **and d = 1, 2, 3, 4 corresponding to depths 7.5, 22.5, 37.5 and 52.5 cm respectively.**

Figure 5: The finite difference grid with boundary values for time $t = 1, 2, 3, 4$ and $d =$ **1, 2, 3, 4 corresponding to depths 7.5, 22.5, 37.5 and 52.5 cm**

The Figure 5 shows the translation of the P.M.E problem into a finite difference problem. The boundary values are the data for the depth from 0 to 52.5 cm. Similarly the grids have been made from the depth 0 to 22.5 and the results have been obtained using the finite difference method. The lower and the upper boundary values are substituted from the given data whereas the left and right boundary values are obtained using the cubic fit. Then the middle values of the grid are obtained using the finite difference method.

10 percent P.M.E	$b_0(t)$	$b_1(t)$	$b_2(t)$	$b_3(t)$
$t = 1$	151.670	-9.1648	.1692	$-.0010$
$t = 2$	262.323	-16.041	.3015	$-.0018$
$t = 3$	405.208	-25.802	.4981	$-.0030$
20 percent P.M.E				
$t = 1$	316.600	-15.915	.2736	$-.0015$
$t = 2$	340.469	-20.406	.4045	$-.0025$
$t = 3$	506.110	-30.564	.5894	$-.0036$
30 percent P.M.E				
$t = 1$	467.220	-21.8890	.35770	$-.002$
$t = 2$	473.8980	-13.9960	.11370	$-.0002$
$t = 3$	262.47	-6.76790	.04340	.00003
40 percent P.M.E				
$t = 1$	516.1420	-15.2510	.09320	.0002
$t = 2$	419.7080	-6.6657	$-.09110$.0014
$t = 3$	320.6210	2.27400	$-.27580$.0025

As seen in Figure 2, $K(t, d) = b_0(t) + b_1(t)d + b_2(t)d^2 + b_3(t)d^3$ $K(t, d) = b_0(t) + b_1(t)d + b_2(t)d^2 + b_3(t)d$

Table 2: The values of b_0 , b_1 , b_2 , b_3 for the wheat crop for different concentrations of **PM.E**

As seen from figure 3 the change in K with respect to time is also cubic in d. That is from equation (1)

K(t +1, d)-K(t, d) = C1(t) *d ³ + C2(t) *d 2 + C3(t) *d +C4……………………..(5) where $C_i(t) = a_{0i} + a_{1i}t, i = 1,...4$

The C_i 's are linear with respect to time.

Table 3: The linear coefficients of the parameters of equation (5) for wheat crop.

For example for 10 percent P.M.E, from equation (4) we get

 $\frac{\partial^2 K(t, d)}{\partial t^* \partial d} = 3 * (.0000666 - .001t) d^2 + 2 * (-.00597 + .164t) * d + (-.365 - 8.319t)$ t) d^2 + 2 * (-.00597 + .164t) * d + (-.365 - 8.319t $\frac{\partial^2 K(t, d)}{\partial t^* \partial d}$ = 3*(.0000666 – .001*t*) d^2 + 2*(-.00597 + .164*t*)* d +(-.365 –

For finite difference method a starting model is needed which is provided by curve fitting in this case. And hence the values of K interpolated by cubic fit and finite difference method are very close to one another with very high level of accuracy ($\mathbb{R}^2 \ge 0.95$). It is also seen that in the case of absence of data coupled with the knowledge of some model (from experience) with boundary conditions, the finite difference method functions very well but in the case presence of data, curve fitting and finite difference function equally well, the former being simple and hence faster than the latter.

Conclusion

The relationships were looked at mathematically and they confirmed their biological properties. This can be seen from Table 1, 2 and 3. In addition, the interesting properties of the soil and of K, which were normally revealed in the laboratory, were discovered while analysing the data. Thus after some replications of the experiment the results can be obtained by data analysis and modelling which in turn saves time and money, which would have to be spent in the laboratory and field to get the same level of information. Figure 6 and Figure 7 reveal the relative performance of both the models in interpolating the values of K between the depths 0 to 52 cm for the four harvests of wheat crops.

Acknowledgement

We are very thankful to Dr. Nicole Marheineke, Department of Industrial Mathematics, University of Kaiserslautern, Germany for very inspiring exchange of ideas.

References

- 1. Aryal Sabita, (1998) Residual effect of distillery effluent application on wheat crop. Unpublished Masters of Science thesis submitted to the faculty of the postgraduate school, Indian Agricultural Research Institute, New Delhi.
- 2. Marheineke Nicole, 2005, Department of Industrial Mathematics, University of Kaiserslautern, Germany. Lecture hand out notes on 'Numerics for Differential Equations', Kathmandu University, School of Sciences, Nepal.