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DEVELOPMENT OF MATHEMATICAL MODEL TO OPTIMIZE THE DEGRADATION RATE

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ABSTRACT

Water is an important renewable and reusable natural resource and a factor of subsistence for all the beings as well as a fundamental element for social welfare. Nevertheless, although water is one of the most abundant resources on planet, still about 18-20% of the world's population have no access to potable water. The degradation rate and concentration dependence for removing the impurities lead, to low efficiency of AOP systems, poor data if obtained and increased number of efforts. Significance of concentration, pH, stirrer speed, time, temperature as various independent and response variables involved in this specific operation for the experimental data-based modelling of this operation is discussed. Formulation and development of mathematical models in the form of relationship amongst responses and causes involved including optimization of deduced models in additional to intensity of influence of various independent variables on responses and the nature of relationship has been focused.

KEYWORDS: Degradation, Concentration, Mathematical model, Experimental data, Kinematic analysis.

1. INTRODUCTION

The ever-increasing population and the standard of living has led to unprecedented growth in agricultural and industrial sector causing a quantum jump in freshwater demand. The industry extracts water from aquifers, from surface water or the public drinking water net and after being used for industrial needs, it is discharged as wastewater. On the other hand, water requirement for agriculture, which corresponds to the highest percentage of world's fresh water (i.e., 66%), is increasing even faster to cater to the extensive irrigation programs which are inevitable for sustaining the industrial agriculture of the "Green Revolution".

Most of the industrial activities are executed manually due to the limitations of mechanization such as technological and cost oriented. The industrial activities such as purification of water are manually performed. Operators are working with different types of machine tools and process machines under different environmental conditions. Experimentation design of the purification of water varies suitable for the operators with different constraints.

Various factors depending on the operations are identified so as to optimize the degradation and concentration in this process. There are many approaches to develop /upgrade industrial activities such as kinematic analysis etc. Experimental data-based modelling approach is proposed to save man machine efforts.

2. Causes and Effects of Relationships

Formulation of logic-based model correlating causes and effects is not possible for these types of complex phenomenon. Only approach appropriate for this type of study is experimental data-based modelling. Experimental data-based model correlates the inputs and causes in other words outputs of such activity by formulating the quantitative mathematical modelling. The indices of the equation responses i.e., mathematical model indicate the most influencing inputs. Such correlation indicates the deficiency and the strength of the process which helps to improve the performance of the system. Hence, for improving system/activity performance it is absolutely essential to form such analytical cause – effect relationships conceptualized as EXPERIMENTAL DATA BASED MODELS.

The physiological cost (dependent/ response variable) / response variable) incurred in operation is recorded for different conditions of these independent variables. Productivity of operation is considered as other dependent/ response variable. These variables are also recorded in order to study the effect of independent variables on quality of operation.

Earlier researchers suggested the experimentation theory to know the output of any activity in terms of various inputs of any phenomenon. In fact, it is felt that such an approach is not yet seen towards correctly understanding the operations. This approach finally establishes an experimental data-based model for the phenomenon.

The various inputs in the industrial activity are i) time ii) pH iii) initial concentration iv) Fe v) Temperature vi) H_2O_2 vii) Reactor, viii) stirrer, ix) UV involved in experimentation.

The response variables of the phenomenon are i) Concentration ii) Percentage degradation.

A quantitative relationship is established amongst the responses and inputs. The inputs as well as the corresponding responses are measured. Such quantitative relationships are known as mathematical models. Two types of models are established viz. the model using the concept of least-square multiple regression curve (here after referred as mathematical model). The interest of the operator lies in arranging inputs so as to obtain targeted responses. From the analysis of models, the intensity of influence of various independent variables on the dependent variables and the nature of relationship between independent and dependent variables is determined. Finally, some important conclusions are drawn based on the analysis of models.

3. Improvement of water quality

The variables affecting the effectiveness of the phenomenon under consideration are pollutant concentration, catalyst concentration, time and details of interacting physical system (details of effluents) and environmental (conditions) variables. The dependent or the response variables are- Concentration (C) and Degradation (D).

Dependent and independent variables for the degradation involved water improvement are present in table 1.

Table 1: Independent and Dependent Variables.

Sr. No.	Description	Variables	Symbol	Dimension
1	Time	Independent	Ti	[M0 L0 T1]
2	Initial Concentration	Independent	IC	[M0 L-3T0]
3	pH	Independent	pH	[M0 L0T0]
4	Fe	Independent	Fe	[M0 L-3T0]
5	Temperature	Independent	θ	[M0 L0T0]
6	H2O2	Independent	H2O2	[M0 L-3T0]
7	Reactor	Independent	Re	[M0 L3T0]

8	Stirrer	Independent	St	[M0 L0T-1]
9	UV	Independent	UV	[M1 L2T-3]
10	Final Concentration (FC)	Dependent	FC	[M0 L-3T0]
11	Degradation (De)	Dependent	De	[M0 L0T0]

Establishment of Dimensionless Group of π terms

These independent variables have been reduced into group of π terms. The Equation (18) ahead shows the relationship of Dimensionless π terms of the phenomenon. List of the Independent & Dependent π terms of the are shown in table 2 and table 3:

Table 2: Independent dimensionless π terms.

Sr. No.	Independent Dimensionless ratios	Nature of basic Physical Quantities
01	π1 = [pH]	pH of system
02	π2 = [Fe / H2O]	Pi term related to Fe and H2O
03	π3 = [θ]	Temperature
04	π4 = [(H2O) (Re)]	Pi term related to Re and H2O
05	π5 = [IC / H2O]	Pi term related to IC and H2O
06	π6 = [(St) (Ti)]	Pi term related to Stirrer speed and time

Table 5.3: Dependent dimensionless π terms

Sr. No.	Dependent Dimensionless ratios or π terms	Nature of basic Physical Quantities
01	Z1 = [De]	Degradation

5. Formulation of Field Data Based Model

Six independent π terms ($\pi_{1,}$ $\pi_{2,}$ $\pi_{3,}$ $\pi_{4,}$ $\pi_{5,}$ π_6) and three dependent π terms ($Z_{1,}$ Z_2) have been identified for field study model formulation.

Each dependent π term is a function of the available independent π terms,

Z_1 = function of ($\Pi_{1,}$ Π_2, $\Pi_{3,}$ $\Pi_{4,}$ Π_5, Π_6)

Z_2 = function of ($\Pi_{1,}$ Π_2, $\Pi_{3,}$ $\Pi_{4,}$ Π_5, Π_6)

Where,

$Z_1 = \Pi_{D1,}$ First dependent π term= Td*R/Dr

$Z_2 = \Pi_{D2,}$ Second dependent π term= Pd*Dr/R

The probable exact mathematical form for the dimensional equations of the phenomenon could be relationships assumed to be of exponential form.

(Z) = K* [pH]a,[Fe / H2O]b, [θ]c, [(H2O) (Re)] d, [IC / H2O]e ,[(St) (Ti)]f

6. Model formulation for Degradation

The multiple regression analysis helps to identify the indices of the different π terms in the model aimed at, by considering six independent π terms and one dependent π term. Let model aimed at be of the form,

$$(Z_1)=k_1*[(\pi_1)^{a1}*(\pi_2)^{b1}*(\pi_3)^{c1}*(\pi_4)^{d1}*(\pi_5)^{e1}*(\pi_6)^{f1}]$$

To determine the values of a_1, b_1, c_1, d_1, $e_1$and f_1 and to arrive at the regression hyper plane, the above equations are presented as follows:

$$\Sigma Z_1 = nK_1 + a_1*\Sigma A + b_1*\Sigma B + c_1*\Sigma C + d_1*\Sigma D + e_1*\Sigma E + f_1*\Sigma F$$

$$\Sigma Z_1*A = K_1*\Sigma A + a_1*\Sigma A*A + b_1*\Sigma B*A + c_1*\Sigma C*A + d_1*\Sigma D*A + e_1*\Sigma E*A + f_1*\Sigma F*A$$

$$\Sigma Z_1*B = K_1*\Sigma B + a_1*\Sigma A*B + b_1*\Sigma B*B + c_1*\Sigma C*B + d_1*\Sigma D*B + e_1*\Sigma E*B + f_1*\Sigma F*B$$

$$\Sigma Z_1*C = K_1*\Sigma C + a_1*\Sigma A*C + b_1*\Sigma B*C + c_1*\Sigma C*C + d_1*\Sigma D*C + e_1*\Sigma E*C + f_1*\Sigma F*C$$

$$\Sigma Z_1*D = K_1*\Sigma D + a_1*\Sigma A*D + b_1*\Sigma B*D + c_1*\Sigma C*D + d_1*\Sigma D*D + e_1*\Sigma E*D + f_1*\Sigma F*D$$

$$\Sigma Z_1*E = K_1*\Sigma E + a_1*\Sigma A*E + b_1*\Sigma B*E + c_1*\Sigma C*E + d_1*\Sigma D*E + e_1*\Sigma E*E + f_1*\Sigma F*E$$

$$\Sigma Z_1*F = K_1*\Sigma F + a_1*\Sigma A*F + b_1*\Sigma B*F + c_1*\Sigma C*F + d_1*\Sigma D*F + e_1*\Sigma E*F + f_1*\Sigma F*F$$

After substituting these values in the equations, one will get a set of 7 equations, which are to be solved simultaneously to get the values of K_1, a_1, b_1, c_1, d_1, e_1 and f_1.The above equations can be verified in the matrix form and further values of K_1, a_1, b_1, c_1, d_1, e_1 and f_1 can be obtained by using matrix analysis.

$Z_1=W_1 \times X_1$

Here,

W_1 = 7 x 7matrix of the multipliers of K_1, a_1, b_1, c_1, d_1, e_1 and f_1

P_1 = 7 x 1 matrix of the terms on L H S and

X_1 = 7 x 1 matrix of solutions of values of K_1, a_1, b_1, c_1, d_1, e_1 and f_1

Then, the matrix obtained is given by,

Matrix

$$\begin{bmatrix} Z_1 \\ A \\ B \\ C \\ D \\ E \\ F \end{bmatrix} = \begin{bmatrix} n & A & B & C & D & E & F \\ A & A^2 & BA & CA & DA & EA & FA \\ B & AB & B^2 & CB & DB & EB & FB \\ C & AC & BC & C^2 & DC & EC & FC \\ D & AD & BD & CD & D^2 & ED & FD \\ E & AE & BE & CE & DE & E^2 & FE \\ F & AF & BF & CF & DF & EF & F^2 \end{bmatrix} \begin{bmatrix} K_1 \\ a_1 \\ b_1 \\ c_1 \\ d_1 \\ e_1 \\ f_1 \end{bmatrix}$$

In the above equations, n is the number of sets of readings, A, B, C, D, E and F represent the independent π terms $\pi 1$, $\pi 2$, $\pi 3$, $\pi 4$, $\pi 5$ and $\pi 6$ while, Z1 matrix represents, dependent π term.

Substituting the values of A, A^2, BA, CA…..…up to F^2 in the above matrix (Refer Annexure), value of constant K_1 and indices a_1, b_1, c_1, d_1, e_1 and f_1 are evaluated by taking the inverse of matrix W_1 and multiplying with Z_1 matrix as shown.

$$\begin{bmatrix} -4.12442 \\ -1.9506 \\ 9.637945 \\ -10.2345 \\ -0.43989 \\ -1.12826 \\ -9.80436 \end{bmatrix} = \begin{bmatrix} 60 & 27.97561 & -137.823 & 148.8866 & 6.791391 & 16.02128 & 159.1729 \\ 27.97561 & 13.30127 & -64.2842 & 69.41986 & 3.153294 & 7.483346 & 74.21597 \\ -137.823 & -64.2842 & 318.8836 & -342 & -15.969 & -36.4329 & -365.628 \\ 148.8866 & 69.41986 & -342 & 369.4535 & 16.85245 & 39.7559 & 394.9784 \\ 6.791391 & 3.153294 & -15.969 & 16.85245 & 1.069863 & 1.5123 & 18.01676 \\ 16.02128 & 7.483346 & -36.4329 & 39.7559 & 1.5123 & 4.579172 & 42.50257 \\ 159.1729 & 74.21597 & -365.628 & 394.9784 & 18.01676 & 42.50257 & 425.7283 \end{bmatrix} \begin{bmatrix} K_1 \\ a_1 \\ b_1 \\ c_1 \\ d_1 \\ e_1 \\ f_1 \end{bmatrix}$$

$K_1 = -0.7771$, $a_1 = -0.1017$, $b_1 = 0.1052$, $c_1 = 0.0307$, $d_1 = 0.2745$, $e_1 = 0.0598$ and $f_1 = 0.3295$

Taking antilog of K

Antilog (-0.7771) = 0.1670

The exact form of model obtained is as under:

$(Z_1)=0.1670*(\pi_1)^{-0.1017}*(\pi_2)^{0.1052}*(\pi_3)^{0.0307}*(\pi_4)^{0.2745}*(\pi_5)^{0.0598}*(\pi_6)^{0.3295}$ (5)

(Z_1) =

$(\mathrm{De})=0.1670*[\mathbf{pH}]^{-0.1017}[\mathbf{Fe/H_2O}]^{0.1052}[\boldsymbol{\theta}]^{0.0307}[\mathbf{(H_2O)(Re)}]^{0.2745}[\mathbf{IC/H_2O}]^{0.0598}[(\mathrm{St})(\mathrm{Ti})]^{0.3295}$

(6)

7. RESULT AND DISCUSSION

The results obtained from the experimentation mathematical model is developed to form the correlation between the experimental inputs and the output. The reading obtained from the experimentation and the calculated from the developed mathematical model is in close agreement as shown in the table 3. This show the developed mathematical model can be used for predicating the further results from any new inputs.

Table 3: Comparison of Experimental calculated values and Mathematical Model Equation base values.

Sr. No.	Dependent Variable Degradation			
	Calculated from Mathematical Model	Experimental Observation	Error = Experimental Observation - Calculated Value	Percentage Error
1	0.548	0.4437	-0.1047	-23.5992
2	0.689	0.6837	-0.0054	-0.7900
3	0.788	0.8613	0.0738	8.5649
4	0.866	0.9380	0.0721	7.6901
5	0.911	0.9720	0.0610	6.2775
6	0.610	0.5570	-0.0527	-9.4597
7	0.766	0.7737	0.0075	0.9750
8	0.876	0.9257	0.0500	5.4054
9	0.963	0.9700	0.0073	0.7532
10	1.013	0.9823	-0.0305	-3.1070

1. The absolute index of π_6 is the highest Viz. 0.3295. Thus, the term related to specification of stirrer speed and time involved are the most influencing π term in this model. The value of this index is positive indicating that the degradation activity (Z_1) is directly proportional to term related to the specification of stirrer speed and time involved, i.e. π_6, indicates that more time is required for degradation.
2. The absolute index of π_3 is the lowest Viz. 0.0307. Thus, the term related to temperature is the least influencing π term in this model. The value of this index is positive indicating that the degradation (Z_1) is directly proportional to the term related to temperature [π_1]. With the temperature increases as [π_1] increases.
3. As it may increase the kinetic energy and stimulating molecules for more degradation.
4. The sequence of influence of other independent π terms present on this model is $\pi_{4,}$ π_5 & π_2 having absolute indices as 0.2745, 0.0598 & 0.1052 in the reducing order respectively.

The degradation activity (Z_1) is inversely proportional to the term related to pH [π_1] with the index as -0.1017. With the increase in pH the degradation is reduced.

Similarly, the time of AOP activity (Z_1) is directly proportional to the term related to the H2O and Re [π_4] with the index as 0.2745, increasing the degradation with the increase in H2O and Re capacity.[284]

The degradation (Z_1) is directly proportional to the term related to IC and H2O [π_5] with the index as 0.0598 indicates that in the proper initial concentration, improve the degradation rate effectively.[285]

Similarly, the time of face drilling activity (Z_1) is directly proportional to the term related to the Fe and H2O [π_2] as the Fe increases degradation increases with the index as 0.1052.

CONCLUSION

Interpretation of model carried out for studying order of influence of various inputs (causes) on outputs (effects), relative influence of causes on effect and interpretation of curve fitting constant. The influence of each individual independent variable on response variable is analysed for face drilling. Values computed by experimental observations and values computed by mathematical models are justified by calculating their respective mean values and standard errors of estimation.

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