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STOCHASTIC MODELING AND OPTIMIZATION OF PROCESS PARAMETER OF A COAGULATION PROCESS IN WATER TREATMENT USING A HYBRID COAGULANT BY RESPONSE SURFACE METHODOLOGY

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ABSTRACT

Design of experiment uses a series of structured analytic method to investigate the relation between parameters and the responses. The particular technique used in this study is response surface methodology. Using the DOE approach, a mathematical based model was developed to study the response prediction. Effectiveness of important process parameters Al/Si molar ratio, OH/Al molar ratio, pH and dosage were determined, optimized and modeled successfully. Significant quadratic polynomial models were obtained.

Key words: PAlSiC, Hybrid coagulant, Coagulation, Turbidity, RSM.

INTRODUCTION

Statistics is a branch of mathematics used extensively in natural science and also in the engineering field as well as in social science, physics and computing. Response surface methodology will be used as a technique for the statistical study. The primary focus of this study will be on predicting the response of a process by statistical means. Statistical approach here refers to an empirical method of describing the relationship between the input factors (parameters) as to how far their influence ranges on the output (responses). It is a mathematical evaluation of signifying the relationship of the parameters to the responses[1].

A general objective for a statistical study is to investigate causality especially to correlate the effect of changes in the parametric values to the responses. It is most helpful to construct a model, which provides a mathematical representation of the given situation for most of the statistical based investigation[2].

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In general, the statistical approach can be divided into three categories:

(1) Mathematical model

(2) Statistical model

(3) Empirical model

Mathematical model

A mathematical model can be described as a theoretical model that uses mathematical language to explain the behavior of a system. Among the forms of a mathematical model are game theory model, differential equation and dynamic system. However, mathematical model are not just limited to these alone. Mathematical model is able to overlap with other models involving an array of abstract structure.

Statistical model

A statistical model normally contains one or more systematic components as well as a random (or stochastic) element[2]. The random element is sometimes referred to as noise. This element arises for various reasons and it is sometimes helpful to differentiate between:

(1) Measurement error

(2) Natural random variability

In the engineering point of view, statistical analysis can be regarded as extracting information about the signal in the presence of noise.

Empirical model

An empirical model can also be referred to as a regression or ANOVA model whereby it aims to capture some sort of smooth average behavior in the long run. The advantage of this model (or in some cases seen as the disadvantage) is that it is not based on highly specific subject-matter consideration[3].

An empirical model is developed to understand the factors that contribute to a process and how they affect each other as well as the output.

An empirical model can be built to explain the existing situation by using the existing data related to it. The empirical model consists of a function that fits the data. A matter to note here is that empirical model cannot be used to explain the system. It can only be used to predict and estimate behavior where data does not exist.

Objectives

(1) Develop an empirical model for Turbidity removal of a hybrid coagulant.

(2) Check the consistency between the mathematical models with actual experimentation data.

(3) To be able to predict the output of the response based on the parametric values.

EXPERIMENTAL

Materials and methods

Preparation of synthetic turbid water

Synthetic turbid water for the jar tests was prepared by adding kaolin clay materials to water. About 30 g of the kaolin clay materials was added to 1 liter of water. The suspension was stirred for about 1 hour to achieve a uniform dispersion of clay particles. Then it was allowed to settle for at least 24 hours for complete hydration of the clay materials. The supernatant suspension of synthetic turbid water was added to the sample water to achieve the desired turbidity just before.

Preparation of coagulants

The 40 mL of 0.25 M aluminium solutions (prepared from aluminum chloride hexahydrate) were taken in 9 beakers, then 2.2 mL, 3.3 mL and 6.7 mL of 0.3 M polysilicic acid solution was added in each set of 3 beakers respectively to make corresponding 15, 10 and 5 molar ratio of Al/Si. Again, after 5 minutes of mixing, 30 mL, 40 mL, and 50 mL of 0.5M NaOH solution was added drop wise to each set of 3 beakers to make 1.5 to 2.5 OH/Al molar ratios, respectively. Final volume was maintained to 100mL by adding water. Thus obtained final volume of 100 mL in each beaker contained the different Al/Si and OH/Al molar ratio with constant aluminum concentration. This process of preparation of coagulant by polymerization is called co-polymerization technique[4].

Methods-Coagulation method

Coagulation test were performed using the synthetic turbid water samples. The initial turbidity of water sample was 11.3 NTU. All coagulation experiments were conducted in 1L glass beakers using conventional jar test apparatus. 500 mL of water sample to be treated was taken in separate beakers. The coagulants having 3 different Al/Si and OH/Al molar ratios had been added to make 1 mg/L, 2 mg/L and 3 mg/L dosage. Fast mixing was set for 10 min, followed by slow mixing for 20 min. Settlement time for the formation of floc was set to 20 min. After the settlement of floc particles, the supernatant liquid was withdrawn for the measurement of residual turbidity. To study the effect of pH, the pH of sample was varied to 5 and 9. Percentage removal of turbidity was calculated by using the following equation,

$$\% \text{ Removal} = (T_1 - T_2)/\, T_1 \text{ X } 100$$

Where, T_1 = Initial turbidity and T_2 = Final turbidity.

Turbidity in solution was measured by Nephlometric turbidity meter. The supernatant solution after coagulant treatment was carefully taken for turbidity measurement.

Design of experiment

For this project, response surface methodology (RSM) was used to develop the mathematical model in order to study the effect of the parameters on the response. From RSM itself, central composite design (CCD) method will be used to develop the matrix for modeling. CCD is known as one the primary design techniques in RSM. This technique is used to build a second order model (quadratic model) and commonly used for process optimization[1]. For this experimental study, DESIGN EXPERTS VERSION 8.0.7.1, software was used to conduct the RSM. Before proceeding with the experiment, we must first identify the high and low value of the parameters that are selected to be used for this experimental study. The parameters under investigation here are Al/Si ratio, OH/Al, pH and Dosage.

Preparation of doe matrix

Once the responses, factors and levels have been selected, the next step is to design the experimental runs. After the parameters and the values input into the software, a DOE model will be automatically generated with specific number of runs coupled with specific parametric settings. In this case, 30 runs were generated as shown in Table 1.

Table 1: Experimental layout for response surface

Run No.	Al/Si	OH/Al	pH	Dosage (mg/L)
1	5	1.5	5	1
2	15	1.5	5	1
3	5	2.5	5	1
4	15	2.5	5	1

Cont…

Run No.	Al/Si	OH/Al	pH	Dosage (mg/L)
5	5	1.5	9	1
6	15	1.5	9	1
7	5	2.5	9	1
8	15	2.5	9	1
9	5	1.5	5	3
10	15	1.5	5	3
11	5	2.5	5	3
12	15	2.5	5	3
13	5	1.5	9	3
14	15	1.5	9	3
15	5	2.5	9	3
16	15	2.5	9	3
17	5	2	7	2
18	15	2	7	2
19	10	1.5	7	2
20	10	2.5	7	2
21	10	2	5	2
22	10	2	9	2
23	10	2	7	1
24	10	2	7	3
25	10	2	7	2
26	10	2	7	2
27	10	2	7	2
28	10	2	7	2
29	10	2	7	2
30	10	2	7	2

Table 2: High and low values of the design parameters

Parameters	Low value	High value
Al/Si ratio	5	15
OH/Al ratio	1.5	2.5
Ph	5	9
Dosage	1 mg/L	3 mg/L

Table 1 shows the parameters and also the high and low values. Based on the runs given with the specific parametric values, the experiment was carried out and the corresponding turbidity removal efficiency values taken were re-entered into the matrix.

RESULTS AND DISCUSSION

ANOVA was used for analyses of the data. The quality of fit polynomial model was expressed by the coefficient of determination R^2 and its statistical significance was checked by F test.

Model terms were evaluated by the P value with 95% confidence level. Three dimensional plots and their respective contour plots were obtained based on the effects of four factors at three levels. Equation (1) presents the models for turbidity removal efficiency (%). The quadratic model statistical results for turbidity removal were summarized as follows:

Std. dev.	0.96
R-Squared	0.9924
Mean	82.35
Adj R-Squared	0.9852
C.V.%	1.17
Pred R-Squared	0.9503

The model F-value of 139.36 implies the model is significant. There is only a 0.01% chance that a "Model F-Value" this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicate model terms are significant. In this case A, B, D, AB, AD, A2, C2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant.

Turbidity removal efficiency = -48.52874 -1.08273 * Al/Si +1.70698 * OH/Al +37.18702 * pH + 6.78331 * DOSAGE +0.35600 * Al/Si * OH/Al +0.044875 * Al/Si * pH +0.26700 * Al/Si * DOSAGE -0.42875 * OH/Al * pH -0.46000 * OH/Al * DOSAGE +1.87500E-003 * pH * DOSAGE -0.063042 * Al/Si^2 +0.79579 * OH/Al^2 -2.61026 * pH^2 -1.14105 * $DOSAGE^2$

They show a high reliability in the estimation of turbidity removal efficiency. A high R^2 value ensures a satisfactory adjustment of the quadratic model to the experimental data. In optimizing a response surface, an adequate fit of model should be achieved to keep away from poor outcome. It also demonstrate that response surface quadratic model for our parameter were significant at the 5% confidence level since P value was less than 0.05. The "Pred R-Squared" of 0.9503 is in reasonable agreement with the "Adj R-Squared" of 0.9852.

"Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. In this we get 43.768 indicates an adequate signal. This model can be used to navigate the design space.

Three dimensional plots

The response surface plots obtained form the software provide a three dimensional view of the turbidity removal efficiency with different combination of independent variable. Some of the interaction effect were shown in following Figures.

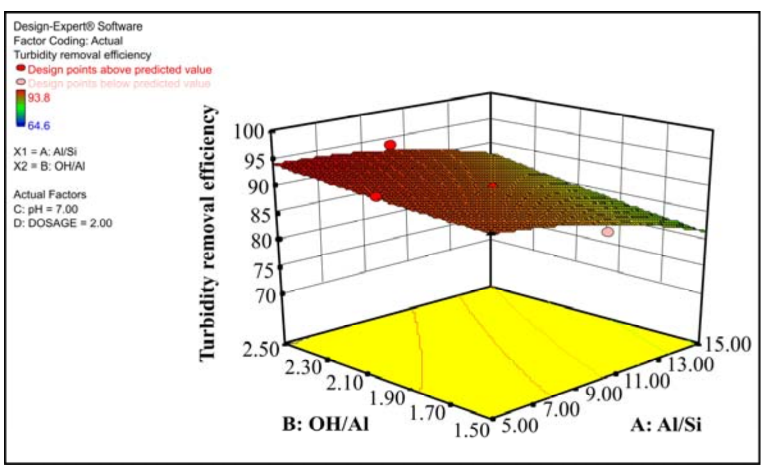

Fig. 1: Interaction between Al/Si and OH/Al

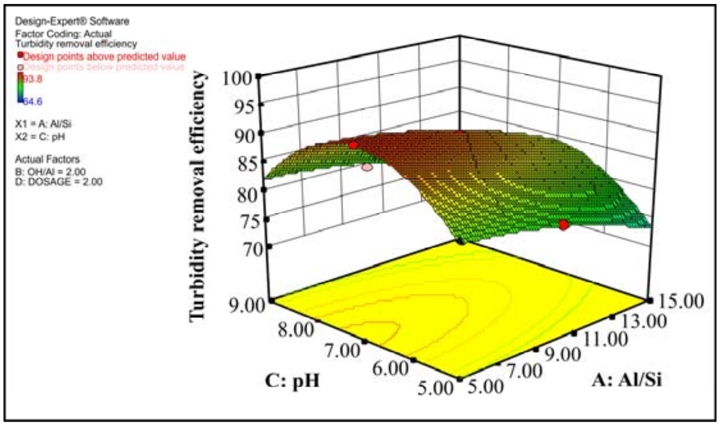

Fig. 2: Interaction between Al/Si and pH

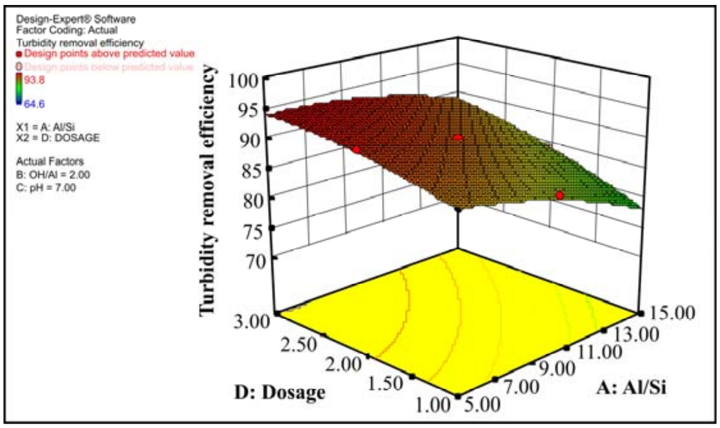

Fig. 3: Interaction between Al/Si and dosage

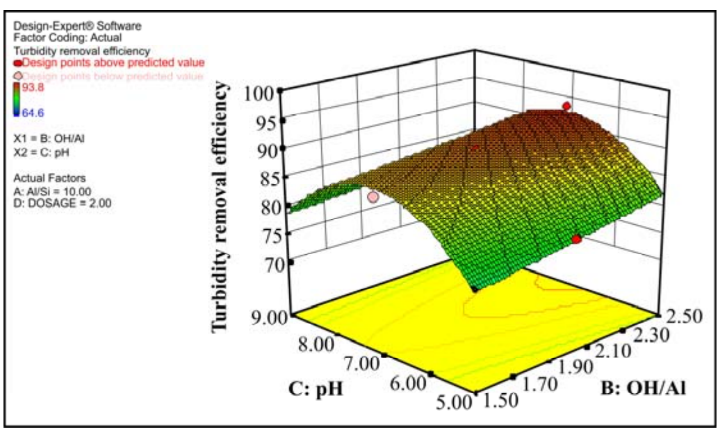

Fig. 4: Interaction between OH/Al and pH

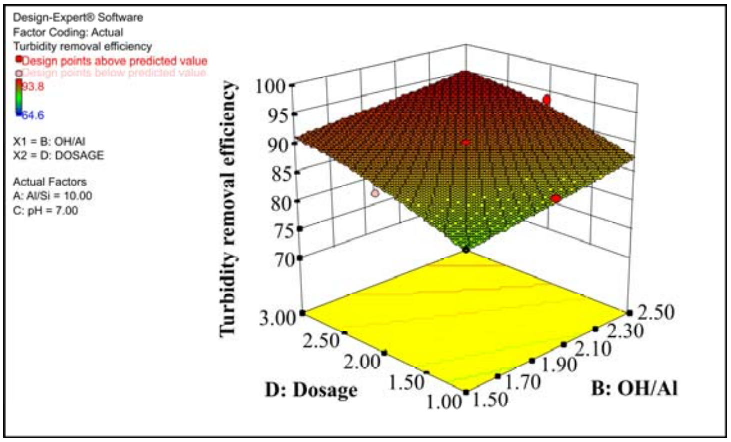

Fig. 5: Interaction between OH/Al and dosage

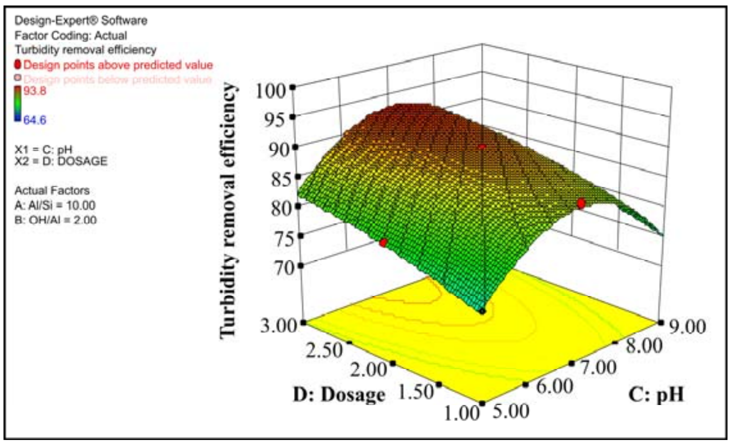

Fig. 6: Interaction between pH and dosage

Optimization and validation experiment

Optimized condition under specified constraints were obtained for highest desirability at Al/Si molar ratio 7.57, OH/Al molar ratio 2.45, pH 6.60 and dosage 2.45. Under this condition, 94.27% turbidity removal was predicted based on desirability function of 1.00. In order to confirm the accuracy of the predicted model and reliability of optimum combination, an additional experiment was carried out at optimum condition. The experimental value 93.4% was found to agree well with predicted 94.27%. The low error in the experimental and predicted value indicates good agreement of the results achieved from models and experiments. These results confirm that RSM is a powerful tool for optimizing the operational condition for turbidity removal in coagulation process.

CONCLUSION

In this study, response surface methodology is used to investigate the relationship between various parameters with the turbidity removal efficiency. The parameters studied here are Al/Si ratio, OH/Al ratio, pH and dosage. From this experimental study, an empirical model was developed from the statistical study. As for the optimization, it can be observed that the deviation error between the observed and the optimized is within acceptable range except for one which can be dismissed due to human error. This shows that the optimization exerts a high level of confident in getting the optimal responses.

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