Global Journal of Engineering Science and Research Management

MODELING AND OPTIMIZATION OF THE RATE OF COAGULANT IN WATER TREATMENT PLANT BY RESPONSE SURFACE METHODOLOGY (RSM)

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KEYWORDS: Modeling, aluminum sulfate, colloidal turbidity, temperature, complete alkalimetric title.

ABSTRACT

Coagulation is one of the most important steps in water treatment process. The main difficulty is to determine the optimal dose of coagulant injection according to the characteristics of the raw water. A bad control of this process can lead to a significant increase in operating costs and failure to comply with the objectives in term of treated water quality.

Aluminum sulfate $Al_2 (SO_4)_3,18H_2O$ is the coagulant the most generally used. The determination of the dose of coagulant is done using jar test .Nevertheless; this experience has the disadvantage of having a long time delay and does not allow an automatic control of the process of coagulation.

Before modeling the coagulation phenomena, we first conducted a study of screening of all parameters that could influence there.

The objective is, therefore, to model the rate of aluminum sulfate with the parameters that have the most influence such as: Colloidal Turbidity (CT), Temperature (T) and Complete Alkalimetric Title (CAT).
We finally found a full degree polynomial model which is therefore given explicitly by the form:

$$Y=b_0+\sum_{i=1}^{k} biXi+\sum_{i=1}^{k} biiXi^2+\sum_{i=1\ ,j=2et\ i\#j}^{k} bijXiXj$$

Y: response of the model
Xi: variables in the model
bi: model coefficients

The final model explains perfectly the phenomenon studied (R^2=0.998), indicating the reliability of the methodology .The results of this study of modeling and optimization are of great importance for the proper management of the water treatment plant since for each tested sample, the calculated rate is very close to the experimental one.

INTRODUCTION

Aluminum sulphate is regarded as the most used coagulant in water treatment given its many advantages includes: low cost, high efficiency particularly in low doses, low toxicity and high availability. (Memento technique de l'eau, tome 1, Degremont – , 1989).On the other hand, it has some disadvantages:

- ✓ Limited coagulation pH range: 5, 5 to 6, 5.
- ✓ Possibility to obtain residual aluminum levels in treated water exceeding acceptable limits if the process is not well controlled.
- ✓ Fragility of alum flocs produced especially in the case of low mineralization. (Gebbie, 2001)

So, these disadvantages can lead to a significant increase in operating costs and failure to achieve the objectives in term of treated water quality. (A.BAZER-BACHI, 1990).

Coagulation is the process in which the negatively charged suspended particles that are present in water in a stable suspension are destabilized. (Freese, 2009).Destabilisation could be achieved along by adding relatively large amounts of cations (Al^{3+} and Fe^{3+}) that interact specifically with negative colloids and neutralise their charge. (Jinming Duana, 2003)Many factors influence its performance, including pH and alkalinity of the suspension, turbidity of the raw water, coagulant dose, organic contents and others (Gurusamy Annadurai, 2004)

Very few studies are conducted to predict the dose of the coagulant using the response surface method:

(A.BAZER-BACHI, 1990)have studiedthe influence of certain parameters on the efficiency of coagulation using aluminum sulfate. The modelisation was divided in two sub-groups:

-a « CALME » model, which fitted very well, showed the primordial influence of the temperature and organic matters, and then of the turbidity. Removal of resistivity was not advisable, as this parameter showed strong interactions with turbidity and organic matters-a « CRUES » model showed the primordial role of the turbidity followed by the temperature and then by organic matters.

(A . L . AHMAD, 2005)have chosen a central composite design (CCD) to explain the effect and interaction of three factors: coagulant dosage, flocculent dosage, and pH.(Shahin Ghafari, 2009)have developed a quadratic models by application of response surface methodology for the four responses: chemical oxygen demand (COD), turbidity, color and total suspended solid (TSS) to optimize coagulation-flocculation.

(Trinh & Kang, 2010)were applied the response surface method and experimental design as an alternative to conventional methods for the optimization of coagulation tests. They have studied, the removal efficiencies of turbidity and total organic carbon (TOC) using a second-order functions of two factors, such as alum dose and coagulation pH.

(Jian-Ping Wang, 2011) have employed a novel approach with a combination of response surface methodology (RSM) and uniform design (UD) to evaluate the effects and interactions of three main influential factors, coagulant dosage, flocculant dosage and pH,

(Xian Liu, 2012)have carried out a study about the performance of coagulation–flocculation (CF) process using iron-based coagulants which is optimized by response surface methodology (RSM).

Optimum alum doses are commonly determined using jar tests; however, of the length of time it takes to conduct it, they cannot be used to respond to rapid changes in raw water quality (Holger R. Maier, 2004).

Viewing these drawbacks, we decided to carry out a mathematical model able to predict availably alum dose including raw water quality parameters as the inputs, and alum dose as the outputs.

MATERIALS AND METHODS

Location of the bab louta dam

Bab louta dam was built on OuedBouSbaa (upstream of OuedBouHellou) is located about 40 km as the crow flies south of the city of TAZA.

It's considered to be the main resource suppling drinking water TAZA city and its regions.

Fig 1: location of bab louta dam (Parc National Tazeka)

Experimental procedure

In order to get a big database, coagulation tests were launched whenever the quality raw water changed.Each experience cannot be started without somephysic-chemical analysis such as: colloidal turbidity (CT), temperature (T), completeAlkalimetric title (CAT), pH, organic matter.

¬ Colloidal turbidity determined by Nephelometric method.
¬ Temperature determined by a calibrated thermometer of 0.5 °C of uncertainty.
¬ CAT determined by the titrimetric method using a strong acid HCl.
¬ pH determined by the electrochemical method.
¬ Organic matter determined by the titrimetric method (permanganate index).

All coagulation tests were conducted on solutions prepared by
dissolution of analytical quality compounds in distilled water (pH = 6.4 to 7.0,
conductivity = 1 to 4 µS/cm and residual chlorine = 0).

During our tests, we used as a powder aluminium sulphate ($Al_2(SO_4)_3$,18 H_2O /17%
Al_2O_3), prepared periodically by dissolution in distilled water to get a concentration of 10 g/l.

Jartest conducted on a flocculator of 6 agitators with individual speed ranging between 0 and 260 RPM.In our study,the raw water and the coagulant are subject for2 min fast agitation at120rpm.Speed is subsequently reduced to 40 rpmfor duration of 20 min. After a settling of 30 min(a phase during destabilized floc is led to the bottom of thebeakers), recoverwater supernatant to determine the physicochemical parameters.After, decanted water flow filtration in order to determine the turbidity and CAT.

RESULTS AND DISCUSSION

Study of screening of the factors

The cause-effect diagram and bibliographic research has helped us to study the influence of five variables on the rate of alum dose. These parameters are: colloidal turbidity (CT), temperature (T), complete Alkalimetric title (CAT), pH, and organic matter.

Screening strategies are used to identify quickly some of the factors in a broad range of potentially influential factors with a low number of experiments. (Nair, Strecher, Fagerlin, Ubel, &Resnicow, 2008)

The best-known screening matrices are matrices of Hadamard or matrix of placket and Burman (1946) (also called matrix effects) in such a way that the number of experiments is close to the number of factors investigated. (Diane L. Beres, 2001)

Table 1: Characteristics of the problem

Objective of the study	the effects
Number of variables	5
Number of experiments	8
Number of coefficients	6
Number of responses	1

Table 2: Experimental field

	Factor	Number levels	Levels
U1	COLLOIDAL TURBIDITY	2	2
			290
U2	TEMPERATURE	2	11

			23
U3	CAT	2	10
			15
U4	PH	2	7.20
			8.30
U5	Organic matter	2	1.2
			3.2

Table 3: experimental response

	Response	Unit
Y1	Rate of coagulant	mg/l

Table 4: Matrix of experiments

N°Exp	X1	X2	X3	X4	X5	Y1
1	1	1	1	-1	1	75.00
2	-1	1	1	1	-1	10.00
3	-1	-1	1	1	1	20.00
4	1	-1	-1	1	1	90.00
5	-1	1	-1	-1	1	20.00
6	1	-1	1	-1	-1	80.00
7	1	1	-1	1	-1	85.00
8	-1	-1	-1	-1	-1	25.00

Table 5: Analysis of variance: response Y1: rate of the coagulant

Source of variation	Sum of the square	degrees of freedom	Mean square	Fisher index	p-values
Regression	8.36563E+0003	5	1.67313E+0003	535.4000	0.154 **
Residues	6.25000E+0000	2	3.12500E+0000		
Total	8.37188E+0003	7			

Table 6: estimates and statistics of coefficients

Standard deviation of the response	1.768
R^2	0.999
R^2A	0.997
R^2pred	0.997
PRESS	25.000
Number of degrees of freedom	2

Name	Coefficient	F.Inflation	Standart deviation	t.exp.	p-values
b0	50.625		0.625	81.00	0.0171 ***
b1	31.875	1.00	0.625	51.00	0.0302 ***
b2	-3.125	1.00	0.625	-5.00	3.46 *
b3	-4.375	1.00	0.625	-7.00	1.64 *
b4	0.625	1.00	0.625	1.00	42.4
b5	0.625	1.00	0.625	1.00	42.4

The p values showed that the Colloidal Turbidity (CT), Temperature (T) and Complete Alkalinity Title (CAT) were highly significant.

It is also concluded that the factors pH and organic matter are significantly different from zero.
The quality of raw water, in summer period, requires generally only low levels of coagulant:

The pH of flocculated water changes very little. On the other hand, during the winter period, the pH variation is lower due to the buffering effect.

The effect of the fifth factor (organic matter) was not considered. Indeed, waters of bablouta dam do not contain a significant rate of organic matter which makes its influence on the rate of the coagulant is not significant.

In conclusion, only the factors: colloidal turbidity (CT), temperature (T) and alkalinity (CAT)
which have been selected for this study to model the rate of coagulant.

Modeling

The aim of our research was to apply Box–Behnken experimental design and response surface methodology for modeling the rate of coagulant.Box–Behnken design is rotatable second-order designs based on three-level incomplete factorial designs. (N. Aslan, 2007).For the three-level three-factorial Box–Behnken experimental design, a total of 15 experimental runs, shown in Table 7 are needed.
The model is of the following form: (A.BAZER-BACHI, 1990)

$$Y=b_0+\sum_{i=1}^{k} biXi+\sum_{i=1}^{k} biiXi^2+\sum_{i=1\,,j=2et\ i\#j}^{k} bijXiXj$$

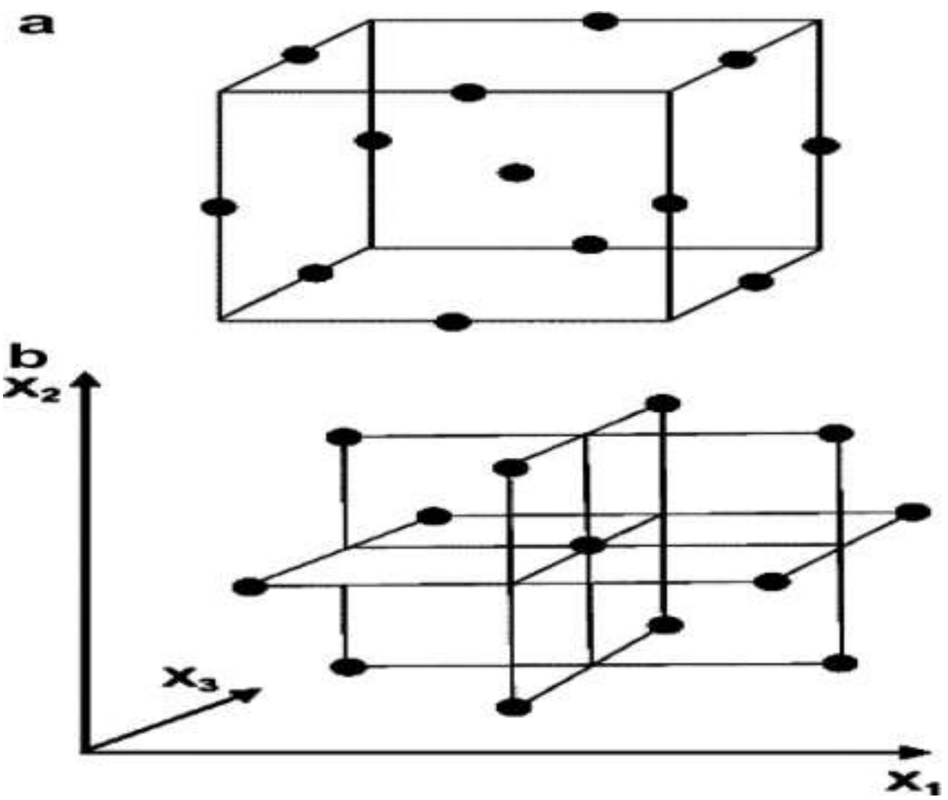

Fig 2: Box–Behnken design. (a) The design, as derived from a cube; (b) Representation as interlocking (N. Aslan, 2007).

In order to achieve a design of experiments, we should define reduced centered variables that can represent matrix format to conduct various tests. The reduced centered variable x corresponds to a change in variable such as:

X = A0-A/P

Where:
A: Value of the original variable
A0: Median value of the studied interval

The model coefficients are calculated by the law of squares, using the software "NEMROD" developed by the laboratory of prospective and analysis of information of the University of Aix-Marseille.

The quality of the forecast will be tested by three criteria:
-the standard deviation of the estimate on the response (σT),
-the adjusted squared (R^2A), multiple regression coefficient
-curves residuals to visualize

Table 7: Experimental field

	Factor	Unit	Center	Step of variation
U1	Colloidal Turbidity	NTU	146.00	144.00
U2	Temperature	°C	17.00	6.00
U3	CAT	°F	12.50	2.50

A classic experiment to estimate the 10 unknown parameters of such a model is given below BOX BENKHEN plan.

It is therefore necessary to carry out a total of 15experiments with 3 experiences at the centre to be able to evaluate the experimental error.

Table 8: Matrix of experiments

N°Exp	CT	T	CAT	Y1
1	-1.0000	-1.0000	0.0000	15.00
2	1.0000	-1.0000	0.0000	115.00
3	-1.0000	1.0000	0.0000	10.00
4	1.0000	1.0000	0.0000	100.00
5	-1.0000	0.0000	-1.0000	15.00
6	1.0000	0.0000	-1.0000	110.00
7	-1.0000	0.0000	1.0000	10.00
8	1.0000	0.0000	1.0000	105.00
9	0.0000	-1.0000	-1.0000	95.00
10	0.0000	1.0000	-1.0000	90.00
11	0.0000	-1.0000	1.0000	85.00
12	0.0000	1.0000	1.0000	80.00
13	0.0000	0.0000	0.0000	75.00
14	0.0000	0.0000	0.0000	80.00
15	0.0000	0.0000	0.0000	80.00

Statistical analysis leads to the following ANOVA table

Table 9: Analysis of variance: response Y1: rate of the coagulant

Source of variation	Sum of the square	degrees of f reedom	Mean square	Fisher index	p-values
Regression	2.05183E+0004	9	2.27981E+0003	273.5778	< 0.01 ***
Residues	4.16667E+0001	5	8.33333E+0000		
Validity	2.50000E+0001	3	8.33333E+0000	1.0000	53.4
Error	1.66667E+0001	2	8.33333E+0000		
Total	2.05600E+0004	14			

The ANOVA 1 p< 5% and VREG>VRES; so the ANOVA 1 is checked so we can judge the validity of the model model according to ANOVA 2, p > 5% and VLOF =VPE the error due to the model equal to the experimental error, the model is considered valid.

The sum of squares due to error is very low this indicates that the model seems to be adjusted.

The analysis of variance table proposed here by the software is more complex because the sum of squares due to residues was decomposed into sum due to the "validity" and amount due to the "error".

Table 10: estimates and statistics of coefficients

Standard deviation of the response	2.887
R^2	0.998
R^2A	0.994
R^2 pred	0.979
PRESS	437.500
Number of degrees of freedom	5

Name	Coefficient	F.Inflation	St deviation	t.exp.	p-values
b0	78.333		1.667	47.00	< 0.01 ***
b1	47.500	1.00	1.021	46.54	< 0.01 ***
b2	-3.750	1.00	1.021	-3.67	1.48 *
b3	-3.750	1.00	1.021	-3.67	1.48 *
b11	-22.917	1.01	1.502	-15.25	0.0109 ***
b22	4.583	1.01	1.502	3.05	2.85 *
b33	4.583	1.01	1.502	3.05	2.85 *
b12	-2.500	1.00	1.443	-1.73	14.2
b13	0.000	1.00	1.443	0.00	100.0
b23	0.000	1.00	1.443	0.00	100.0

The final model is given by the following form:

$$\mathbf{Y = 78.333 + 47.500CT - 3.750\,T - 3.750CAT - 22.917\,CT^2 + 4.583\,T^2 + 4.583\,CAT^2}$$

$\sigma_T = 2.887$
$R^2 = 0.998$
$R^2A = 0{,}994$

Statistical checks (ANOVA table, R^2 and R^2A value, model lack of fit test, and p value) indicated that the model was adequate for representing the experimental data.

The standard deviation and the regression coefficient show that this model is excellent.
This is confirmed by the curve of residues (fig. 3 and 4). Indeed, there is one sample that deviate by more than 3 g/m3 of the experimental rate either only 6.6% of samples and an another sample more than 2 g/m3 or 6.6% of the 13 data. Most experiences (about 87%) remaining does not deviate from 1.67 g/m3 maximum.
This shows that the adjustment is of very good quality.

For example, the figure 5 shows the optimum rate of its calculated from the model when a variable scans the experimental area, the other being in the middle.

The value of 48.9 g/m3, for example, corresponds to water with the following characteristics:

C T= 74.0 NTU ($X_1 = -0.5$); T = 17 ° C ($X_2 = 0$); CAT = 12, 5 ° F ($X_3 = 0$)
In these cases, the rate of coagulant increases with the turbidity and decreases with temperature and the CAT.

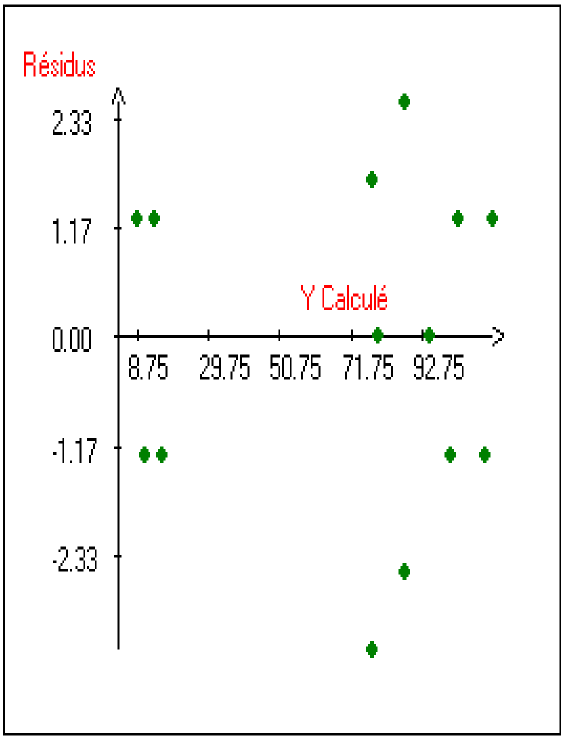

Fig 3: Residue = F (Y calculated)

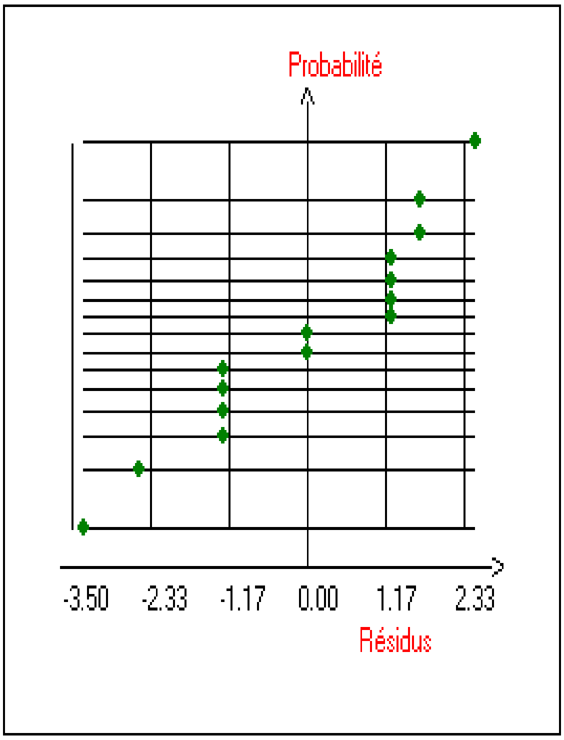

Fig 4: Distribution of residues on the right side of Henry

Figure 3 shows the good distribution of residues of part and other axis 0.
Figure 4 shows that all residues are well aligned themselves on the right side of Henry.
The graphical study of two figures proves that all residues follow a normal distribution.
The largest error of adjustment made (about -3, 33) for an observed response (78,33) was one of the Central experiments (experiment n° 13)

To gain a better understanding of the two variables for optimal coagulation performance, the model was presented as both 3-D response surface and 2-D contour graphs (Fig 5 and 6).

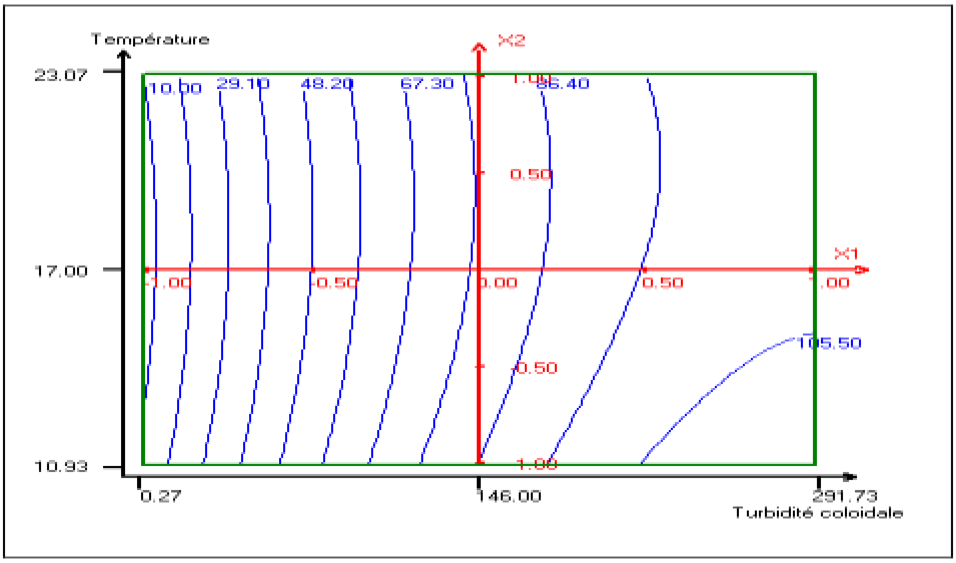

Fig 5 Variation in the response - rate of the coagulant in the plan: turbidity colloidal, Temperature FACTORS FIXED:- CAT = 12.50 ° F (2D graphic study)

-At average alkalinity (CAT = 12.5 ° F) the rate increases when the temperature drops.
-At average temperature (17 ° C), the rate increases when the TAC is reduced.
-At average turbidity (NTU 146), the rate is almost constant regardless of temperature and the CAT.

The very strong influence of turbidity on the optimum rate can be explained in part by its very wide range of variation. On the other hand, the temperature and alkalinity seem to have less influence on the response.

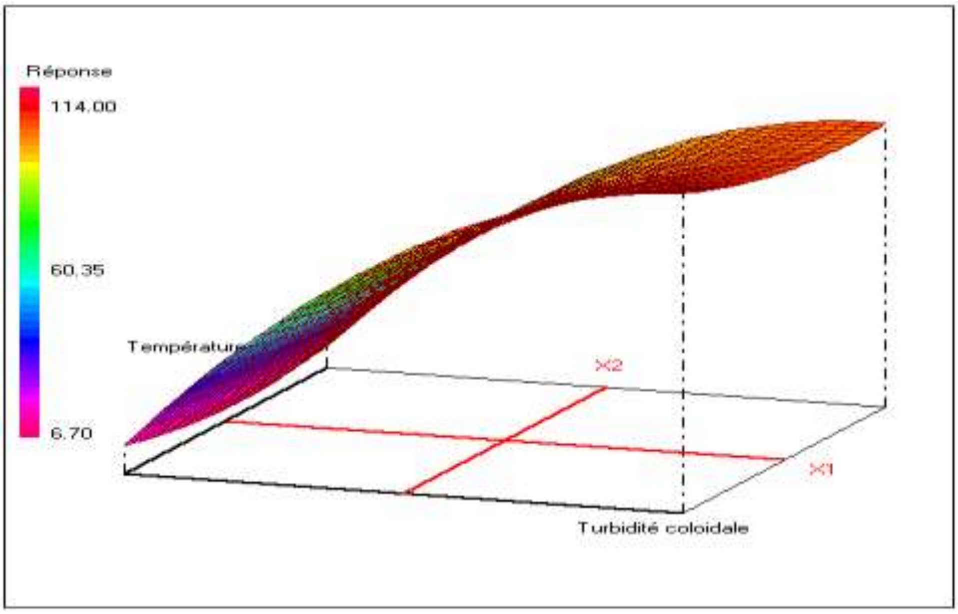

Fig 6 Variation in the response - rate of the coagulant in the plan: turbidity colloidal, Temperature FACTORS FIXED:-CAT = 12.50 ° F (3D graphic study)

CONCLUSION

A study of screening of the factors has shown that the most influential factors on the phenomenon under study are: CT, T and CAT.

The predicted response from the model showed close agreement with the experimental data (R^2 Values of 99.8% and $\sigma_T = 2.887$) which demonstrates the effectiveness of this approach in achieving good predictions, while minimizing the number of experiments required.

This study has shown that a polynomial model of order two no interacting seems to correctly model the phenomenon studied here.

The adaptation of this modeling on treatment is encouraging .Indeed, the final model allowed us to reduce, in average, the consumption of 5 g/m3 aluminum sulfate and therefore save nearly 147 kg/day in full flow.

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