Response surface methodology for predicting the dimethylphenol removal from wastewater via reverse osmosis process

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Abstract

Reverse Osmosis (RO) process can be considered as one of the intensively used pioneering equipment for reusing wastewater of several applications. The recent study presented the development of an accurate model for predicting the dimethylphenol removal from wastewater via RO process. The Response Surface Methodology (RSM) was applied to carry out this challenge based on actual experimental data collected from the literature. The independent variables considered are the inlet pressure (5.83 to 13.58) atm, inlet temperature (29.5 to 32) ^{o}C, inlet feed flow rate (2.166 to 2.583)×10^{-4} m^3/s, and inlet concentration (0.854 to 8.049)×10^{-3} kmol/m^3 and the dimethylphenol removal is considered as the response variable. The analysis of variance showed that the inlet temperature and feed flow rate have a negative influence on dimethylphenol removal from wastewater while the inlet pressure and concentration show a positive influence. In this regard, F-value of 240.38 indicates a considerable contribution of the predicted variables of pressure and concentration against the process dimethylphenol rejection. Also, the predicted R^2 value of 0.9772 shows the high accuracy of the model. An overall assessment of simulating the performance of RO process against the operating parameters has been systematically demonstrated using the proposed RSM model.

Key words: Wastewater treatment; RO process; Dimethylphenol removal; Modelling; Response surface methodology (RSM).

1. Introduction

Water pollution is a crucial issue of health due to its link to a variety of diseases with hazardous environmental consequences. The corresponding emerging pollutants and toxic contaminants in water are of a great concern due to its carcinogenic impact. The rapid growth of population besides the uncontrolled expansion of industries, and agricultural and domestic activities are the main factors for water pollution.[1] Therefore, the elimination of these pollutants from wastewater is of a high priority today. In this regard, intensive endeavors from research institutions were made to encounter the water pollution by innovating feasible and efficient technologies.[2,3]

Nowadays, a clear global increase of highly toxic and carcinogenic compounds in wastewater is being noticed. Modern industrial applications associated with different types of technologies are disposing vast amounts of wastewater with a variety of chemicals, fats, alcohols, and acids into the environment. Undoubtedly, the main concern of wastewater is the wide range of complex harmful chemicals and highly toxic pollutants that have been restricted by several environmental agencies.[4] Therefore, it is recommended to employ a proper technology that would reduce not only the water deficiencies but also the energy consumption leading to reduced impact on climate change. Having said this, the reuse of wastewater would reduce the reliance on potable water. However, this needs a comprehensive development of efficient, affordable, and low-cost treatment methods compared to the prevailing technologies. However, the reuse of wastewater may be forbidden as a result to the presence of complex compounds such as phenolic compounds. Note, 0.05 ppm has been assigned as the constraint of dimethylphenol in water

bodies based on the Agency of Toxic Substances and Disease Registry (ATSDR).[5] Therefore, a variety of wastewater treatment approaches were consequently industrialised to reduce the highly toxic phenolic compounds such as adsorption, oxidation and membrane technology. Adsorption technology has been used to treat water with a wide range of emerging pollutants. Amongst other treatment technologiess, adsorption characterises as an easy and inexpensive operation with the use of wide range of adsorbents capturing various kinds of contaminants.[6,7] Furthermore, the RO process has outweighed other membrane technologies due to its successfulness of removing a wide range of micropollutants including phenolic compounds.[8,9,10]

In recent years, a number of model based research has been noted in the area of wastewater treatment.[11] Accurate process models consisting of several partial (or ordinary) differential and algebraic and non-linear equations can describe the interaction of various design and operating conditions and process performance indicators. Therefore, the effect of the process input parameters on the process responses and the optimum performance can be conducted via simulation and optimisation studies, respectively, using detailed model-based techniques. However, the associated modelling of wastewater treatment using RO process has a considerable complexity of nonlinear behavior with many degrees of freedom.

On the other hand, Srinivasan et al.[12,13,14] and Sundaramoorthy et al.[15] investigated the performance of RO process for the wastewater treatment containing phenolic compounds experimentally accompanied by simple models to predict the rejection of phenolic compounds from synthesised wastewater. However, these simple models were not accurate enough. It is important to know that the trustworthiness of any model in calculating the system performance principally depends on an accurate evaluation of model parameters using parameter estimation and experimental data. Specifically, solvent, and solute membrane transport parameters and feed

channel friction parameter were estimated graphically using linear fit that resulted in inaccurate predictions. To address these inaccuracies, Al-Obaidi and Mujtaba[16] and Al-Obaidi et al.[17] developed more rigorous models. However, the open literature confirms the scarcity of a very accurate model with uncertainty in their parameters that can efficiently estimate the dimethylphenol removal from wastewater using RO process. In addition, computational time can be another factor for not using high infidelity models for optimisation and control purposes. Therefore, models based on advanced multivariate statistical approaches such as Response Surface Methodology (RSM) and Artificial Neural Network (ANN) technique for complex processes can provide alternative to rigorous first principle based models with high computation time.[18,19,20,21] Note, ANN has been extensively and successfully used as a prediction, classification, optimisation, and control methodology for a wide range of processes.[22,23,24] For instance, Khayet et al.[25] employed ANN and RSM to create models for simulation and optimisation of spiral wound RO seawater desalination process. In this respect, the feed concentration of sodium chloride, operating temperature, feed flow rate and pressure were considered as the input variables. However, the sodium chloride rejection and permeate flux were considered as the output variables. This assist to configure ANN and RSM models based on the obtainable experimental data. The adequacy of RSM model was very good to estimate the RO performance over the whole range of sodium chloride in the feed solution. Recently, Abdulrahman et al.[11] used ANN combined with Genetic Algorithm to create a new model to predict the chlorophenol removal from wastewater based on experimental data obtained from an individual membrane of RO process. However, a thorough study exploring the feasibility of RSM based mathematical model to precisely predict the rejection of phenolic compounds from wastewater via the RO process has not yet been established and hence demonstrates the novelty

of this work. The RSM model developed and validated in this work is then used to predict the performance of the RO process for removing dimethylphenol from wastewater under a wide range of operating and design conditions, which also reflects the novelty of this study. Experimental data from the open literature is used to validate the RSM model before using the model for further simulation.

2. Description of RO system and experimental data

Srinivasan and his co-authors carried out explicit experimental works to remove several pollutants of phenolic compounds family from wastewater via a simple design of RO process. In this regard, Srinivasan et al.[14] used a pilot-scale of an individual spiral wound module of RO process to abate the existence of dimethylphenol from wastewater. Figure 1 shows a schematic diagram of the treatment process. The membrane used was Ion Exchange, India Ltd., TFC Polyamide of 7.845 m^2. The data sets included the flow rate, pressure, temperature, concentration as the operating parameters and dimethylphenol rejection as the response. A wide range of these parameters was used to explore the influence of these parameters on the process rejection (see Table 1).

The feed solution splits into two main streams of low (permeate) and high (retentate) concentrations, after being processed in the membrane module and collected in two separate stainless tanks with a manual valve at the retentate stream to adjust the feed velocity inside the module via controlling the operating pressure. Therefore, two flow meters were instilled in the permeate and retentate streams to measure the flow rate. Moreover, another specific valve was set to control the high-pressure pump as can be seen in Figure 1. Furthermore, the operating pressure and retentate pressure were measured using Bourdon pressure gauges that fixed in the

inlet and outlet streams. Feed, permeate, and retentate dimethylphenol concentrations were analysed using A HPLC (Perkin Elmer, USA make) unit fitted with a UV detector and C-18 column.

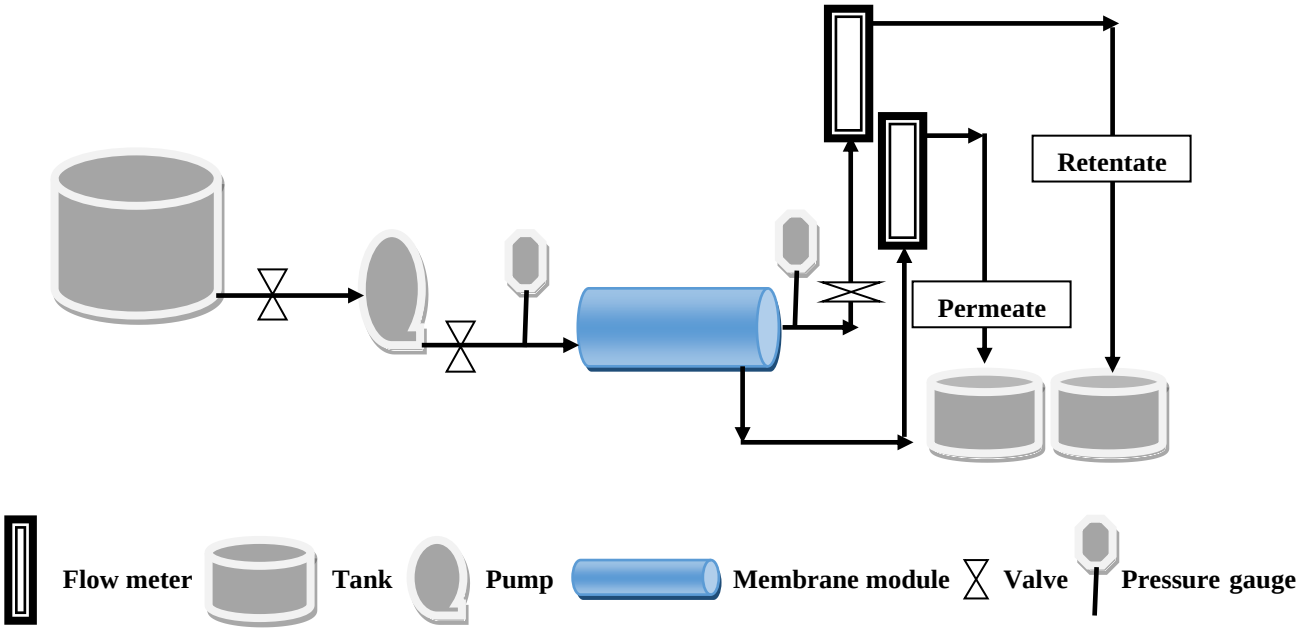

Figure 1. Schematic diagram of individual RO system (Adapted from Srinivasan et al.[14])

Table 1. Experimental results of dimethylphenol removal from wastewater (Adapted from Srinivasan et al.[14])

P_b (atm)	T_b (^oC)	$C_b x10^3$ (kmol/m^3)	F_b (m^3/s)	Rej (-)	P_b (atm)	T_b (^oC)	$C_b x10^3$ (kmol/m^3)	F_b (m^3/s)	Rej (-)
5.83	32.5	0.819	0.0002166	0.902	7.77	31	2.455	0.000233	0.928
7.77	32.5	0.819	0.0002166	0.915	9.71	31	2.455	0.000233	0.944
9.71	32.5	0.819	0.0002166	0.927	11.64	31	2.455	0.000233	0.950
11.64	32.5	0.819	0.0002166	0.936	13.58	31	2.455	0.000233	0.956
13.58	32.5	0.819	0.0002166	0.942	5.83	30	4.092	0.000233	0.936
5.83	31	1.637	0.0002166	0.919	7.77	30	4.092	0.000233	0.943
7.77	31	1.637	0.0002166	0.934	9.71	30	4.092	0.000233	0.951
9.71	31	1.637	0.0002166	0.943	11.64	30	4.092	0.000233	0.957
11.64	31	1.637	0.0002166	0.949	13.58	30	4.092	0.000233	0.964
13.58	31	1.637	0.0002166	0.953	7.77	31.5	6.548	0.000233	0.953
5.83	31	2.455	0.0002166	0.908	9.71	31.5	6.548	0.000233	0.962
7.77	31	2.455	0.0002166	0.926	11.64	31.5	6.548	0.000233	0.969
9.71	31	2.455	0.0002166	0.943	13.58	31.5	6.548	0.000233	0.973
11.64	31	2.455	0.0002166	0.949	5.83	32.5	0.819	0.0002583	0.907
13.58	31	2.455	0.0002166	0.952	7.77	32.5	0.819	0.0002583	0.92
5.83	30	4.092	0.0002166	0.935	9.71	32.5	0.819	0.0002583	0.941
7.77	30	4.092	0.0002166	0.94	11.64	32.5	0.819	0.0002583	0.950
9.71	30	4.092	0.0002166	0.949	13.58	32.5	0.819	0.0002583	0.959
11.64	30	4.092	0.0002166	0.955	5.83	31	1.637	0.0002583	0.921
13.58	30	4.092	0.0002166	0.963	7.77	31	1.637	0.0002583	0.937
7.77	31.5	6.548	0.0002166	0.952	9.71	31	1.637	0.0002583	0.943
9.71	31.5	6.548	0.0002166	0.962	11.64	31	1.637	0.0002583	0.948
11.64	31.5	6.548	0.0002166	0.97	13.58	31	1.637	0.0002583	0.951
13.58	31.5	6.548	0.0002166	0.973	5.83	31	2.455	0.0002583	0.917
5.83	32.5	0.819	0.000233	0.903	7.77	31	2.455	0.0002583	0.931
7.77	32.5	0.819	0.000233	0.915	9.71	31	2.455	0.0002583	0.944
9.71	32.5	0.819	0.000233	0.93	11.64	31	2.455	0.0002583	0.953
11.64	32.5	0.819	0.000233	0.935	13.58	31	2.455	0.0002583	0.958
13.58	32.5	0.819	0.000233	0.948	9.71	29	4.092	0.0002583	0.953
5.83	31	1.637	0.000233	0.919	11.64	29	4.092	0.0002583	0.958
7.77	31	1.637	0.000233	0.935	13.58	29	4.092	0.0002583	0.965
9.71	31	1.637	0.000233	0.943	5.83	31.5	6.548	0.0002583	0.946
11.64	31	1.637	0.000233	0.949	7.77	31.5	6.548	0.0002583	0.954
13.58	31	1.637	0.000233	0.953	9.71	31.5	6.548	0.0002583	0.963
5.83	31	2.455	0.000233	0.917	11.64	31.5	6.548	0.0002583	0.969

3. Response Surface Methodology

The RSM is characterised by coding each variable to be optimised at three specific levels of -1, 0, and +1. In this regard, the prediction of individual Y variables has been based on a quadratic polynomial regression model. The model projected for each response variable is

$$Y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ii} x_i^2 + \sum\sum \beta_{ij} x_i x_j \quad (1)$$

$\beta_0, \beta_i, \beta_{ii}$, and β_{ij} are constant, linear, square, and interaction regression coefficient terms, respectively. Also, xi and xj are independent variables.

The multiple regression analysis and analysis of variance (ANOVA) were carried out using the Minitab software version 14 (Minitab Inc., USA).[26] The accuracy of fit of the proposed model was appraised by the R^2 (coefficient of determination) and its statistical significance, which was tested by the *F*-test. A three-factor D-optimal design (statistical analysis method in ANOVA) was engaged to study the response of the dimethylphenol removal from wastewater via RO process.

4. Results and response surface analysis

The perception of any industrial process performance is quite important to comprehensively predict the associated response indicators in case of any expected change of operating conditions. Therefore, the process modelling including the RO process plays an important role as a superior tool to inclusively forecasting the process behavior within the constraints' limits of inlet parameters. In this regard, several methodologies of process modelling can be used to attain this aim including RSM and ANN. In this study, response surface methodology based on experimental data is applied to understand the relationship between four predictor variables named: the inlet pressure, temperature, concentration and flow rate and their effect on

dimethylphenol removal from wastewater via RO process. It is important to mention that the pollutant removal from wastewater is highly recommended to guarantee disposing of wastewater with regulated limits. Therefore, this study was concerned with dimethylphenol removal from wastewater with the aim of developing an accurate model for RO process. In this regards, quadratic regression with a second order and interaction terms is used to describe the analysis of variance. However, F-ratio at a probability (P) of 0.01 is used to judge the significance of the model terms. More importantly, the model appropriateness is measured using model analysis, lack of fit test, coefficient of determination (R^2), predicted error sum of squares (PRESS), and coefficient of variation (C.V). According to the quadratic regression Eq. 1, the regression equation of dimethylphenol removal as a function of the four input predictor variables can be described as

$$Rej = 0.95 + 0.015\ P_b - 9.374\times10^{-3}\ T_b + 0.012\ C_b - 7.122\times10^{-5}\ F_b - 4.592\times10^{-3}\ (P_b)^2 - 4.524\times10^{-3}\ (T_b)^2 + 5.643\times10^{-3}\ (C_b)^2 + 2.720\times10^{-3}\ P_b\ T_b - 4.166\times10^{-3}\ P_b\ C_b + 1.997\times10^{-3}\ P_b\ F_b + 2.275\times10^{-3}\ T_b\ F_b$$

It is observed that inlet temperature and volume flow rate have a negative influence while inlet pressure and concentration have a positive influence on the dimethylphenol removal. However, the negative impact of temperature is worse than the influence of feed flow rate. This is specifically opposite for both feed pressure and concentration which showed a higher positive contribution of feed pressure compared to lower contribution of concentration.

The regression coefficients of the proposed model and their significant on the response are summarised in Table 2. Specifically, the presented rejection model includes linear, quadratic, and interacted parameters. Generally, the P-value (less than 0.01) signifies that the obtained model is considered high-significant and fits well with experimental results. However, the P-value (less

than 0.05) signifies the model is significant compared to P-value of less than 0.1 of not notability. Moreover, the probability of the model is less than 0.01, which shows that the model is high-significant in its part linear model. In other words, this is a desirable action as it specifies that the individual terms in the model have a significant influence on the process response. In this case, P_b, T_b, and C_b are significant model terms. The main effect of linear order of the inlet pressure P_b and the inlet concentration C_b are the most significant factors with first class of notability (*) associated with dimethylphenol removal more than the inlet temperature Tb with second class of notability (**). In this regard, the effect of the feed flow rate has less significance with third class of notability (***). On the other hand, the inlet pressure has significance in the quadratic part of the model with first class of notability (*) compared to temperature, concentration, and feed flow rate of third class of notability and not notability, respectively. In interaction part model, the combination of the effect of inlet pressure and inlet concentration has more significant with first class of notability (*). However, the combination of inlet temperature and concentration has no effect.

The F-value represents the effect of predictor parameters variation on the response. Table 2 depicts higher values of F for inlet pressure and concentration which means that the variation of these parameters makes a considerable change on the dimethylphenol removal from wastewater. However, the low values of F for the inlet temperature and flow rate indicate that the variation of these parameters are less significant on the dimethylphenol removal from wastewater.

Table 2. Regression coefficients of the predicted quadratic polynomial model for response variables

Predictors	Coefficient (β)	F-value	Probability	Notability
Intercept	+0.95	---	0.0001	*
		Linear		
P_b	+0.015	388.39	0.0001	*
T_b	$- 9.374\times10^{-3}$	7.23	0.0150	**
C_b	+ 0.012	28.27	0.0001	*
F_b	$- 7.122 \times10^{-5}$	0.00175	0.9670	***
		Quadratic		
$P_b P_b$	$- 4.592\times10^{-3}$	32.23	0.0001	*
$T_b T_b$	-4.524×10^{-3}	2.38	0.1404	***
$C_b C_b$	$+ 5.643\times10^{-3}$	8.62	0.4414	***
$F_b F_b$	--------	----	------	----
		Interaction		
$P_b T_b$	$+2.720 \times10^{-3}$	5.81	0.0269	**
$P_b C_b$	-4.166×10^{-3}	10.41	0.0046	*
$P_b F_b$	$+1.997 \times10^{-3}$	2.53	0.128	***
$T_b C_b$	-----	---	-----	
$T_b F_b$	$+ 2.275 \times10^{-3}$	0.87	0.3631	***
$C_b F_b$	------	-----	-----	

*P<0.01; **P<0.05; ***P<0.1

The analysis of variance (ANOVA) for the proposed model is summarised in Table 3. This in turn shows that the F-value of the model is recorded as 240.38, which indicate that the predictor variable has a strong and significant influence on the performance of the model. Moreover, the sum of squared error of the model, residual, lack of fit, and pure error are recorded low values of $8.48x10^{-3}$, $5.77x10^{-5}$, $5.77x10^{-5}$, and 0, respectively. Also, these results are associated with low values (C.V) and (PRESS). Consequently, the overall performance of the model as referred to the coefficient of determination R^2 depicts the R^2-predicted of 0.9772 with a plausible corroboration with R^2-adjusted of 0.9891 with a minor difference of 0.0119.

Table 3. ANOVA table of the proposed model

Variable and source	D_f	Sum of squares	F- value
Model	11	$8.48x10^{-3}$	240.38
Residual	18	$5.77x10^{-5}$	---
Lack of fit	17	$5.77x10^{-5}$	---
Pure error	1	0	---
C.V=19%,		PRESS=$1.94x10^{-4}$	
R^2- predicted=0. 9772,		R^2 -adjusted= 0.9891	

The normal probability plot of Figure 2 for the dimethylphenol removal from wastewater using RO process shows that the predicted (the proposed model) and actual (experimental results of Table 1) values are generally distributed on a straight line, which means that the errors are normally distributed as depicted in Figure 2. Interestingly, the predicted values are found to be statistically similar to the actual one. Therefore, it is fair to claim that the RSM method is able to constitute an accurate model for the prediction of dimethylphenol from wastewater via the RO process. Very small differences (high R^2) between the predicted values and experimental data signify the merits of using the RSM. Additionally, the RSM model is quicker to estimate the response compared to other sophisticated mathematical methods. It is important to mention that once the RSM model is developed, the calculation of rejection parameter is very fast as it is just functions of operating conditions. Also to demonstrate the robustness of the RSM model, note that the obtained results of RSM model are closer to the experimental data compared to other models developed in the literature. For instance, the model of Al-Obaidi and Mujtaba[16] has entailed a higher discrepancy of 11.4% for the removal of chlorophenol from wastewater between the model's predictions and observational data. Moreover, the model of Al-Obaidi et al.[17] was overestimated the permeate concentration of a maximum of 15% error, which reflects the limitation of the previous models.

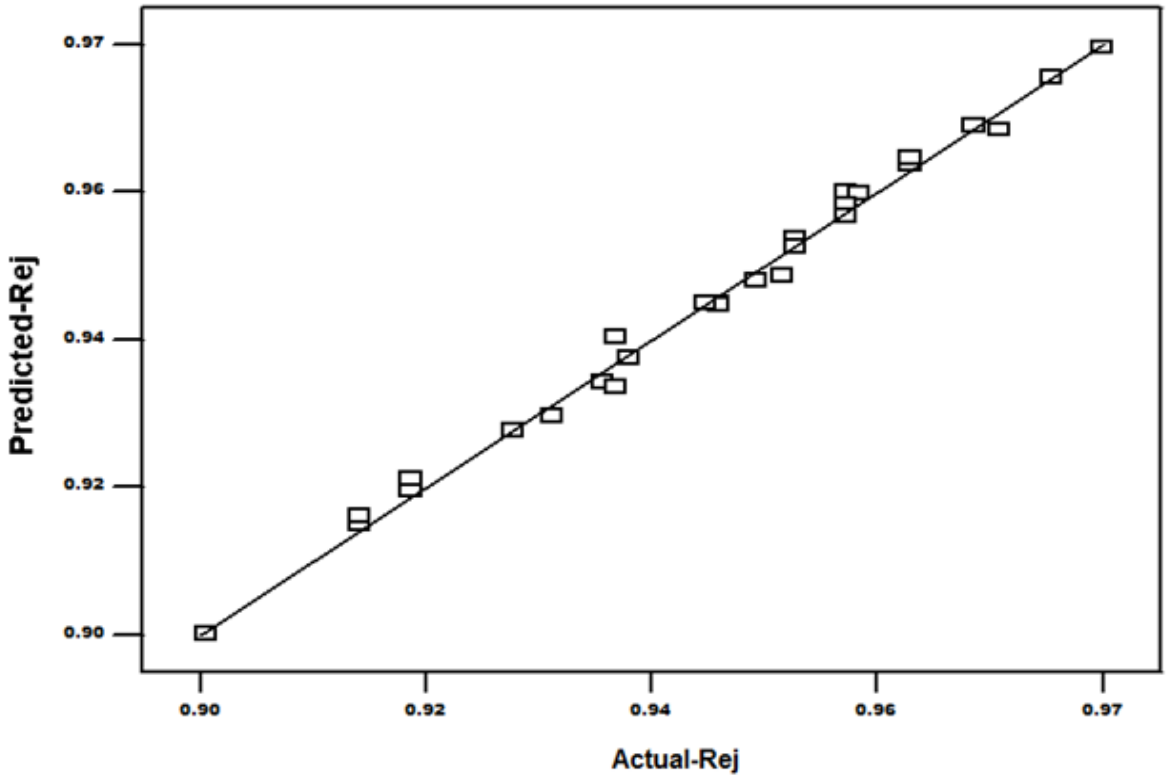

Figure 2. Plot of predicted dimethylphenol rejection against actual one (response)

5. Effect of operating parameters on the dimethylphenol removal

The performance of any industrial process including RO process can be studied via simulation and based on a successful model, which able to forecast the process behavior under the variation of operating conditions. In this regard, the simulation of any industrial process has many advantages. For instance, it offers a conceptual perception of the influence of individual and combined operating conditions on the process responses. Moreover, it would map the selection of proper values of operating conditions to sustain the process at elevated performance. Lastly, it would aid to optimise the process to attain the most requested objective functions. Interestingly, the RSM developed in this research was able to develop a rigorous and simple model to explore the removal of dimethylphenol from wastewater without the need of realising the detailed

transport phenomenon inside the module and guessing the transport parameters of water and dimethylphenol of the membrane. More importantly, RSM has relaxed the addiction on complex models established in the open literature that are essentially built on strict assumptions besides a significant level of arbitrariness. This is already confirmed by Popović et al.[27] who used RSM to analyse and optimise the enhanced ultrafiltration treatment process of cutting oil wastewater.

In this section, the model presented in section 4 of dimethylphenol rejection is used to explore the influence of the main control variables of RO process on the abatement of dimethylphenol from wastewater. This is basically based on the experimental data presented in Table 1. For the preceding discussions, it has been decided to analyse the conjugated influence of two parameters on the removal of dimethylphenol in three-dimensional contour plots. This would be helpful tool in better understanding the interconnection between the operating conditions in a way to optimising their contribution in the next studies. It is important to mention that the preceding simulation results were plotted using ANOVA.

Figure 3 shows the conjugated profile of two parameters namely the operating pressure and temperature on the removal of dimethylphenol. This in turn showed the significant contribution of operating condition on the retention of dimethylphenol. Increasing the operating pressure will lead to enhance the permeate flux due to increasing the trans-membrane pressure between the two sides of the membrane.

It is also interesting to observe an opposite contribution of temperature on dimethylphenol rejection if compared to pressure (Figure 3). Specifically, the removal of dimethylphenol is deteriorated due to elevated temperature for all the tested operating pressure. This deterioration is much more pronounced at the highest applied pressure which might be attributed to combining two parameters (pressure and temperature) to lift the permeate flux compared to the lowest

applied pressure. One would expect this behavior due to increasing the pollutant passage through the membrane due to increasing the membrane pore size as a reply to increasing temperature.

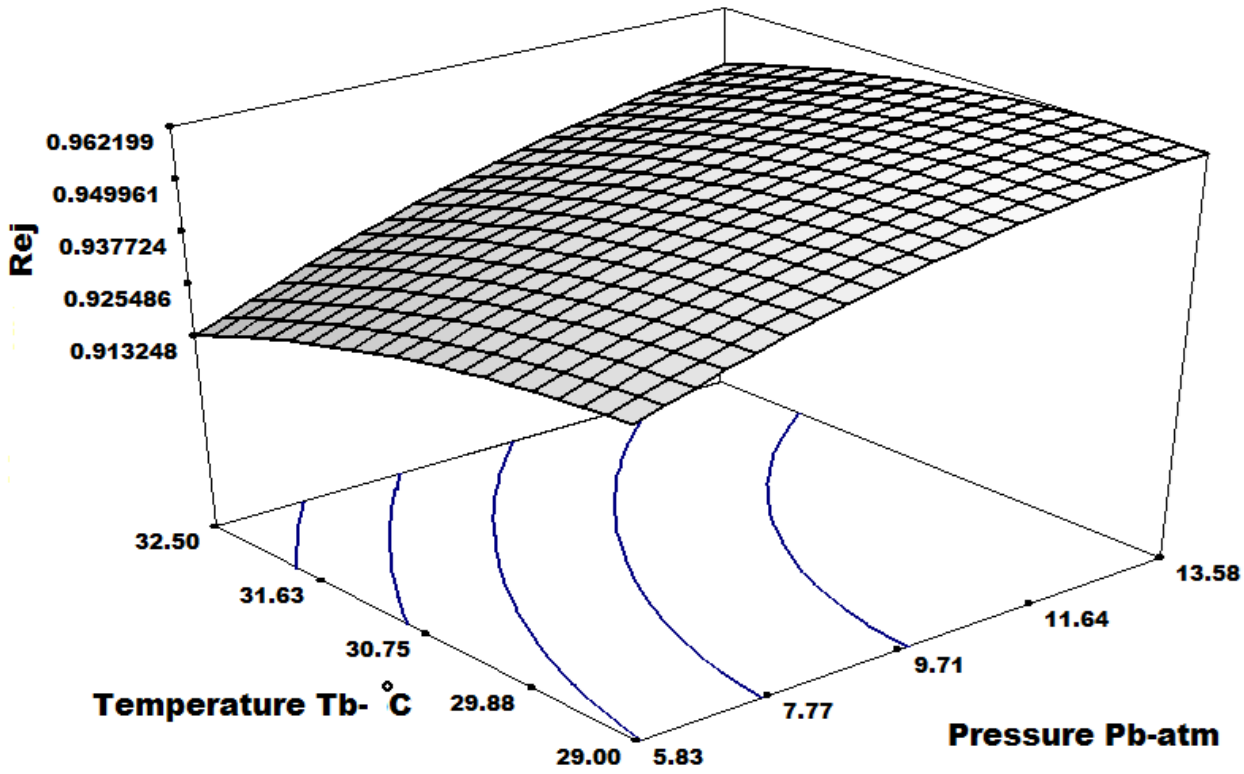

Figure 3. Response surfaces as contour plot of the effect of temperature and pressure on dimethylphenol removal

The influence of feed concentration of dimethylphenol on the removal of dimethylphenol from wastewater at different operating pressures is elucidated in the counter plot of Figure 4. As the inlet concentration increases, the permeate flux would retard due to increasing the osmotic pressure, which entirely decreases the total water recovery (not presented here to economise space). However, increasing the feed concentration at the feed channel is much more the one accumulated in the permeate channel. Therefore, this would increase the dimethylphenol rejection as a consequence of increasing feed channel concentration, which is already pictured in Figure 4. Interestingly, the operation of RO process at the lowest feed concentration and

increased pressure from 5.83 atm to 13.58 atm has pronounced a higher promotion in dimethylphenol rejection compared to the highest feed concentration. This is conceptually ascribed to lower concentration polarisation at the lower feed concentration.

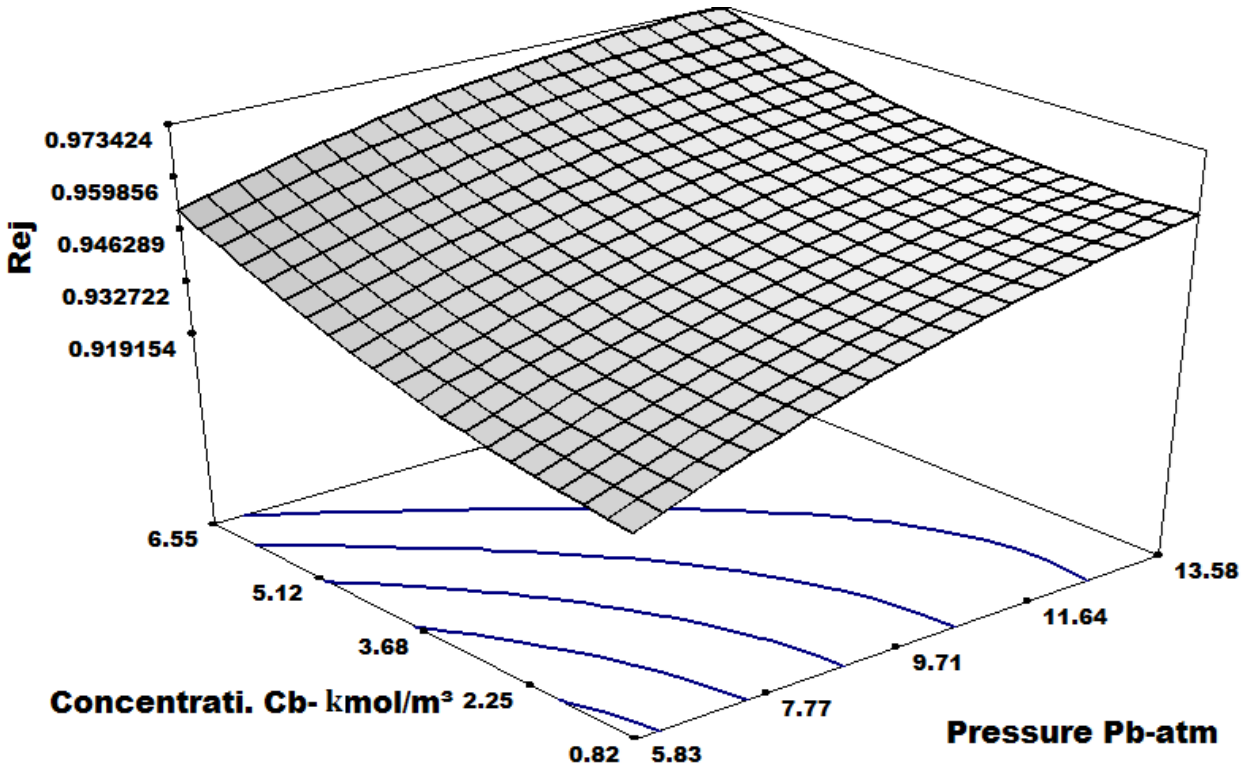

Figure 4. Response surfaces as contour plot of the effect of concentration and pressure on dimethylphenol removal

To neutralise the influence of feed flow rat and pressure on the removal of dimethylphenol, Figure 5 exhibits this influence. Insignificant change in dimethylphenol removal is noticed due to increasing the feed flow rate for all the tested pressures. The unique behavior of dimethylphenol rejection against feed flow rate might attributed to different mechanisms occur with increasing feed flow rate. Firstly, increasing bulk velocity would in fact limit the dimethylphenol concentration at the membrane wall due to increasing the shear stress. This would promote the turbulence inside the feed channel and increases the permeate flux. However, a contrasted

mechanism would be occurred as a result to increasing the bulk velocity. Lower residence time of water will be the result of increasing the bulk velocity, which means lesser opportunity to permeate flux that would contrast the first mechanism. Therefore, it is fair to expect inconsiderable influence of feed flow rate on dimethylphenol removal as depicted in Figure 5.

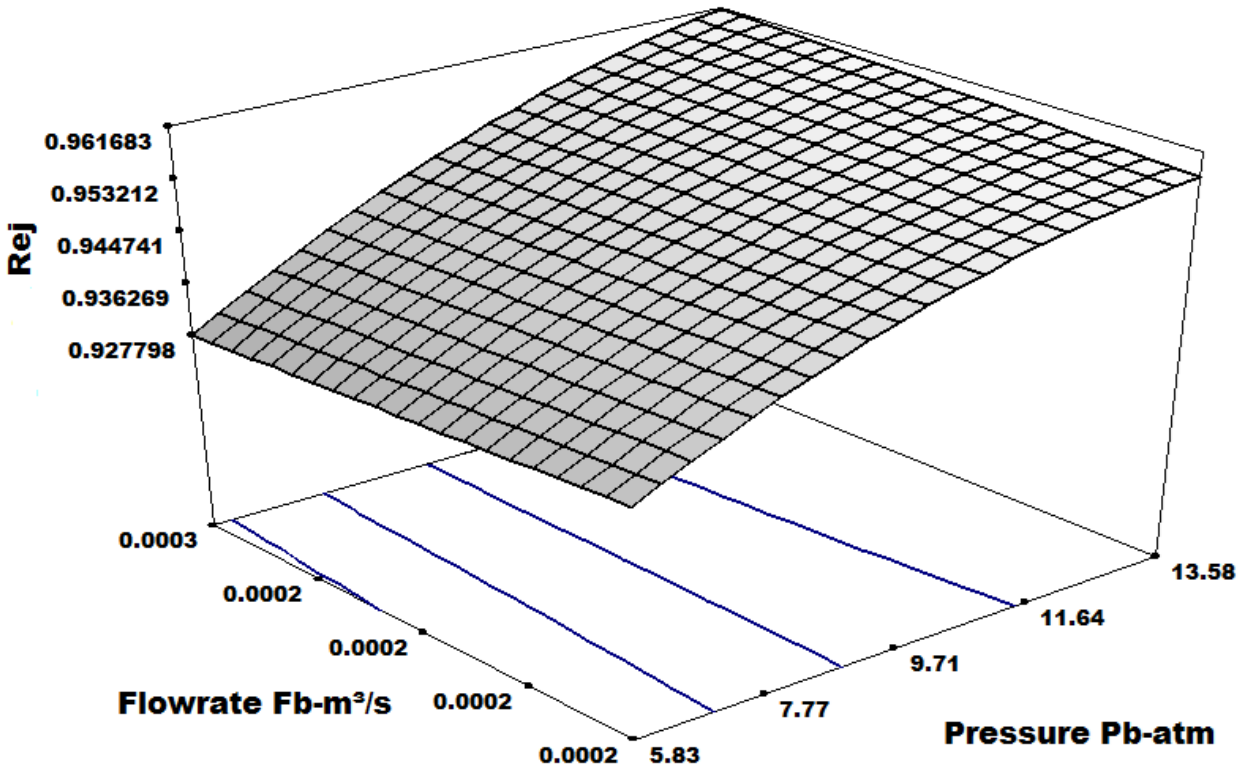

Figure 5. Response surfaces as contour plot of the effect of feed flow rate and pressure on dimethylphenol removal

Figure 6 illustrates the combined influence of temperature and concentration on dimethylphenol retention. This is specifically showed that the dimethylphenol removal is conspicuously increased due to growing the feed concentration from 0.82 kmol/m³ to 6.55 kmol/m³ at high temperature of 32.5 °C compared to low temperature of 29 °C. This would fit the above findings of higher permeate flux at high temperatures, which elaborated a higher promotion of rejection.

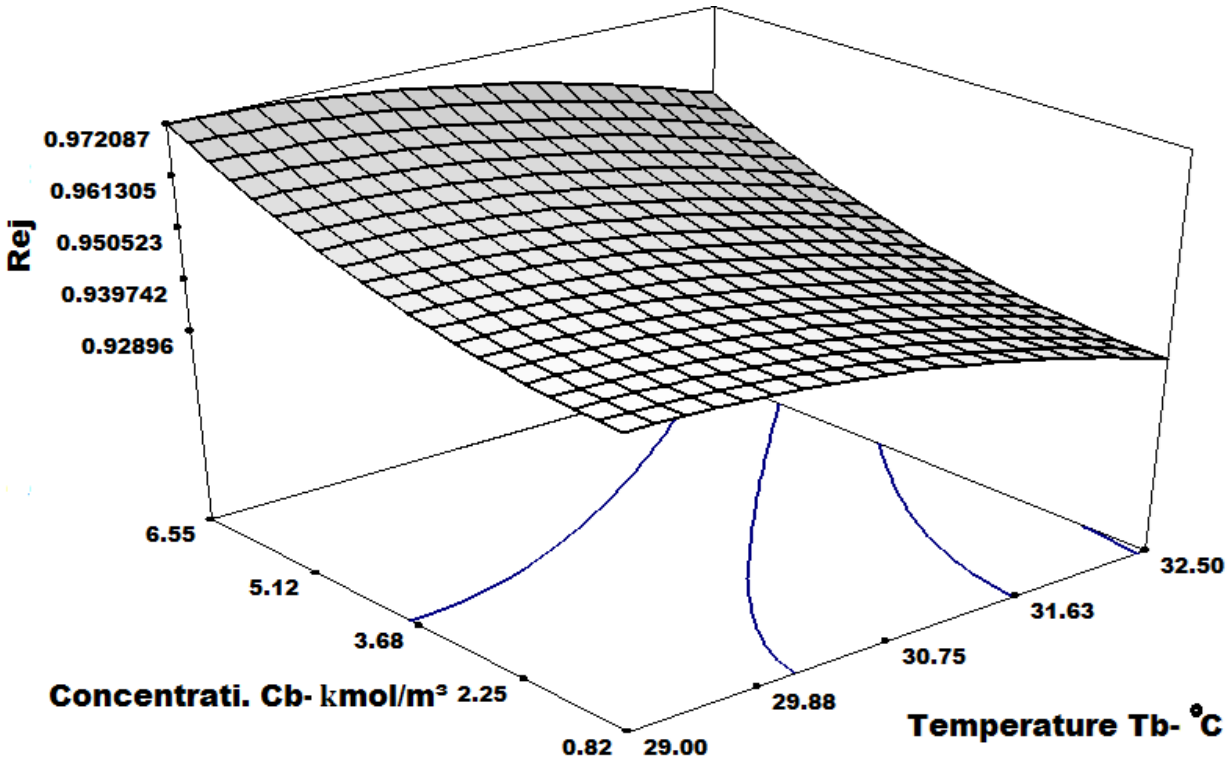

Figure 6. Response surfaces as contour plot of the effect of concentration and temperature on the dimethylphenol removal

Finally, the influences of feed flow rate variation at variable temperature and concentartion on dimethylphenol removal are pictured in Figures 7 and 8, respectively. For the first time, the impact of temperature is clearly depicted on the dimethylphenol retention following the variation of feed flow rate. This is specifically shown a drop of rejection as temperature rises. Therefore, it is recommended to implemnt low temperature at any operational feed flow rate. Moreover, Figure 8 presents a clear improvement of rejection as feed concentration increases despite insignificant change of rejection with increasing feed flow rate.

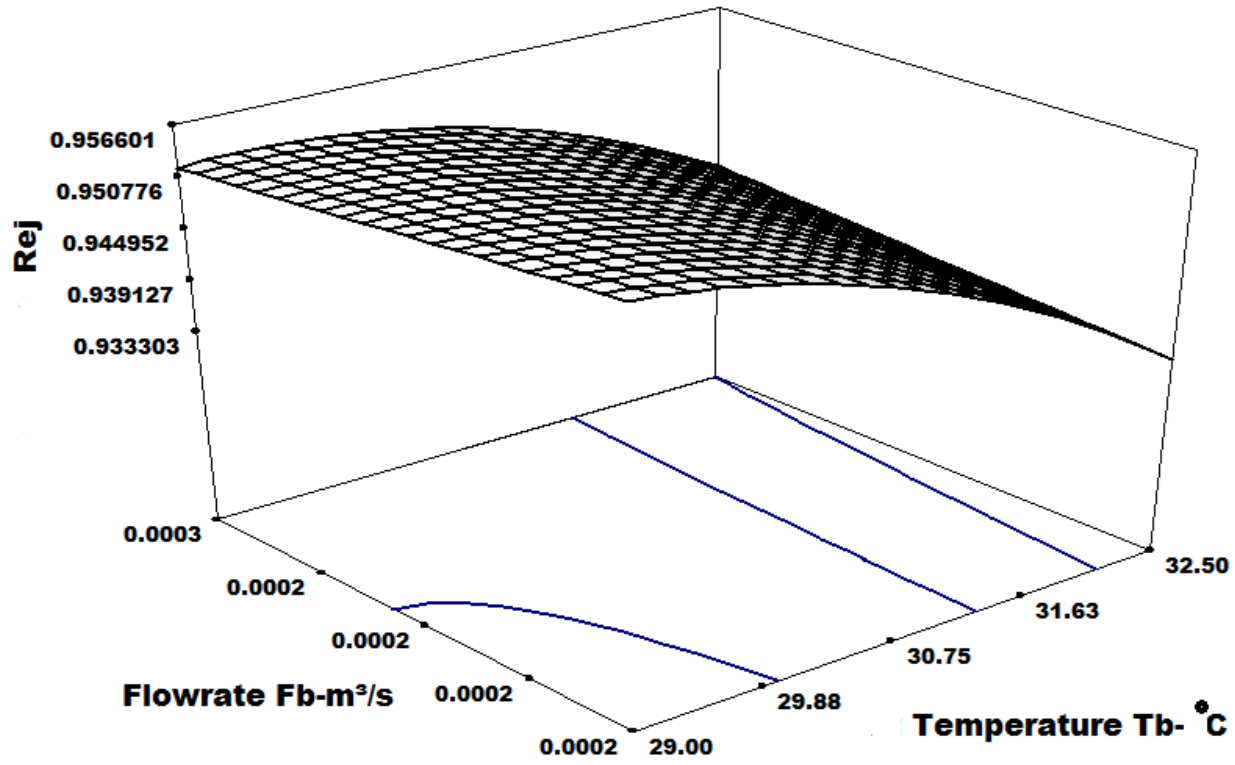

Figure 7. Response surfaces as contour plot of the effect of feed flow rate and temperature on the dimethylphenol removal

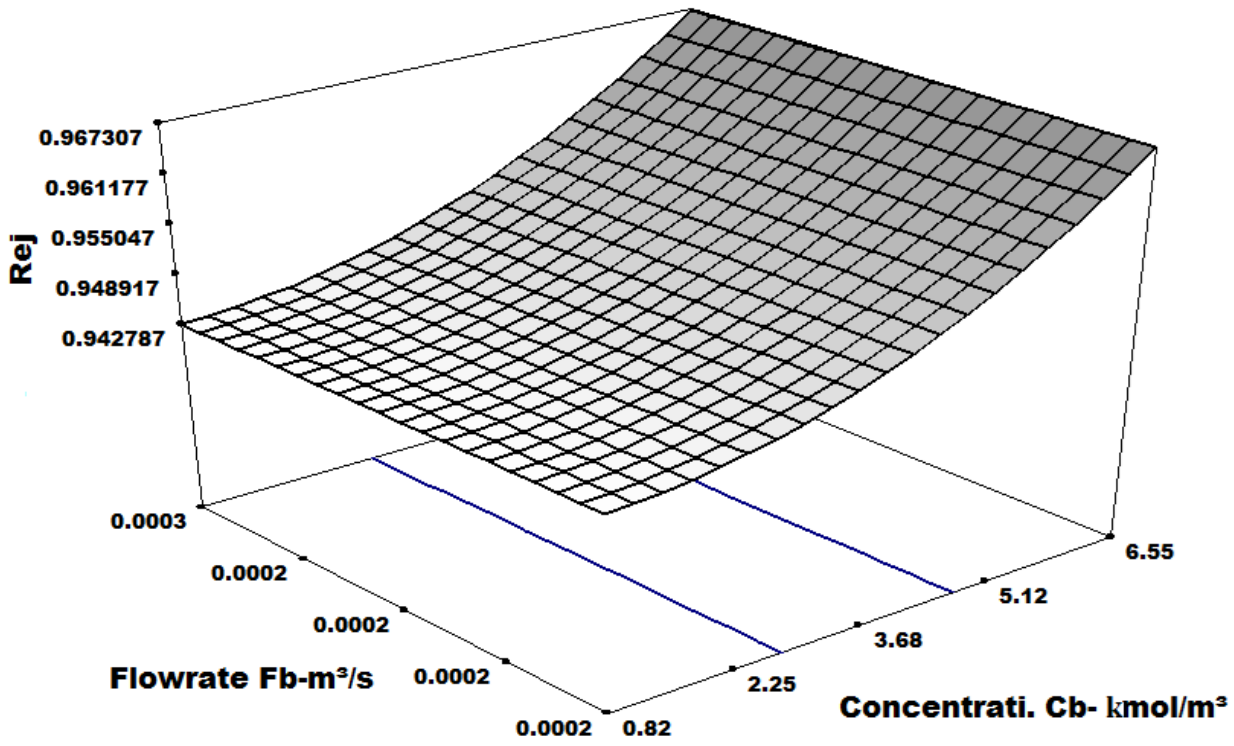

Figure 8. Response surfaces as contour plot of the effect of feed flow rate and concentration on the dimethylphenol removal

6. Conclusions

Quadratic regression analysis using response surface methodology (RSM) was employed to develop an accurate statistical model to forecast the performance of a spiral wound RO process to retain dimethylphenol from wastewater. In this respect, RSM developed has considered four predictor variables of RO process of operating pressure, concentration, flow rate and temperature as input parameters of the model. On the other hand, dimethylphenol rejection has been used as the response parameter.

The following conclusions can be made from the analysis of the proposed model as follows:

1. The probability for the linear part of the proposed model is less than 0.01, which elaborated its consistency.

2. The interaction part of the proposed model that signifies the combination of the effect of pressure and concentration has more significant with first class of notability compared to the combination of the effect of the temperature and concentration of no effect.
3. The prediction of the proposed model for dimethylphenol rejection showed a high-degree of agreement with the experimental data. This is due to the gain of a predicted R^2 of 0.9772 with the adjucted R^2 of 0.9891 with differnce of 0.0119.

The research dedicated on appraising the effect of the operating variables on the dimethylphenol rejection. It is observed that the pressure and concentration have a positive influence on the dimethylphenol removal from wastewater compared to a negative impact of the temperature and feed flow rate. Finally, to appraise the validity of the proposed model of RSM with the scale up of RO process is recommended for the next research.

Nomenclature

C_b: Dimethylphenol concentration (kmol/m^3)

F_b: Feed flow rate (m^3/s)

P_b: Feed pressure (atm)

Rej: Dimethylphenol rejection (dimensionless)

T_b: Feed temperature (^{o}C)

References

1. Ali I., Alharbi O.M., Tkachev A., Galunin E., Burakov A., Grachev V.A., 2018. Water treatment by new-generation graphene materials: hope for bright future. *Environmental Science and Pollution Research*, 25(8), 7315–7329.

2. Basheer A.A., 2018. Chemical chiral pollution: impact on the society and science and need of the regulations in the 21st century. *Chirality*, 30(4), 402–406.
3. Basheer A.A., 2018. New generation nano-adsorbents for the removal of emerging contaminants in water. *Journal of Molecular Liquids*, 261, 583–593.
4. Ali I., Mbianda X.Y., Burakov A., Galunin E., Burakova I., Mkrtchyan E., Tkachev A., Grachev V., 2019. Graphene based adsorbents for remediation of noxious pollutants from wastewater. *Environment international*, 127, 160–180.
5. Agency for toxic substances and disease registry (ATSDR), division of toxicology and human health sciences, 2015. Substance Priority List. https://www.atsdr.cdc.gov/spl/index.html
6. Ali I., 2018. Microwave assisted economic synthesis of multi walled carbon nanotubes for arsenic species removal in water: batch and column operations. *Journal of molecular liquids*, 271, 677–685.
7. Nodeh H.R., Ibrahim W.A.W., Ali I., Sanagi M.M., 2016. Development of magnetic graphene oxide adsorbent for the removal and preconcentration of As (III) and As (V) species from environmental water samples. *Environmental Science and Pollution Research*, 23(10), 9759–9773.
8. Al-Obaidi M.A., Kara-Zaïtri C., Mujtaba I.M., 2017a. Simulation of full-scale reverse osmosis filtration system for the removal of N-nitrosodimethylamine from wastewater. *Asia-Pacific Journal of Chemical Engineering*, e2167, 1–13.
9. Ochando-Pulido J.M., Martinez-Ferez, A., 2018. Optimization of the fouling behaviour of a reverse osmosis membrane for purification of olive-oil washing wastewater. Process *Safety and Environmental Protection*, 114, 323–333.

10. Al-Obaidi M.A., Kara-Zaïtri C., Mujtaba I.M., 2019. Evaluation of chlorophenol removal from wastewater using multi-stage spiral-wound reverse osmosis process via simulation. *Computers and Chemical Engineering*, 130, 106522.
11. Abdulrahman Th. Mohammad, Mudhar A. Al-Obaidi, Emad Majeed Hameed, Basil N. Basheer, Iqbal M. Mujtaba., 2020. Modelling the chlorophenol removal from wastewater via reverse osmosis process using a multilayer artificial neural network with genetic algorithm. *Journal of Water Process Engineering*, 33, 100993.
12. Srinivasan G., Sundaramoorthy S., Murthy D.V.R., 2009. Separation of dimethyl phenol using a spiral-wound RO membrane — Experimental and parameter estimation studies. *Desalination*, 243 (1) 170–181.
13. Srinivasan G., Sundaramoorthy S., Murthy D.V.R., 2010. Spiral wound reverse osmosis membranes for the recovery of phenol compounds-experimental and parameter estimation studies. *American Journal of Engineering and Applied Sciences*, 3 (1) 31–36.
14. Srinivasan G., Sundaramoorthy S., Murthy D.V.R., 2011. Validation of an analytical model for spiral wound reverse osmosis membrane module using experimental data on the removal of dimethylphenol. *Desalination*, 281 (Supplement C) 199–208.
15. Sundaramoorthy S., Srinivasan G., Murthy D.V.R., 2011. An analytical model for spiral wound reverse osmosis membrane modules: Part II — Experimental validation. *Desalination*, 277 (1–3) 257–264.
16. Al-Obaidi M.A., Mujtaba I.M., 2016. Steady state and dynamic modeling of spiral wound waste water reverse osmosis process. *Computers and Chemical Engineering*, 90, 278–299.

17. Al-Obaidi M.A., Kara-Zaïtri C., Mujtaba I.M., 2017b. Wastewater treatment by spiral wound reverse osmosis: Development and validation of a two dimensional process model. *Journal of Cleaner Production*, 140, 1429–1443.
18. Samarbaf S., Birgani Y.T., Yazdani M., Babaei A.A., 2019. A comparative removal of two dyes from aqueous solution using modified oak waste residues: process optimization using response surface methodology. *J. Ind. Eng. Chem*. 73, 67–77.
19. Baştürk E., Alver A., 2019. Modeling azo dye removal by sono-fenton processes using response surface methodology and artificial neural network approaches. *Journal of Environmental Management*, 248, 109300.
20. Zin M.M.T., Kim D.J., 2019. Struvite production from food processing wastewater and incinerated sewage sludge ash as an alternative N and P source: Optimization of multiple resources recovery by response surface methodology. *Process Safety and Environmental Protection*, 126, 242–249.
21. Krishnan S., Zulkapli N.S., Md Din M.F., Abd Majid Z., Honda M., Ichikawa Y., Md Sairan F., Nasrullah M., Guntor N.A..A., 2020. Statistical optimization of titanium recovery from drinking water treatment residue using response surface methodology. *Journal of Environmental Management*, 255, 109890.
22. Tehlah Noree, Kaewpradit Pornsiri, Mujtaba Iqbal M., 2017. Development of molecular distillation based simulation and optimization of refined palm oil process based on response surface methodology. *Processes*, 5, 40, 1–15.
23. Ekpo E.E., Mujtaba I.M., 2008. Evaluation of Neural Networks Based Controllers in Batch Polymerisation of Methyl Methacrylate. *Neurocomputing*, 71, 1401–1412.

24. Ali I., Alharbi O.M., Alothman Z.A., Badjah A.Y., Alwarthan A., 2018. Artificial neural network modelling of amido black dye sorption on iron composite nano material: kinetics and thermodynamics studies. *Journal of Molecular Liquids*, 250, 1–8.
25. Khayet M., Cojocaru C., Essalhi M., 2011. Artificial neural network modeling and response surface methodology of desalination by reverse osmosis. *Journal of Membrane Science*, 368(1-2), 202–214.
26. Wu M., Ding H., Wang S., Xu Sh, 2008. Optimization conditions for the purification of linoleic acid from sunflower oil by urea complex fractionation. *J. Am. Oil Chem. Soc*., 85, 677–684.
27. Popović S., Karadžić M., Cakl J., 2019. Optimization of ultrafiltration of cutting oil wastewater enhanced by application of twisted tapes: Response surface methodology approach. *Journal of Cleaner Production*, 231, 320–330.

Highlights

1. Response Surface Method forms RO model to remove dimethylphenol from wastewater.
2. The model validation is realised based on actual data of dimethylphenol removal.
3. RSM model shows high F-value that pointed out high contribution of the variables.
4. RSM model depicts R^2 of 0.9772 of high-support of the model and experimental data.
5. Effect of main parameters on dimethylphenol removal analysed by 3D counter plots.

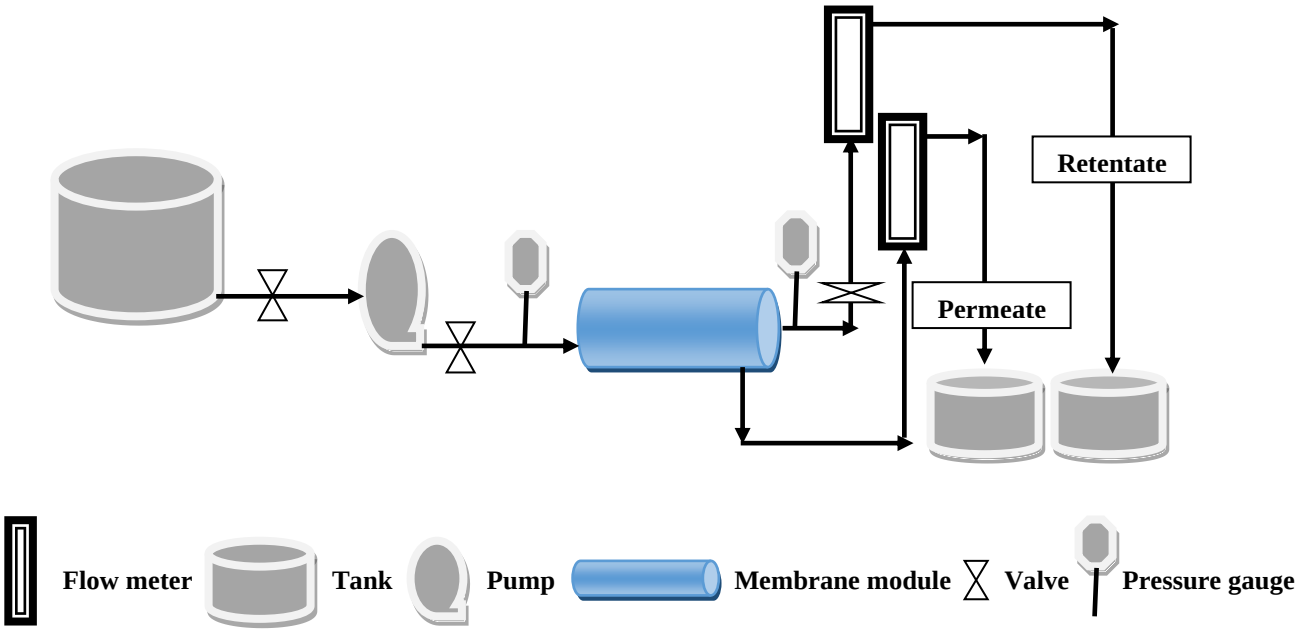

Figure 1. Schematic diagram of individual RO system (Adapted from Srinivasan et al.[8])

Table 1. Experimental results of dimethylphenol removal from wastewater (Adapted from Srinivasan et al.[14])

P_b (atm)	T_b (^oC)	$C_b x10^3$ (kmol/m^3)	F_b (m^3/s)	Rej (-)	P_b (atm)	T_b (^oC)	$C_b x10^3$ (kmol/m^3)	F_b (m^3/s)	Rej (-)
5.83	32.5	0.819	0.0002166	0.902	7.77	31	2.455	0.000233	0.928
7.77	32.5	0.819	0.0002166	0.915	9.71	31	2.455	0.000233	0.944
9.71	32.5	0.819	0.0002166	0.927	11.64	31	2.455	0.000233	0.950
11.64	32.5	0.819	0.0002166	0.936	13.58	31	2.455	0.000233	0.956
13.58	32.5	0.819	0.0002166	0.942	5.83	30	4.092	0.000233	0.936
5.83	31	1.637	0.0002166	0.919	7.77	30	4.092	0.000233	0.943
7.77	31	1.637	0.0002166	0.934	9.71	30	4.092	0.000233	0.951
9.71	31	1.637	0.0002166	0.943	11.64	30	4.092	0.000233	0.957
11.64	31	1.637	0.0002166	0.949	13.58	30	4.092	0.000233	0.964
13.58	31	1.637	0.0002166	0.953	7.77	31.5	6.548	0.000233	0.953
5.83	31	2.455	0.0002166	0.908	9.71	31.5	6.548	0.000233	0.962
7.77	31	2.455	0.0002166	0.926	11.64	31.5	6.548	0.000233	0.969
9.71	31	2.455	0.0002166	0.943	13.58	31.5	6.548	0.000233	0.973
11.64	31	2.455	0.0002166	0.949	5.83	32.5	0.819	0.0002583	0.907
13.58	31	2.455	0.0002166	0.952	7.77	32.5	0.819	0.0002583	0.92
5.83	30	4.092	0.0002166	0.935	9.71	32.5	0.819	0.0002583	0.941
7.77	30	4.092	0.0002166	0.94	11.64	32.5	0.819	0.0002583	0.950
9.71	30	4.092	0.0002166	0.949	13.58	32.5	0.819	0.0002583	0.959
11.64	30	4.092	0.0002166	0.955	5.83	31	1.637	0.0002583	0.921
13.58	30	4.092	0.0002166	0.963	7.77	31	1.637	0.0002583	0.937
7.77	31.5	6.548	0.0002166	0.952	9.71	31	1.637	0.0002583	0.943
9.71	31.5	6.548	0.0002166	0.962	11.64	31	1.637	0.0002583	0.948
11.64	31.5	6.548	0.0002166	0.97	13.58	31	1.637	0.0002583	0.951
13.58	31.5	6.548	0.0002166	0.973	5.83	31	2.455	0.0002583	0.917
5.83	32.5	0.819	0.000233	0.903	7.77	31	2.455	0.0002583	0.931
7.77	32.5	0.819	0.000233	0.915	9.71	31	2.455	0.0002583	0.944
9.71	32.5	0.819	0.000233	0.93	11.64	31	2.455	0.0002583	0.953
11.64	32.5	0.819	0.000233	0.935	13.58	31	2.455	0.0002583	0.958
13.58	32.5	0.819	0.000233	0.948	9.71	29	4.092	0.0002583	0.953
5.83	31	1.637	0.000233	0.919	11.64	29	4.092	0.0002583	0.958
7.77	31	1.637	0.000233	0.935	13.58	29	4.092	0.0002583	0.965
9.71	31	1.637	0.000233	0.943	5.83	31.5	6.548	0.0002583	0.946
11.64	31	1.637	0.000233	0.949	7.77	31.5	6.548	0.0002583	0.954
13.58	31	1.637	0.000233	0.953	9.71	31.5	6.548	0.0002583	0.963
5.83	31	2.455	0.000233	0.917	11.64	31.5	6.548	0.0002583	0.969

Table 2. Regression coefficients of the predicted quadratic polynomial model for response variables

Predictors	Coefficient (β)	F-value	Probability	Notability
Intercept	+0.95	---	0.0001	*
		Linear		
P_b	+0.015	388.39	0.0001	*
T_b	$- 9.374\times10^{-3}$	7.23	0.0150	**
C_b	+ 0.012	28.27	0.0001	*
F_b	$- 7.122 \times10^{-5}$	0.00175	0.9670	***
		Quadratic		
$P_b P_b$	$- 4.592\times10^{-3}$	32.23	0.0001	*
$T_b T_b$	-4.524×10^{-3}	2.38	0.1404	***
$C_b C_b$	$+ 5.643\times10^{-3}$	8.62	0.4414	***
$F_b F_b$	--------	----	------	----
		Interaction		
$P_b T_b$	$+2.720 \times10^{-3}$	5.81	0.0269	**
$P_b C_b$	-4.166×10^{-3}	10.41	0.0046	*
$P_b F_b$	$+1.997 \times10^{-3}$	2.53	0.128	***
$T_b C_b$	-----	---	-----	
$T_b F_b$	$+ 2.275 \times10^{-3}$	0.87	0.3631	***
$C_b F_b$	------	-----	-----	

*P<0.01; **P<0.05; ***P<0.1

Table 3. ANOVA table of the proposed model

Variable and source	D_f	Sum of squares	F- value
Model	11	$8.48\text{x}10^{-3}$	240.38
Residual	18	$5.77\text{x}10^{-5}$	---
Lack of fit	17	$5.77\text{x}10^{-5}$	---
Pure error	1	0	---
C.V=19%,		PRESS=$1.94\text{x}10^{-4}$	
R^2- predicted=0. 9772,		R^2 -adjusted= 0.9891	

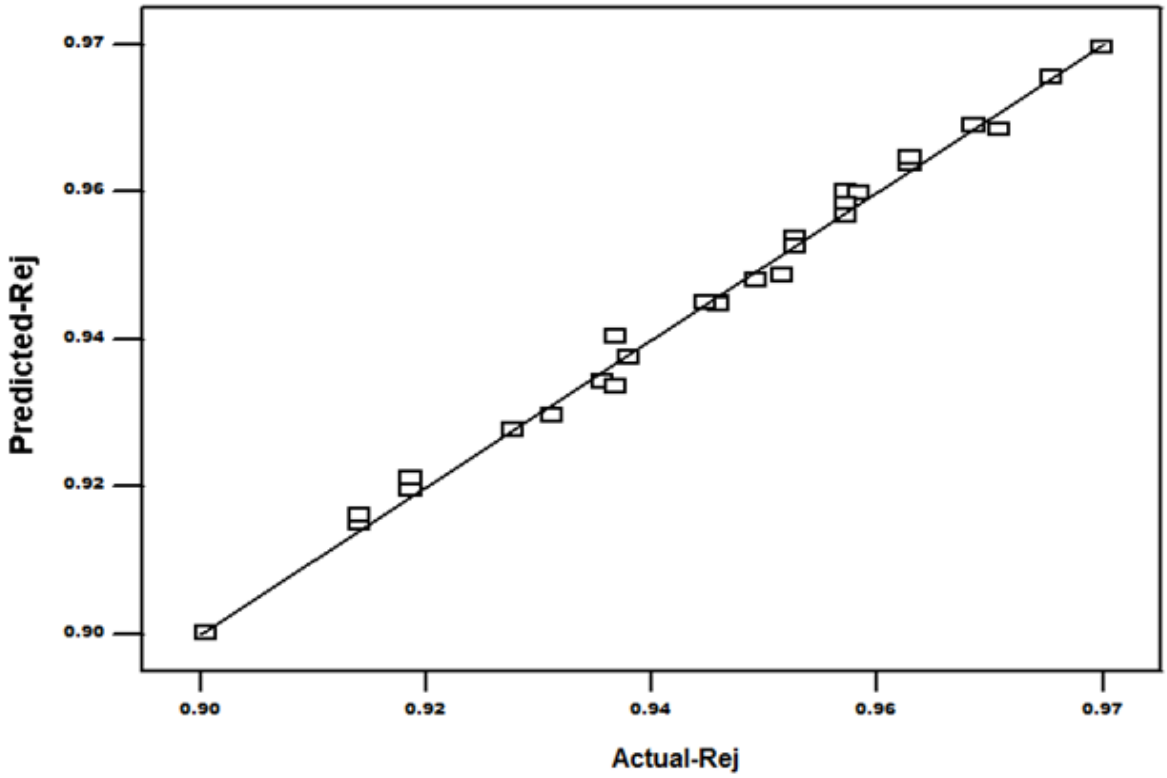

Figure 2. Plot of predicted dimethylphenol rejection against actual one (response)

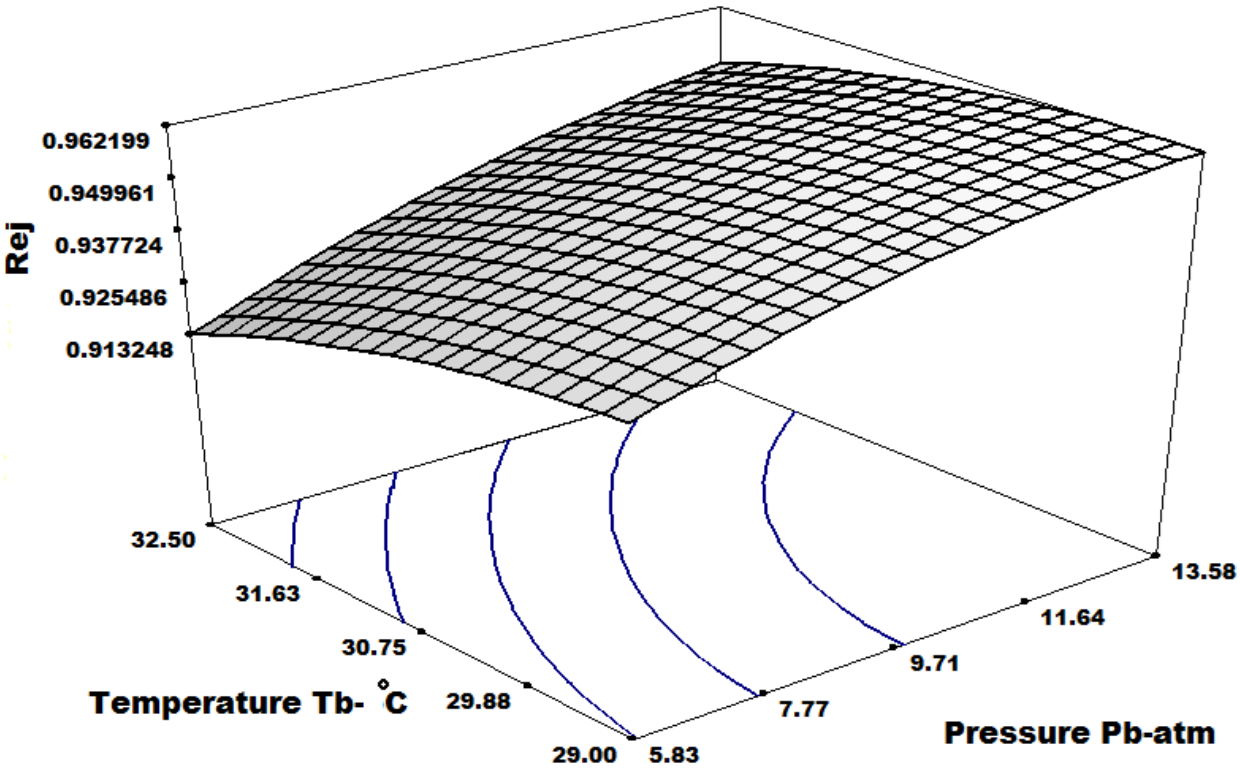

Figure 3. Response surfaces as contour plot of the effect of temperature and pressure on dimethylphenol removal

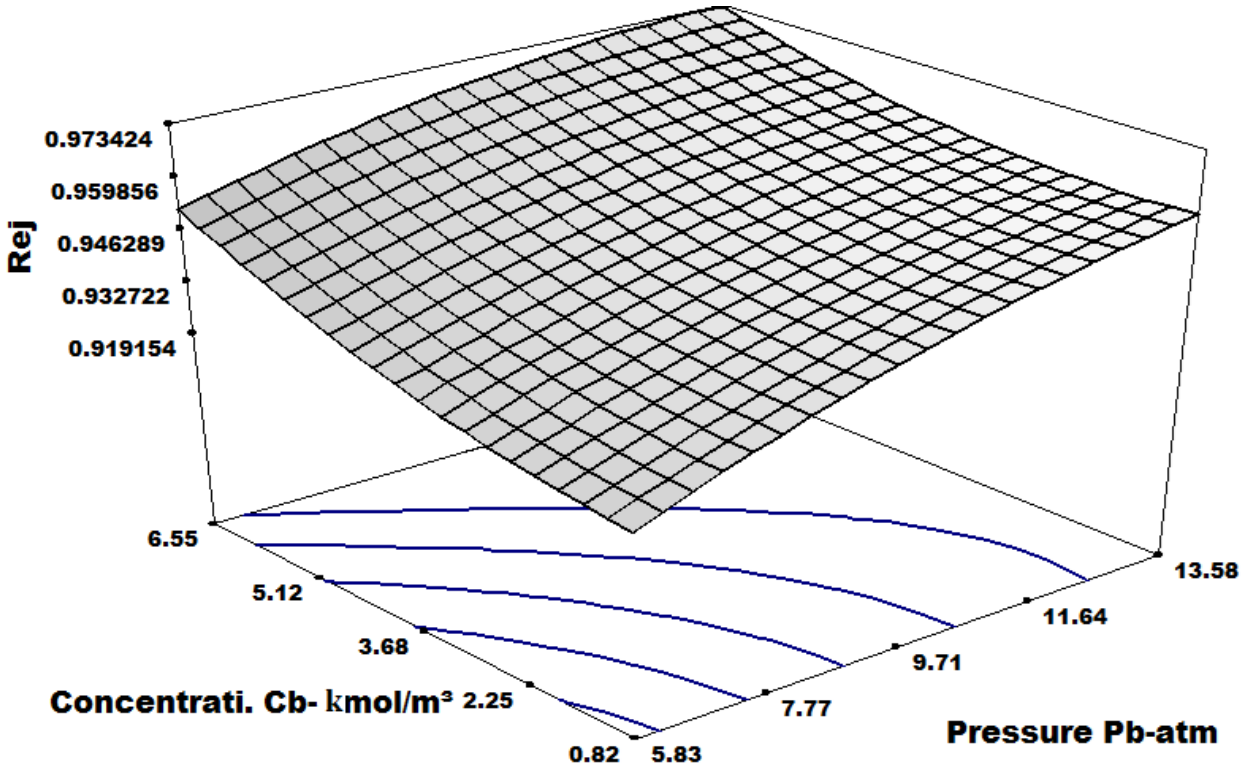

Figure 4. Response surfaces as contour plot of the effect of concentration and pressure on dimethylphenol removal

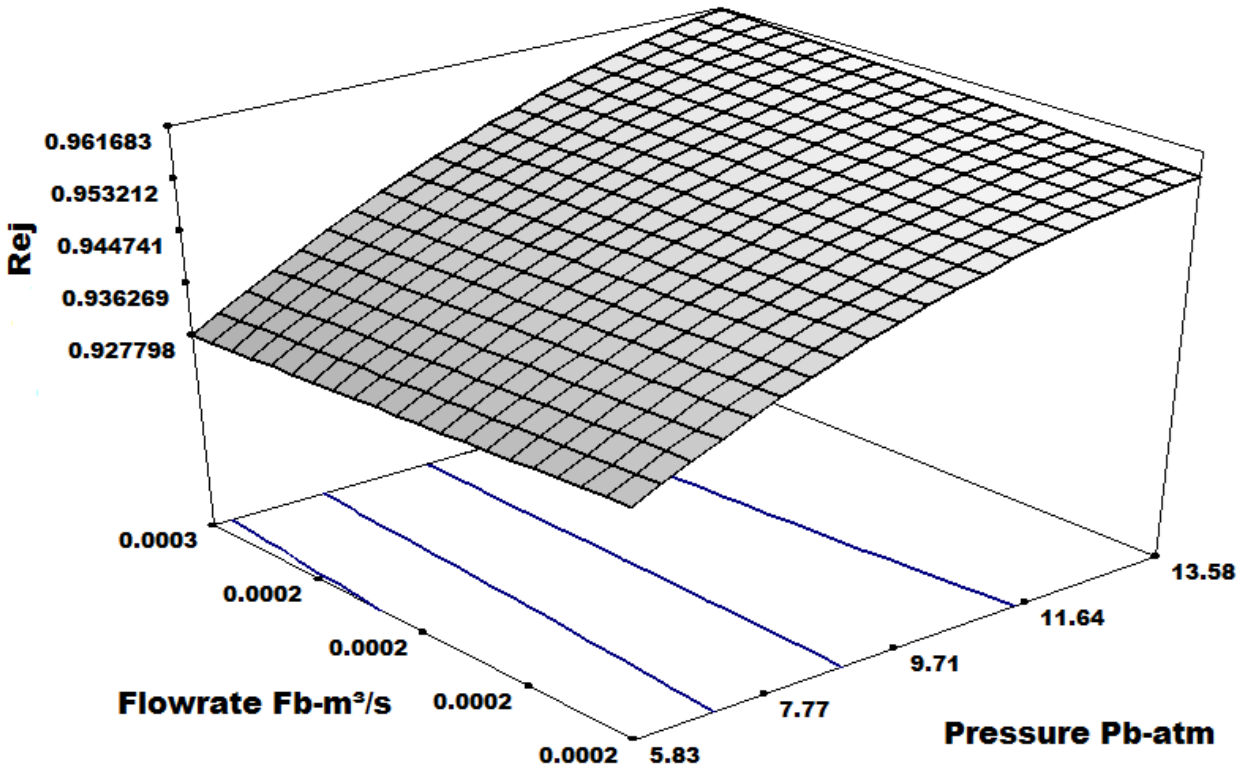

Figure 5. Response surfaces as contour plot of the effect of feed flow rate and pressure on dimethylphenol removal

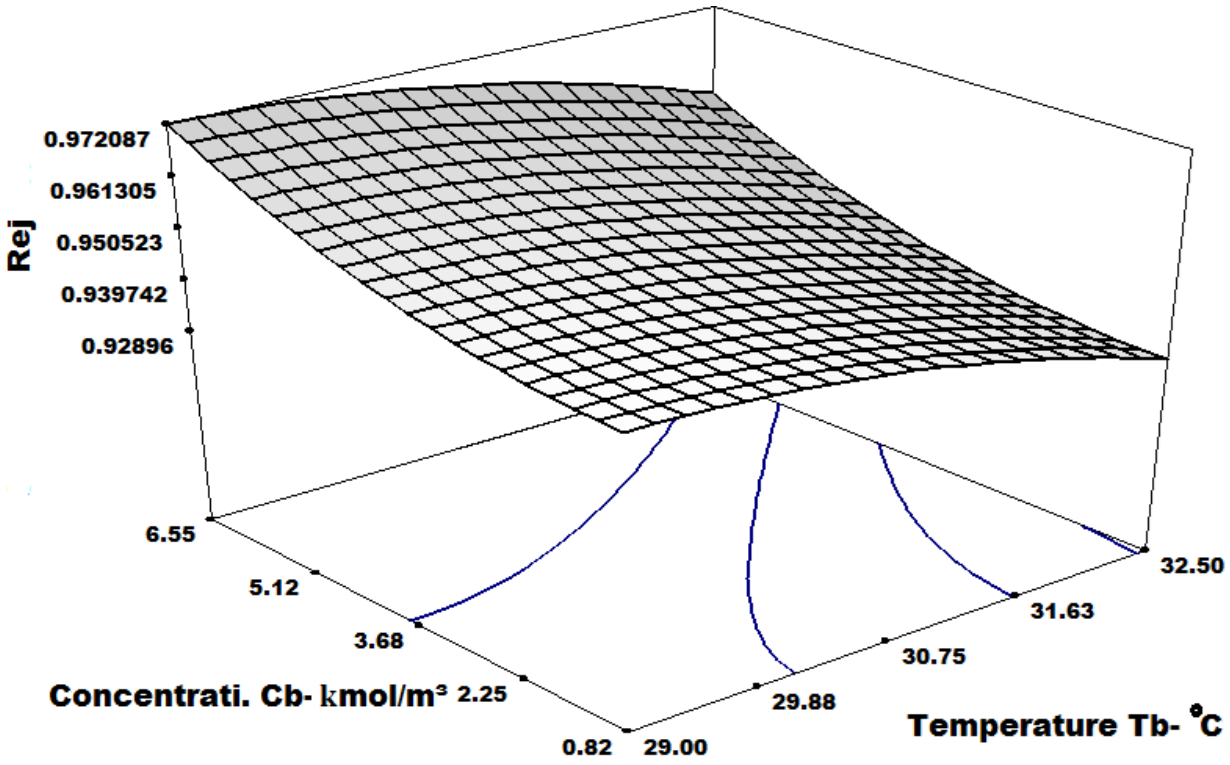

Figure 6. Response surfaces as contour plot of the effect of concentration and temperature on the dimethylphenol removal

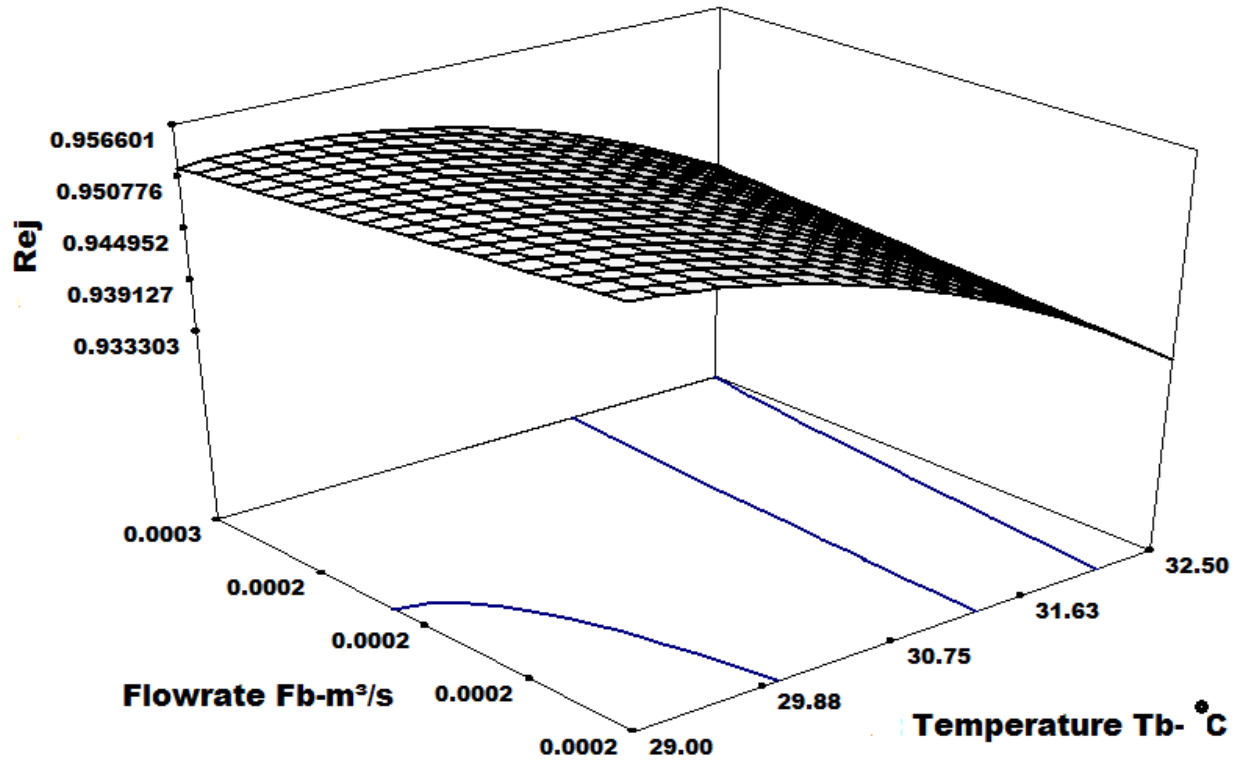

Figure 7. Response surfaces as contour plot of the effect of feed flow rate and temperature on the dimethylphenol removal

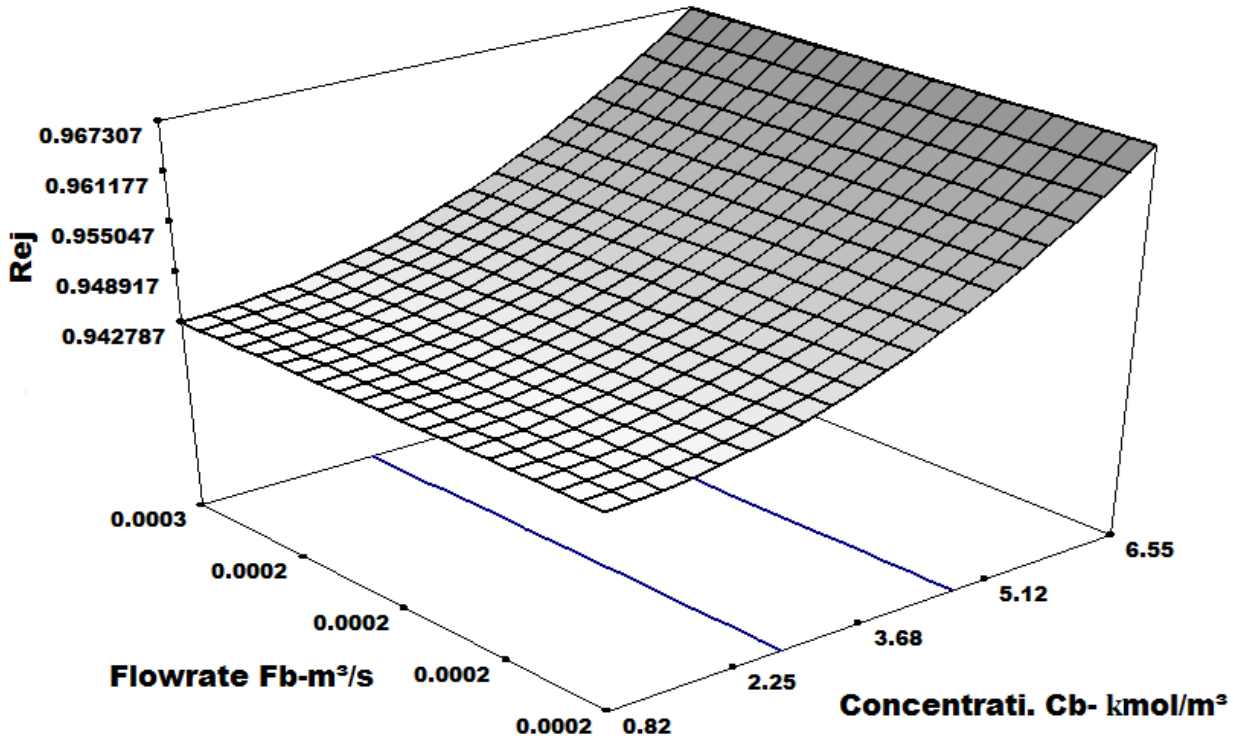

Figure 8. Response surfaces as contour plot of the effect of feed flow rate and concentration on the dimethylphenol removal