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RSM-BASED ANALYSIS AND OPTIMIZATION APPROACH FOR CHEMICAL PROCESSES

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Abstract: -

This research addressed a convenient analysis and optimization approach for chemical process based on software simulation, Response Surface Methodology (RSM) and the mathematical software Matlab simultaneously. A case study of CO_2 dehydration was used to showcase the capabilities of the model. In this paper, the objective of the model was to analyze the separate effects and interaction effects of factors to total energy cost of the CO_2 dehydration process, and obtain explicit formulae between independent parameters and response values. With Matlab, the minimum energy consumption was determined by optimization of parameter setting.

Keywords: - RSM, BBD, chemical process, optimization.

I. INTRODUCTION

Producing qualified product with minimal energy consumption is always the pursuit of chemical industry. Therefore, obtaining energy economization by giving proper parameter setting is imperative and valuable when adjust a plant or design a new process. In recent years, conventional methods using deterministic or stochastic techniques have been widely employed to identify optimal solutions from the formulated optimization model in various industrial applications^[1]. Usually, more than one factor which affects the energy consumption of a process exists. From the mathematic point of view, the relation between factors and energy cost can be concluded as follow:

$$f(x_1, x_2, \cdots x_n) = E$$

Where *E* is the total energy consumption of a process; x_i is the factor which has influence on the total energy consumption. According to whether the chemical process investigated is linear or not, function $f x x(1_2, x_n)$ "represents the linear/nonlinear mapping from the input space to the output space. Obviously, optimization is conducted within the space based on the scales of parameters.

However, most of the time, the relation are not explicit formulae in actual field^[2]. Even in the simulation software, the overall formulae are usually invisible or not straightforward to derive. Hence, univariate studies are often employed to investigate each factor's influence on energy consumption. Namely, adjust only one factor while keep other factors at a fixed level to study the change regulation of dependent value. Unfortunately, the evaluation of the interaction effects between the factors by univariate studies is impossible. If significant interaction effects between factors exist, the optimal conditions indicated by the univariate studies will be different from the correct results of the multivariate optimization^[3-5]. The larger the interaction effects, the greater the difference that will be found using univariate and multivariate optimization strategies^[6]. So the univariate procedure may fail since the effect of one variable can be dependent on the level of the others involved in the optimization. In another word, the combination of each factor at their local optimums doesn't guarantee that it is the global optimum when all the variables are changed simultaneously. Therefore, it is vital to conduct process optimization to attain global optimum based on explicit formulae. Herein, Response Surface Methodology (RSM), which combines experimental design with statistical analysis, can be utilized to investigate the single factor effects and interaction effects of parameters on the response values quantitatively^[7].

In this paper, a case study of CO_2 dehydration was implemented to showcase the capabilities of the RSM model. Based on the Aspen Hysys simulation of the dehydration unit, RSM model was established as the explicit water content and energy consumption quadratic models of the dehydration unit. After analyzing, the parameter setting was optimized with mathematical software Matlab. The merit of simplicity makes it convenient and practical for energy consumption analysis and optimization in process design and parameter adjustment.

II. CASE STUDY OF CO2 DEHYDRATION

A. Process description

To investigate the method of analysis and optimization to energy consumption in chemical process, this paper use CO_2 dehydration process as the case study. CO_2 capture, utilization, and sequestration (CCUS)^[8] is taken as a promising reduction alternative. However, CO_2 , comes from sources such as power plants, gas field, and facilities that consume fossil fuels, is always saturated with water^[9-11], which make it inefficient to transport and utilize CO_2 immediately. Moreover, when temperature decreases, high pressure in pipeline make it easy to result in pipeline blocking caused by the formation of carbon dioxide hydrate^[12]. Besides, free water in acid gas will contribute to corrosion of the plant and the pipeline^[13]. To avoid transport inefficiency, corrosion and hydrate formation, the water volume fraction in CO_2 stream should be limited within $500 \times 10^{-6[14-15]}$. To meet the water content requirement, acid gas dehydration by simple cooling and compression is not enough to avoid corrosion and hydrate problem^[16-17]. M. M. Faruque Hasan et al. suggested use the most economical alternative TEG-absorption^[8] for flue gas dehydration. The detailed configurations and description of the water absorption processes are presented in Figure 1.



Figure 1: The simplified flowsheet of CO₂ dehydration process A-Filter separator; B-Absorber; C-Flash tank; D-Desorber; E-Filter

Feed gas, removed free water and mechanical impurity in filter separator, is injected into the absorber bottom, reversely contact the Lean TEG to get dehydrated. Dried product gas is discharged from the top of absorber to the next unit, while

water-rich TEG is subsequently got throttled, flashed, and then regenerated in a distillation column (desorber) and the temperature of reboiler in this column is typically limited to 204 °C to avoid TEG thermal degradation. After regeneration, lean TEG gets pressure boosted by pump and enters into the absorber overhead.

B. Process simulation by Hysys

Herein, Aspen Hysys, commercially available software, was used as a prophase process simulator. Chen $Xi^{[18]}$ demonstrates that it is accurate to employ Aspen Hysys to describe CO_2 dehydration process. To model the thermodynamic properties of TEG and the dehydration process, the Peng–Robinson equation fluid package was utilized^[19].

Flow rate of feed gas, temperature of feed gas, pressure of absorber, plate number of absorber and concentration of lean TEG were set the same as the literature^[18]. Tray efficiency of absorber in TEG absorption is usually 25 %^[20]. The temperature of lean TEG entering into the absorber overhead is also vital for dehydration process, because too low temperature would result in TEG foaming while too high temperature would lead to TEG loss. So the inlet temperature of lean TEG was set 40 °C.

The parameters setting and their initial values are listed in Table 1 and the compositions of acid feed gas from article are given in Table 2.

Simulation parameters	unit	value
Flow rate of feed gas	kmol/h	867
Temperature of feed gas	°C	30
Pressure of absorber	kPa	4000
Plate number of absorber	floor	8
Tray efficiency	%	25
Concentration of lean TEG	%	98.7
Inlet temperature of lean TEG	°C	40
TEG circulation volume rate	L/h	200

Table 1: Parameters setting and variable value of simulation

Table 2: Composition of acid feed gas of CO₂ dehydration unit^[18] (y %)

CO ₂	N_2	H ₂ O	CH ₄	C2H6	C3H8
95.27976	1.24688	1.20000	2.21400	0.02968	0.02968

C. Parameter selection for RSM modeling

RSM is based on the work proposed by Box and Wilson^[7] in which experimental design and procedures were introduced for determining a path of steepest ascent and for exploring maxima and ridges. It was defined as a group of mathematical and statistical techniques for analyzing problems by investigating a response of interest influenced by variables or factors to be optimized. Modeling can be performed by extracting quantitative data from a set of experiments with an appropriate experimental design and fitting them into mathematical equations.

The energy consumption to CO2 dehydration process was calculated by Eq.2^[21]

(2)

$$=E_p+E_r$$

Ε

Where *E* is the total energy consumption of CO_2 dehydration unit, kW; E_p is energy consumption of circulation pump, kW; E_r is the calefaction heat quantity of reboiler, kW.

Flow rate of feed gas (X_1 , kmol/h), temperature of feed gas (X_2 , °C), pressure of absorber (X_3 , kPa) and TEG circulation volume rate (X_4 , L/h) usually have greater effect on the performance of absorption ^[22], which affect the water content of product gas and energy consumption of the process. Hence, these four factors and the response variables water content ($Y_{H2}O$, 10⁻⁶) and energy consumption (E, kW) were chosen.

The flow rate of feed gas and the temperature of feed gas were selected as the feed gas varying parameters, whose ranges were 693.6~1040.4 kmol/h (± 20 % of the flow rate value 867 kmol/h set in literature^[18]) and 20~30 °C (general temperature in industrial field), respectively. The investigation scale of absorption pressure was set ranging from 2000~4000 kPa and the variation range of TEG circulation volume rate was 140~200 L/h.

D. Sample points design

In general, a bulk of data is needed for regression to manifest the multivariate relation. For the sake of obtaining a precise fitting model with less data, some complex experimental sample point designs are introduced based on the orthogonal design, such as Doehlert matrix (DM), central composite designs (CCD) and three-level designs such as the Box-Behnken design (BBD)^[23,24].

Box-Behnken designs (BBD) are a class of rotatable or nearly rotatable second-order designs based on three-level incomplete factorial designs^[25]. It can be applied to evaluate the independent effects and interaction effects of parameters on the response values effectively with fewer experimental sample points^[6]. For three factors its graphical representation can be seen as the form below:



Figure 2: The cube for BBD and three interlocking 2² factorial design

A comparison between the BBD and other response surface designs (central composite, Doehlert matrix and threelevel full factorial design) has demonstrated that the BBD and Doehlert matrix are slightly more efficient than the central composite design but much more efficient than the three-level full factorial designs where the efficiency of one experimental design is defined as the number of coefficients in the estimated model divided by the number of experiments^[6].

Another advantage of the BBD is that it does not contain combinations for which all factors are simultaneously at their highest or lowest levels. So these designs are useful in avoiding experiments performed under extreme conditions, for which unsatisfactory results might occur.

According to Box-Behnken Design, flow rate of feed gas (X_1) , temperature of feed gas (X_2) , pressure of absorber (X_3) and TEG circulation volume rate (X_4) were arrayed with the assistance of software Design Expert. The factors distribution of response surface is listed in Table 3.

Table 3: Factors distribution of response surf
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F a atau 1aaa1		Factors selected in CO ₂ d	ehydration process	
	X_l , kmol/h	<i>X</i> ₂ , ℃	X3, kPa	<i>X</i> ₄ , L/h
-1	693.6	20	2000	140
0	867	25	3000	170
1	1040.4	30	4000	200

The formulae to the response surface model can be abstracted as follow:

$$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i< j}^{m} \beta_{ij} x_i x_j + \varepsilon$$
(3)

Where y is response value; x_i , x_j are the value of parameters investigated in different levels; *m* is the number of variables; β_0 is the constant term; β_i is the linear coefficient; β_{ii} is the quadratic coefficient; β_{ij} is the interaction coefficient; ε is the error term.

E. Model regression

The water content of product gas $(Y_{H2}O)$ and the energy consumption (E) of CO₂ dehydration process under different condition are listed in Table 4.

test number	X_l , kmol/h	<i>X</i> ₂ , ℃	X₃, kPa	<i>X</i> ₄ , L/h	YH2O, 10-6	E, kW
1	-1	-1	0	0	311	21.85
2	1	-1	0	0	359	25.21
3	-1	1	0	0	680	26.47
4	1	1	0	0	813	31.45
5	0	0	-1	-1	763	25.38
6	0	0	1	-1	480	22.76
7	0	0	-1	1	653	31.15
8	0	0	1	1	417	28.09
9	-1	0	0	-1	495	21.24
10	1	0	0	-1	590	25.25
11	-1	0	0	1	434	26.39
12	1	0	0	1	505	30.96
13	0	-1	-1	0	454	25.24
14	0	1	-1	0	1071	31.73
15	0	-1	1	0	306	23.08
16	0	1	1	0	645	28.19
17	-1	0	-1	0	637	25.82
18	1	0	-1	0	759	30.65
19	-1	0	1	0	407	23.33
20	1	0	1	0	478	27.5
21	0	-1	0	-1	360	20.86
22	0	1	0	-1	817	26.04
23	0	-1	0	1	317	25.95
24	0	1	0	1	698	31.94
25	0	0	0	0	501	26.11

 Table 4: Experimental design and simulation results of response surface

Based on the regression results, two formulae of the RSM model were obtained. Eq.4 describes the relation between the four factors and the water content of product gas. Eq.5 implies the relation between the four factors and the energy consumption of the CO_2 dehydration process.

$$Y_{H_2O} = 442.72222 + 0.2004x_1 - 0.4x_2 - 0.22625x_3 - 0.32778x_4 + 0.02451x_1x_2 - 7.35294 \times 10^{-5}x_1x_3 -1.1534 \times 10^{-3}x_1x_4 - 0.0139x_2x_3 - 0.12667x_2x_4 + 3.91667 \times 10^{-4}x_3x_4 - 7.89888 \times 10^{-5}x_1^2 +1.72x_2^2 + 7.2875 \times 10^{-5}x_3^2 + 5.83333 \times 10^{-3}x_4^2 E = 7.76019 + 2.63841 \times 10^{-3}x_1 - 0.21533x_2 - 2.9725 \times 10^{-3}x_3 + 0.074093x_4 + 4.67128 \times 10^{-4}x_1x_2$$
(4)

$$9.51557 \times 10^{-7} x_1 x_3 + 2.69127 \times 10^{-5} x_1 x_4 - 6.9 \times 10^{-5} x_2 x_3 + 1.35 \times 10^{-3} x_2 x_4 - 3.66667 \times 10^{-6} x_3 x_4 - 2.06479 \times 10^{-6} x_1^2 + 6.96667 \times 10^{-3} x_2^2 + 7.87917 \times 10^{-7} x_3^2 - 8.42593 \times 10^{-5} x_4^2$$
(5)

F. Model verification

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The variance analysis of the quadratic regression model using Design Expert is listed in Table 5, and the variance analysis of the RSM model is shown in Table 6.

	1 .	1.	c ·	C /1	•	1	• 1	1
Table 5. An	alveie r	esults of	t variance	for the	regression	noly	vnomial	mode
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		Formula 1				Formula 2				
source	Sum of Squares	Mean Square	F Value	p-value	Sum Squares	of Mean Square	F Value	p-value		
Model	885300	63239.16	181.73	< 0.0001	270.47	19.32	1391.48	< 0.0001		
X_{I}	24300	24300.00	69.83	< 0.0001	55.99	55.99	4032.45	< 0.0001		
X_2	570700	570700	1640.13	< 0.0001	94.25	94.25	6788.17	< 0.0001		
X_3	214400	214400	616.14	< 0.0001	24.14	24.14	1738.67	< 0.0001		
X_4	19280.08	19280.08	55.41	< 0.0001	90.48	90.48	6516.43	< 0.0001		
$X_1 X_2$	1806.25	1806.25	5.19	0.0459	0.66	0.66	47.26	< 0.0001		
$X_1 X_3$	650.25	650.25	1.87	0.2016	0.11	0.11	7.84	0.0188		
$X_1 X_4$	144.00	144.00	0.41	0.5345	0.078	0.078	5.65	0.0389		
$X_2 X_3$	19321.00	19321.00	55.52	< 0.0001	0.48	0.48	34.29	0.0002		
$X_2 X_4$	1444.00	1444.00	4.15	0.0690	0.16	0.16	11.81	0.0064		
$X_3 X_4$	552.25	552.25	1.59	0.2364	0.048	0.048	3.49	0.0914		
X21	15.93	15.93	0.046	0.8349	0.011	0.011	0.78	0.3968		
X22	5220.71	5220.71	15.00	0.0031	0.086	0.086	6.17	0.0323		
X23	14995.10	14995.10	43.09	< 0.0001	1.75	1.75	126.25	< 0.0001		
X24	77.82	77.82	0.22	0.6464	0.016	0.016	1.17	0.3049		
Residual	3479.75	347.98			0.14	0.014				
Cor Total	888800				270.61					

Table 6:	Variance a	analysis	of the	RSM model
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	Std. Dev.	R-Squared	Adj R-Squared	Adeq Precision
Model 1	18.65	0.9961	0.9906	51.098
Model 2	0.12	0.9995	0.9988	121.579

Both the p-values of Formula 1 and Formula 2 were less than 0.0001, and the relative Error between predicted values and Hysys values were low, which suggest that the regression model was significant to describe the water content of product gas and energy consumption of the process when feed gas condition changed. The high correlation ratio R-Squared (0.9961 and 0.9995 of Formula 1 and 2, respectively) guaranteed that the model is reliable. The adjusted correlation ratio R-Squared were 0.9906 and 0.9988, which mean the regression model can describe 99.06 % variance of the water content and 99.88 % variance of the energy consumption. The Adequate Precision values 51.098 and 121.579 (higher than required value: 4) of Formula 1 and 2 show the rationality. Comparison between predicted values and Hysys values are listed in Table 7. The low Relative Error demonstrated the accuracy of the RSM model.

	Input	Value		RSM Out	put Value	Hysys Output Value		
X_{l} ,	X_2 ,	Хз,	X4,	Y_{H_2O} ,	Ε,	Y_{H_2O} ,	Е,	
kmol/h	°C	kPa	L/h	10-6	kW	10-6	kW	

 Table 7: Comparison between predicted values and actual values

	Input	t Value		RSM Out	tput Value	Hysys Ou	itput Value	Relative Error		
X_{l} ,	X2,	Хз,	X4,	Y_{H_2O} ,	Ε,	Y_{H_2O} ,	Е,	$Y_{H_2O}\%$,	<i>E%</i> ,	
kmol/h	°C	kPa	L/h	10-6	kW	10-6	kW	%	%	
750	29	3800	150	592.4	24.15	603.1	24.23	1.81	0.330	
800	27	3400	160	537.3	24.96	543.3	25.03	1.12	0.280	
850	25	3000	170	496.6	25.90	497.2	25.89	0.121	0.0386	
900	23	2600	180	470.3	26.95	466.4	26.86	0.829	0.335	
950	21	2200	190	458.5	28.12	451.3	28.03	1.57	0.321	

III. Analysis and optimization

A. Analysis of response surface model

Response surfaces were attained utilizing Design Expert based on the regression model. The single factor effects and interaction effects on the response values were shown by three-dimension graphs directly.

The slight curvature of the surface and the irregular frontier in Figure 3 and Figure 4 suggested that high order relation rather than simple linear relation existed in the model. The unequal distance of contour line suggested that the interaction effect existed between parameters.

According to Figure 3 and Figure 4, the higher the flow rate of feed gas and temperature of feed gas, the higher the water content and energy consumption. Higher flow rate make feed gas carry more water, which resulted in inadequate water absorption and higher energy penalty for TEG regeneration. Higher temperature leads to higher absolute humidity of feed gas. Under saturation state, feed gas contains more water, so it exhibited the same effect. By combining this information with the p-value in Table 5, the temperature of feed gas had stronger effect than flow rate of feed gas on the response values. Correspondingly, when feed gas conditions varied and the water content and the energy consumption went higher, the rise of TEG circulation volume and pressure of absorber were helpful to mitigate the undesired effect. That is because higher pressure is good for absorption and higher TEG circulation is beneficial to carry more water. And the pressure of absorber played a greater role.

The interaction effect between parameters on the response values is also worth to be discussed. From Figure 3 and Figure 4 along with p-value in Table 5, the interaction effect between temperature of feed gas and pressure of absorber had significant influence on the water content. From Figure 3(b), the pressure had more influence on the water content when temperature was higher. While the interaction effect between flow rate of feed gas and temperature of feed gas had significant influence on the energy consumption. From Figure 4(a) the equivalent rise of flow rate resulted in more energy consumption at high temperature level than low temperature level. Apart from these two extremely significant interaction effects, other significant mutual effects also existed. Remarkable on water content were the flow rate and temperature of feed gas. Significant on energy consumption were temperature of feed gas and pressure, temperature of feed gas and TEG circulation rate, flow rate of feed gas and pressure, flow rate of feed gas and TEG circulation rate. Interaction effects between other parameters were negligible in this study.





Figure 3: Influence of factors on water content of product gas





Figure 4: Influence of factors on energy consumption

Combined with Table 5, it can be concluded that, the degree of significance on the water content and the energy consumption for single factor, in an order from high to low, are $X_2 > X_3 > X_1 > X_4$ and $X_2 > X_4 > X_1 > X_3$ respectively. The degree of significance on the water content and the energy consumption for interaction effect, in an order from high to low, covers: $X_2 X_3 > X_1 X_2$ and $X_1 X_2 > X_2 X_3 > X_2 X_4 > X_1 X_3 > X_1 X_4$, respectively (items whose significant degree p-value > 0.05 were omitted).

B. Optimization of parameters in dehydration process

In the operation process, the appropriate setting of parameters for device is beneficial to ensure the dehydration plants operate more efficiently and economically. Based on the characteristics of the process, achieving parameter optimization with software can be instructive for field operation.

In reality, once given the variation scales of parameters, the minimum consumption is definitely existent, so a convergent solution for the problem of the original nonlinear response surface model is guaranteed theoretically.

Based on the analysis above, flow rate of feed gas, temperature of feed gas, pressure of absorber and TEG circulation volume rate were taken into consideration in the parameter setting optimization. Both flow rate of feed gas and temperature of feed gas are the conditions of feed gas. Flow rate of feed gas is usually uncontrollable in field, so its value was set 867 kmol/h (the same as initial setting value). While temperature of feed gas can be adjusted by additional water cooler. According to Eq.3 and the three-dimension graphs, the nonlinear relation exhibited between the four parameters and water content. To meet the water content requirement and obtain the minimum energy consumption simultaneously, Matlab was used in this paper to solve the Minimax Problem in parameter optimization by Nonlinear Programming.

Here, the minimum energy consumption *E* was taken as the objective function, the variation range of each parameter was taken as linear constraint condition, while keeping the water content $Y_{H2}O$ within 500×10^{-6} was regarded as the nonlinear constraint condition to meet the water content requirement.

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$$\min E = 7.76019 + 2.63841 \times 10^{-3} x_{1} - 0.21533x_{2} - 2.9725 \times 10^{-3} x_{3} + 0.074093x_{4} + 4.67128 \times 10^{4} x_{1}x_{2} - 9.51557 \times 10^{-7} x_{1}x_{3} + 2.69127 \times 10^{-5} x_{1}x_{4} - 6.9 \times 10^{-5} x_{2}x_{3} + 1.35 \times 10^{-3} x_{2}x_{4} - 3.66667 \times 10^{-6} x_{3}x_{4} - 2.06479 \times 10^{-6} x_{1}^{2} + 6.96667 \times 10^{-3} x_{2}^{2} + 7.87917 \times 10^{-7} x_{3}^{2} - 8.42593 \times 10^{-5} x_{4}^{2} s.t. Y_{H_{2}O} = 442.72222 + 0.2004x_{1} - 0.4x_{2} - 0.22625x_{3} - 0.32778x_{4} + 0.02451x_{1}x_{2} - 7.35294 \times 10^{-5} x_{1}x_{3} - 1.1534 \times 10^{-3} x_{1}x_{4} - 0.0139x_{2}x_{3} - 0.12667x_{2}x_{4} + 3.91667 \times 10^{-4} x_{3}x_{4} - 7.89888 \times 10^{-5} x_{1}^{2} + 1.72x_{2}^{2} + 7.2875 \times 10^{-5} x_{3}^{2} + 5.83333 \times 10^{-3} x_{4}^{2} \le 500 x_{1} = 867 200 \le x_{3} \le 4000 140 \le x_{4} \le 200$$

Eq.6 was calculated with Matlab to obtain optimization. The comparison of parameter setting, water content and energy consumption before and after optimization are shown in Table 8.

	Table 8	: Com	parison	of	parameters and	i res	ponse va	lues	before a	and af	ter o	ptimization
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	X ₁ , kmol/h	<i>X</i> ₂ , ℃	<i>X</i> ₃ , kPa	<i>X</i> ₄ , L/h	<i>YH2O</i> , 10- 6	E, kW	Energy rate, %	saving
Initial value Optimized value	867 867	30 20	4000 3611.3	200 140	602 334	30.97 20.51	33.77	

Table 8 showed that, compared with the initial response values, the energy consumption decreased by 33.77% theoretically after optimization, and the water content was within the requirement(lower than initial water content) at the optimum parameters setting. The lower water content and lower energy consumption showed that, based on the explicit formulae, optimizing the parameter setting with mathematical software to improve the performance of CO₂ dehydration process is feasible.

IV. CONCLUSIONS

According to the investigation of CO₂ dehydration process, results showed that:

- 1、 RSM model was significant manifest the single factor effects and interaction effects of parameters on energy consumption of the device.
- 2. With the assistance of BBD sample point design method, RSM Modeling could be performed by extracting quantitative data from a set of experiments and fitting them into mathematical equations.
- 3. Based on the regressed explicit formulae and constraint relation, using Matlab, the optimal energy consumption could be obtained by optimization of parameter setting theoretically.

Given similar parameter setting adjustment and design problem widely exist in chemical process, analysis and optimization with RSM is a convenient method to put into practical engineering applications.

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