Modeling and Optimization of Fiber Optic Chemical Vapor Sensor

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***Abstract*—This paper discusses the application of Box–Behnken Design (BBD) to get a mathematical model for chemical vapor liquid detection with the objective of optimizing the optical fiber optic sensor probe. The parameters of input process were considered as variables to create the output parameters (response) using Response Surface Methodology (RSM). Input parameters such as length of probe, diameter of probe, photo-initiator liquid, vacuum pressure of chamber and purity of liquid detector were processed with Box – Behnken design approach for making POF (plastic optical fiber) probe of chemical sensor. Design Expert software was used to design the experiments with randomized runs. The main aim is to create an equation model as a platform for the probe design of POF chemical vapors detection similar to acetone, ethanol and methanol liquid. The experimental data were processed by considering the input parameters. The contribution of this research is the mathematic equation model that applies the polynomial equation. The final result of the wavelength application was between five to be three wavelengths, 434.05 nm, 486.13 nm and 656.03 nm. These wavelengths are the significant result of optimization measured using three chemical vapors. The optimization process uses the analysis of variables (ANOVA) to produce the quadratic model equation.**

***Index Terms*—Box–Behnken Design; Design–Expert Software; Fiber Optic Chemical Vapor Sensor; Math-Optimization Model.**

I. INTRODUCTION

Plastic optical fiber probe for chemical vapor detection has been widely used in experimental and industrial scale [1, 2]. Most of POF (plastic optical fiber) probe usually were created with the many of custom variables. One of the main variables is cladding modification of POF by substituting Zinc Oxide (ZnO) layer. The method of measurement uses fabry–perot interferometer and LED super bright as a light source to get sufficient reflection of light from the end of probe tip.

In order to function as a sensor, chemical vapor detection is conducted in a chamber that can regulate air pressure. Three chemical liquid such as Acetone, Ethanol and Methanol were chosen in this experiment to get the chemical vapor that drives the changes of refractive index from the sensor probe. To produce the optimum optical probe, it must be considered other variables, such as the length of probe as x_1, diameter of probe as x_2, doping of photoinitiator liquid as x_3, vacuum pressure in chamber as x_4 and purity of chemical vapor detection as x_5, as the independent variables. The reflection intensity from five particular wavelengths was used as dependent variables.

Box–Behnken experimental design or BBD, which is a well known and most common multi-factorial design of response surface methodology (RSM) in various experiments[3] has been applied in the optimization of probe sensing design. The second-order model has always been used in RSM due to its many advantages: It consists of less number of experiments, suitable with multi-variables and able to explain correlation of each variable [4-6].

The final result determined the optimum values generated from the mathematical model platform. In this study, the authors investigated the chemical vapor detection using plastic optical fiber probe [7] created by the modification of the cladding site with ZnO nano-powder.

II. EXPERIMENTAL PROCEDURE

In this experiment, the vacuum chamber was used as a place of POF probe for detection of chemical vapor from the liquid chamber. The chamber circumstances were set to low-pressure using the vacuum pump that was intended to take up the chemical vapor so that it can change the refractive index of POF probe. The air pressure was regulated by two air valves positioned at the top of the testing chamber.

Figure 1 shows the set-up experiment of chemical vapor detection at the vacuum chamber. Air pressure was sucked using the oil vacuum pump. Light source was injected into the POF Y-coupler to allow it to transmit until the end of probe. When the chemical vapor affected the probe surface area, the POF probe changed the refractive index, which then caused the reflecting light to move the spectrometer.

POF probe was inserted into the hole of the detection chamber. Here, the chemical vapor moved into the chamber when the vacuum pump sucked the air vapor. This situation was controlled until the air pressure was positioned at low level by regulating the outlet valve. In this set-up, white

light source was used to read the changing of the light reflection intensity. Spectrometer USB4000 VIS-NIR used to detect the light was connected to the data recorder.

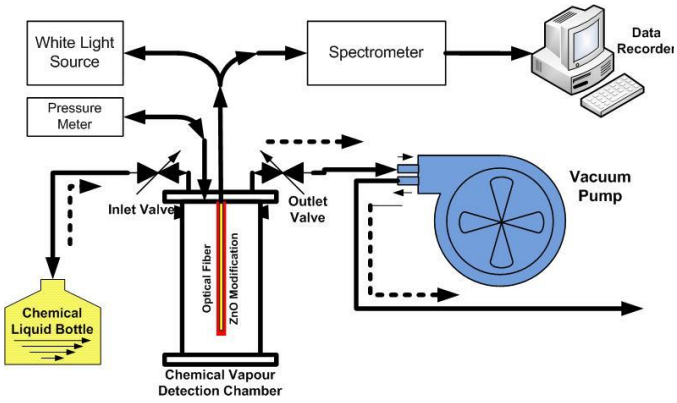

Figure 1: Set-up experiment of chemical vapor

Figure 2 exhibits all parts used in this experiment, together with three chemical vapors detector, namely the Acetone, Ethanol and Methanol that were tested at separate places and different time. Data were collected from the recorder created by SPECTRASUITE application from Ocean Optic. The number of experiment was adjusted according to the methodology of the experiment.

Figure 2: Setup Experiment with three chemical vapors; Acetone, Ethanol and Methanol

III. COATING MATERIAL

ZnO nano powder from SIGMA – ALDRICH was mixed with the methanol liquid. Additional adhesive liquid called photo-initiator was granted with the amount of 0.05 ml, 0.10 ml and 0.20 ml. It was given based on the code of -1, 0 and 1, where -1 as the lowest and +1 as the highest value. The coating liquid was mixed following the process of probes coating as shown in Table 1. After this process, it was dried for six hours until the powder can be attached to the probe head. The mixed liquid was used in the coating process of the optical fiber as shown in Table 1. After the coating process, the optical fiber was left to dry for about 24 hours, so that the ZnO powder can stick into the end of the probe tip.

Figure 3(a) shows ZnO nano powder as coating material. The mixing process consists of 30 ml methanol that is mixed with 0.4884 gram of ZnO material. This process is shown in Figure 3(b) that used the hotplate and stirrer.

(a) (b)

Figure 3: ZnO material;(a). Intake of ZnO nanopowder adjusted with mixing ratio. (b). Mixing process of ZnO with Methanol liquid using hotplate and stirrer

IV. METHODOLOGY

It can be shown from the references [8-10] the development and current applications can be improved using RSM for explaining the parameters of output in many variables input. The response surface methodology promotes the relations between the two or more response variables. The main idea of RSM is to apply a sequence of designed experiments to find an optimal response. The design procedure of RSM is as follows; (1) creating a series of experiments for adequate and reliable measurement, (2) extending a mathematical model of the second order response, (3) searching for the optimum experimental parameters that generate a maximum or minimum value of response, (4) explaining direct and interactive effects of the parameter procedure using graphs. Figure 4 shows the flowchart of the design experiment that aims for efficiency to get more information from fewer experiments by focusing on collecting required information only

RSM design recommends us to calculate interaction and even quadratic effects. It gives us an idea of the local shape of response surface under investigation. Box-Behnken design is one of design experiments of RSM. It is an efficient design for fitting second-order polynomials to response surface because it applies relatively small number of observation to calculate the parameters. The detection process of POF probe,

V. BOX BEHNKEN DESIGN

Box Behnken is an experimental design for response surface methodology (RSM) to achieve the following aims:

i. Each factor or independent variable is placed at one of three equally spaced values, usually coded as -1, 0 and 1.
ii. It should be sufficient to fit a quadratic model that is one containing squared terms and products of two factors.
iii. The ratio of experimental number points the number of coefficients in the quadratic model that should be reasonable in the range 1.5 to 2.6.
iv. The estimation variance should more or less depend

on the distance from the center only.

The Box–Behnken proposed three level designs for fitting response surface. These designs were created by combining 2^k factorials with incomplete block design [11]. Figure 5 shows the three variables of Box–Behnken design. It can be remarked that Box–Behnken design is a spherical scheme with all points lying on radius sphere. Box–Behnken design does not contain any point at the nodes of the cubic region created by the upper and lower limits. BBD needs fewer treatment combinations than a CCD and rotatable in problem with 3 and 5 factors.

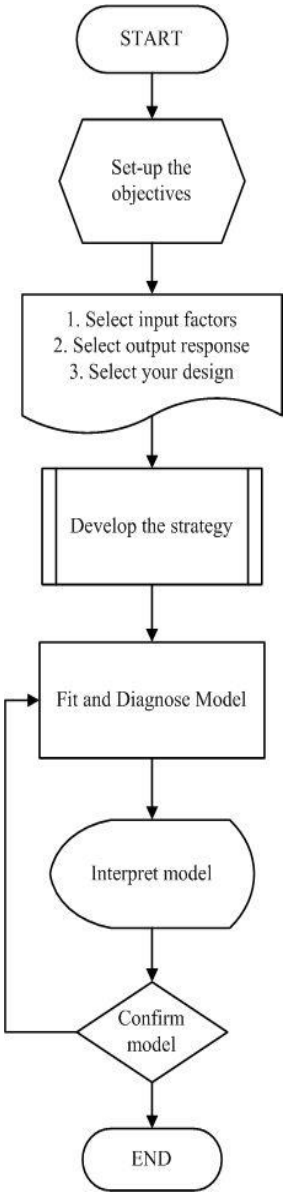

Figure 4: Design of experiments flowchart

The design of RSM allows the calculation of variable interaction and even-quadratic effect. It also gives the ideas from RSM form that was being investigated. The Box-Behnken design has a maximum efficiency for RSM problems involving five factors with three-level factorial. The process number lower than the center composite design (CCD) is required. The RSM is an optimum way to assess the relationship between the experiment output (response) and any factors called as X_1, X_2, X_3, and others. This method is always used in the combination form with factorial design method like the Box–Behnken design and CCD design. The application of Box–Behnken can reduce the sum of constant number without the lack of optimization constant in comparison to the traditional factorial design [11-14].

Run	x_1	x_2	x_3
1	−1	−1	0
2	−1	1	0
3	1	−1	0
4	1	1	0
5	−1	0	−1
6	−1	0	1
7	1	0	−1
8	1	0	1
9	0	−1	−1
10	0	−1	1
11	0	1	−1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0

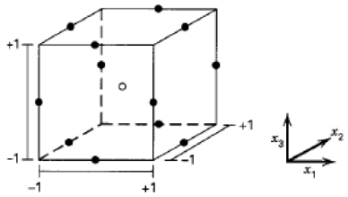

Figure 5: Three variables of Box – Behnken design[8].

Table 1
Minimum and maximum level from four variables factors at coded and un-coded symbol.

Variables	Symbol		Level		
	Coded	Un-Coded	-1	0	1
Probe length (cm)	x_1	X_1	2.5	6.25	10
Probe Diameter (mm)	x_2	X_2	0.51	0.69	0.87
Doping Photo-initiator (ml)	x_3	X_3	0.05	0.125	0.2
Pressure of Vacuum Chamber (mBar)	x_4	X_4	0	50	100
Purity of Liquid detector (%)	x_5	X_5	10	55	100

The minimum and maximum interval of five variables represented by coded and un-coded symbols are shown in Table 2. The correlation of coded and un-coded variables are explained by the following equations [15-17]:

$$x_1 = \frac{(X_1 - 6.25)}{3.75} \quad (1)$$

$$x_2 = \frac{(X_2 - 0.69)}{0.18} \quad (2)$$

$$x_3 = \frac{(X_3 - 0.125)}{0.075} \quad (3)$$

$$x_4 = \frac{(X_4 - 50)}{50} \quad (4)$$

$$x_5 = \frac{(X_5 - 55)}{45} \quad (5)$$

where X_1, X_2, X_3, X_4, X_5 are the un-coded variables and x1, x2, x3, x4,x5 are the coded variables. Two types of variable that have particular unit and effects of variables on detection efficiency can be approached by using a second order of polynomial model that is written in equation [14, 18-20],

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_i {x_i}^2 + \sum_i \sum_j \beta_{ij} x_i x_j + \varepsilon \quad (6)$$

where ε is random error, β_0 is defined as the intercept coefficient, β_i is the linear and quadratic interaction coefficient, β_{ij} is the second order of interaction coefficient and k is the number of independent parameter. Equation (6) can be rewritten into the matrix form as in (7):

$$y = \beta x + \varepsilon \quad (7)$$

Detail solution of Equation (6) and (7) can be explained with the matrix approach with reference to [10]. The preparation of chemical vapor experiment using optical fiber is shown in Figure 2. This experiment consists of chemical liquid chamber, chemical vapor detection chamber, vacuum suction pump, pressure meter, white light source and spectrometers Ocean Optic (USB4000VIS-NIR). In the internal part of the detection chamber, it is a place of probe position that performs the experiment of fiber optic with variety of sizes which are detectable in each of the probes.

Vacuum suction pump was used to attract the chemical vapor in the liquid chamber. Chemical vapor escaped through the output line from the suction pump. The air pressure on the detection chamber was controlled by the alignment of outlet valve with the suction power by the pump. Spectrometer was used as a detector of spectrum from the light source transmitted by the fiber optic.

VI. Result and Discussion

The proposed Box–Behnken design requires 46 processes for response surface model [4, 21, 22]. The parameter process for experimental runs was selected based on the standard design shown in Figure 5. Detail of the experimental runs with input data set that has been carried out is shown in Table 2.

Design expert application software was used to design the experiment and randomized process [4]. Randomized process is more useful to ensure that the conditions in the term do not depend on the previously run process and predict the situation in the next run. The randomized process is important in the experiment as it helps to follow the right track and can be defended, depending on the result of the run.

The experiment result requires meaningful analysis of each variable. Table 3 shows that F-Value is 1.87 implying that the model was not significant for the surrounding disturbance. There is a 12.20% chance that a large F-value could occur due to noise and the values of "prob > F". P-value less than 0.05 indicates that the model is significant. In this case, *A-Probe Length* is a significant model. Values greater than 0.1 indicate the model terms are not-significant [3, 4, 23].

If many parts of the model terms are not significant (not including models that is required to support the hierarchical modeling), the model reduction can improve the proposed model. The lack of fit from F-value is 0.80, implying that the relative value is not significant to the Pure Error. There is 69.45% chance that the lack of fit from F-value can cause disturbance. No significant value due to lack of fit is a good value because the model expectancy is suitable to be applied.

Table 4 shows that F-value is 3.07, implying that the model is significant. There is 0.44% chance that one of the F-values can occur due to disturbances. P-value less than 0.05 means that the part of the model term is significant.

In the case of *E-Purity of Detection Liquid*, *E^2* is a significant part of the model. If there are many parts that are not significant (not including model that is required to support hierarchical modeling), model reduction can improve the proposed model. The lack of fit value is 0.90, implying that it is not obvious to a Pure Error. There is a 61.13% chance that a lack of fit that indicates good conditions because it is considered as suitability of the model.

In addition, the model is validated using analysis of variable (ANOVA). As shown in Table 4, the model is validated by experiments with new parameter to measure the value of ranged reactions and compare with the prediction of equation model. The details of the experiments and calculated from the output variables are given in Table 6, 7 and 8.

Table 2
Box – Behnken Design for the Experiment

Run	Probe Length (cm)	Probe Diameter (mm)	Doping Photo-initiator (ml)	Pressure of Vacuum Chamber (mBar)	Purity of detection liquid (ml)
1	10	0.87	0.125	50	55
2	10	0.69	0.125	50	100
3	6.25	0.87	0.05	50	55
4	10	0.69	0.125	50	10
5	6.25	0.69	0.125	50	55
6	6.25	0.69	0.05	50	10
7	2.5	0.69	0.125	50	10
8	2.5	0.69	0.125	100	55
9	6.25	0.51	0.2	50	55
10	6.25	0.69	0.125	50	55
11	6.25	0.51	0.125	50	10
12	6.25	0.69	0.05	0	55
13	6.25	0.51	0.125	100	55
14	6.25	0.69	0.2	50	100
15	10	0.69	0.125	0	55
16	6.25	0.87	0.125	0	55
17	6.25	0.69	0.125	100	100
18	6.25	0.51	0.125	0	55
19	2.5	0.69	0.125	0	55
20	6.25	0.87	0.125	50	10
21	6.25	0.69	0.125	50	55
22	2.5	0.69	0.2	50	55
23	10	0.69	0.05	50	55
24	6.25	0.69	0.05	100	55
25	10	0.51	0.125	50	55
26	6.25	0.87	0.125	100	55
27	6.25	0.51	0.05	50	55
28	2.5	0.69	0.125	50	100
29	6.25	0.69	0.2	50	10
30	2.5	0.87	0.125	50	55
31	6.25	0.69	0.125	0	100
32	6.25	0.69	0.125	50	55
33	6.25	0.69	0.125	0	10
34	2.5	0.69	0.05	50	55
35	6.25	0.69	0.2	100	55
36	6.25	0.69	0.125	50	55
37	6.25	0.69	0.2	0	55
38	6.25	0.51	0.125	50	100
39	2.5	0.51	0.125	50	55
40	6.25	0.69	0.05	50	100
41	6.25	0.87	0.125	50	100
42	6.25	0.87	0.2	50	55
43	10	0.69	0.2	50	55
44	6.25	0.69	0.125	50	55
45	10	0.69	0.125	100	55
46	6.25	0.69	0.125	100	10

VII. RESEARCH CONTRIBUTION

The experimental result discussed in the design of chemical detection is a mathematic equation as a platform for the probe design by considering five variables, namely the probe length, probe diameter, doping photo-initiator, pressure of vacuum chamber and purity of detection liquid.

Mathematic equation model can be applied with the calculated significant value. For chemical vapor detection, the formation of polynomial equation is drawn from Equation (8).

$$\begin{aligned} y(\lambda_n, \omega_m) = a_{0,\lambda_n,\omega_m} &+ b_{1,\lambda_n,\omega_m}X_1 + b_{2,\lambda_n,\omega_m}X_2 + b_{3,\lambda_n,\omega_m}X_3 \\ &+ b_{4,\lambda_n,\omega_m}X_4 + b_{5,\lambda_n,\omega_m}X_5 + c_{1,\lambda_n,\omega_m}X_1X_2 \\ &+ c_{2,\lambda_n,\omega_m}X_1X_3 + c_{3,\lambda_n,\omega_m}X_1X_4 \\ &+ c_{4,\lambda_n,\omega_m}X_1X_5 + d_{1,\lambda_n,\omega_m}X_2X_3 \\ &+ d_{2,\lambda_n,\omega_m}X_2X_4 + d_{3,\lambda_n,\omega_m}X_2X_5 \\ &+ e_{1,\lambda_n,\omega_m}X_3X_4 + e_{2,\lambda_n,\omega_m}X_3X_5 \\ &+ f_{1,\lambda_n,\omega_m}X_4X_5 + g_{1,\lambda_n,\omega_m}(X_1)^2 \\ &+ g_{2,\lambda_n,\omega_m}(X_2)^2 + g_{3,\lambda_n,\omega_m}(X_3)^2 \\ &+ g_{4,\lambda_n,\omega_m}(X_4)^2 + g_{5,\lambda_n,\omega_m}(X_5)^2 \end{aligned} \quad (8)$$

where, a, b, c, d, e, f and g are defined as constant equation depending on the wavelength and purity of detection liquid, λ_n is the wavelength used for vapor detection and n = 434.05 nm, 486.13 nm, and 656.03 nm, ω_m is the chemical vapor material and m is an integer represented as 1 for Acetone, 2 for Ethanol and 3 for Methanol.

The application of mathematical model in Equation (8) must be considered with the environment situation, the experiment of vacuum chamber at each chemical vapor detection and the positioning of probe. Table 5 shows the results of the different stage of responsive based on Equation (8) to re-test with the variables randomly. The result of re-testing was then compared with the results of the existed prediction.

Parameter of X_1, X_2, X_3, X_4 and X_5 was tested to get the validity of the data that is randomly valued to re-create the probe. This remake was the objective of testing the model that has been designed in Equation (8).

Table 6, 7 and 8 do not provide the information of the wavelength response for 397.14 nm and 410.05 nm. The reaction at these wavelengths from the beginning was to provide a non-significant value. Both of these wavelengths used custom processing methods of models design, namely the average, linear, two-factor interaction, quadratic, cubic, order-5 and order-6 that produce a non-discriminant analysis significantly.

VIII. CONCLUSION

Box–Behnken design and the experimental design were conducted by selecting five input variables and levels. The minimum of the experiment process, data collection and models were explained and developed. Confirmation of the suitability of each model was conducted using ANOVA technique (analysis of variance). The results show that the whole model can be used with a confidence level of 0.95 into the next stage of design. The model validation was conducted by collecting additional experimental data where it has a high confident level to adopt the chosen parameters.

Mathematical equation model in equation (8) was explained as a platform to design optical probe for three chemical vapor detection, namely the acetone, ethanol and methanol. The optimization set of input parameters can be identified by getting into consideration the probe length, probe diameter, doping photo-initiator, pressure of vacuum chamber and purity of detection liquid. By reducing the number of experimental runs, the expected result was very convincing and logically acceptable. It can be followed to obtain a solution for planning purposes as well as saving time and cost.

For future work, we plan that the application of un-cladding plastic optical fiber to be included with the optimization of chemical vapor detection based on the absorbance rate with the other liquid concentrations. In addition, the comparison of ANOVA process method, such as modification process, model design, linearity process and two-factor interaction process. Finally, the model and optimization of chemical vapor detection with high pressure or zero pressure will be conducted.

Table 3
The Result Analysis of ANOVA for the Linear Model of Acetone Vapor Detection (λ = 410.05 nm)

Source	Sum of Squares	df	Mean square	F-Value	p-value "Prob > F"	
Model	1.741E+5	5	34810.78	1.87	0.1220	Not significant
A-Probe Length	96064.35	1	96064.35	5.15	0.0287	significant
B-Probe diameter	51548.30	1	51548.30	2.76	0.1042	Not significant
C-Doping photo-initiator	12.83	1	12.83	6.881E-4	0.9792	Not significant
D-Pressure of Vacuum chamber	15017.89	1	15017.89	0.81	0.3749	Not significant
E-Purity of detection liquid	11410.51	1	11410.51	0.61	0.4387	Not significant
Residual	7.461E+5	40	18651.85			
Lack of fit	6.327E+5	35	18077.87	0.80	0.6945	Not significant
Pure Error	1.133E+5	5	22669.74			
Cor Total	9.201E+5	45				

Table 4
The Result Analysis of ANOVA for the Quadratic Model of Acetone Vapor Detection (λ=434.05nm)

Source	Sum of Squares	df	Mean square	F-Value	p-value "Prob > F"	
Model	1.058E+6	20	52876.05	3.07	0.0044	Significant
A-Probe Length	3477.76	1	3477.76	0.20	0.6569	
B-Probe diameter	51972.60	1	51972.60	3.02	0.0945	
C-Doping photo-initiator	109.67	1	109.67	6.375E-3	0.9370	
D-Vacuum pressure of chamber	2630.66	1	2630.66	0.15	0.6991	
E-Purity of detection liquid	83706.06	1	83706.06	4.87	0.0368	
AB	28170.27	1	28170.27	1.64	0.2124	
AC	25937.10	1	25937.10	1.51	0.2309	
AD	805.99	1	805.99	0.047	0.8304	
AE	49375.06	1	49375.06	2.87	0.1027	
BC	10315.45	1	10315.45	0.60	0.4460	
BD	6771.64	1	6771.64	0.39	0.5361	
BE	12729.48	1	12729.48	0.74	0.3979	
CD	16961.16	1	16961.16	0.99	0.3303	
CE	20049.14	1	20049.14	1.17	0.2907	
DE	8840.70	1	8840.70	0.51	0.4801	
A^2	7668.68	1	7668.68	0.45	0.5105	
B^2	26676.32	1	26676.32	1.55	0.2246	
C^2	266.85	1	266.85	0.016	0.9019	
D^2	21856.38	1	21856.38	1.27	0.2704	
E^2	4.891E+5	1	4.891E+5	28.43	< 0.0001	
Residual	4.301E+5	25	17204.89			
Lack of fit	3.370E+5	20	16850.07	0.90	0.6113	Not significant
Pure error	93120.77	5	18624.15			
Cor Total	1.488E+6	45				

Table 5
The Constant Value from Mathematic Equation Model for Three Chemical Vapors

Constant	Acetone Liquid			Ethanol Liquid			Methanol Liquid		
	λ_{434}	λ_{486}	λ_{656}	λ_{434}	λ_{486}	λ_{656}	λ_{434}	λ_{486}	λ_{656}
a_0	462.80908	755.38509	376.33258	3098.4	3442.58	3372.01	1823.51	1725.73	1180.4
b_1	111.85802	123.79383	109.07676	8.44198	-20.4043	-30.6251	132.3	158.367	150.794
b_2	3439.89815	5031.91204	4630.22492	1330.18	43.0143	-856.992	-436.562	1449.14	1231.6
b_3	6687.63241	8080.87685	7813.96944	-1418.42	635.625	-559.467	7238.74	9356.86	9732.82
b_4	1.95036	3.41617	2.53363	-3.18158	-3.46232	-6.29731	-6.82407	-2.34541	-1.15765
b_5	-6.89487	-12.85265	-9.44871	-9.69591	-12.6787	-10.0643	-5.84429	-8.14692	-3.18591
c_1	-124.32593	-160.04444	-129.22222	-23.5148	-16.4111	-25.8556	-25.0296	-47.0259	-46.9593
c_2	-286.31111	-338.59556	-360.60444	-72.6489	-142.658	-68.6667	-458.738	-513.031	-518.818
c_3	0.075707	0.057600	0.068520	-0.0935867	0.00893333	-0.0148933	0.146973	0.08044	0.0767067
c_4	0.65839	0.32464	0.32960	0.332919	-0.0394519	0.0090963	0.201081	-0.314696	-0.307259
d_1	-3761.66667	-5637.22222	-4916.48148	-2489.26	-4171.85	-3210	-2358.33	-4475.19	-3606.48
d_2	4.57167	5.47667	5.71472	6.76944	7.4625	10.2139	8.19194	4.54611	3.30944
d_3	-6.96451	-8.60216	-6.86111	-6.92438	-10.5157	-10.0562	-4.85	-9.06759	-9.95247
e_1	-17.36467	-27.74000	-29.06933	-8.688	-18.1587	-14.6713	9.43267	-0.521333	-4.518
e_2	-20.97704	-9.06074	-15.48741	-1.87481	0.937778	-0.386667	0.372593	-2.17852	-0.8
f_1	-0.020894	-0.027512	-0.022776	-0.0194856	-0.0265833	-0.02532	0.000248889	-0.00835778	-0.00591667
g_1	-2.10794	-0.43567	-0.42230	1.4917	3.02308	3.66424	-5.65467	-4.42421	-3.60622
g_2	-1706.39146	-2522.96811	-2495.71116	1270.41	494.2	976.44	429.874	-397.492	-239.712
g_3	-983.03704	-843.55556	886.18519	14351.3	13978.4	14326.7	-14475.8	-12690.6	-16369
g_4	-0.020017	-0.020745	-0.014564	0.00421983	0.0129458	0.018253	-0.00613917	-0.0034505	-0.00350433
g_5	0.11691	0.19073	0.14974	0.136087	0.20626	0.173746	0.0986574	0.182593	0.136242

Table 6
Prediction and Experiment Results for Validation Data in Acetone Vapors

X1	X2	X3	X4	X5	λ (434.05nm)		λ (486.13nm)		λ (656.03nm)	
					R*	U*	R*	U*	R*	U*
2.5	0.83	0.2	100	100	2165.12	2160.01	3227.04	3225.01	2649.58	2640.97
2.5	0.8	0.15	100	100	2245.22	2250.12	3317.19	3320.93	2733.65	2740.27
5	0.79	0.05	50	100	2495.46	2490.02	3428.77	3410.40	2854.04	2840.66
7.5	0.81	0.2	50	100	2326.64	2329.72	3203.82	3210.72	2636.61	2639.18

R* = Prediction; U* = Experiment

Table 7
Prediction and Experiment Results for Validation Data in Ethanol Vapors

X1	X2	X3	X4	X5	λ (434.05nm)		λ (486.13nm)		λ (656.03nm)	
					R*	U*	R*	U*	R*	U*
2.5	0.83	0.2	100	100	4614.06	4611.33	3381.631	3370.67	2861.15	2840.16
2.5	0.8	0.15	100	100	4510.44	4530.21	3386.003	3400.03	2849.37	2860.18
5	0.79	0.05	50	100	4670.43	4611.89	3486.888	3450.96	2911.03	2920.63
7.5	0.81	0.2	50	100	4614.06	4599.98	3297.87	3210.78	2757.09	2760.27

R* = Prediction; U* = Experiment

Tabel 8
Prediction and Experiment Results for Validation Data in Methanol Vapors

X1	X2	X3	X4	X5	λ (434.05nm)		λ (486.13nm)		λ (656.03nm)	
					R*	U*	R*	U*	R*	U*
2.5	0.83	0.2	100	100	2469.97	2470.01	3537.78	3540.39	2846.70	2810.93
2.5	0.8	0.15	100	100	2462.09	2440.12	3582.20	3550.88	2902.08	2920.00
5	0.79	0.05	50	100	2436.08	2450.32	3454.13	3425.74	2797.97	2783.80
7.5	0.81	0.2	50	100	2366.08	2390.97	3242.91	3290.94	2605.50	2620.59

R* = Prediction; U* = Experiment

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