

Characterization of ozone production from multi-cylinder reactor in non-thermal plasma device using multivariable power least squares method

L S Tan¹, M T Lim^{2,*} and W Y Tey^{1,3}

¹Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia, 54100, Kuala Lumpur, Malaysia.

² Biomass Plasma Technologies, Renewable Energy and Green Technology, TNB Research Sdn. Bhd., 43000 Kajang, Selangor, Malaysia.

³Faculty of Engineering, UCSI University, 56000 Kuala Lumpur, Malaysia.

* mook.tzeng@tnb.com.my

Abstract. Other than usage for environmental remediation, ozone is also increasingly studied for its potential in combustion enhancement. In this study, the characterization of the ozone production at varied voltage, duty cycle and cylinder configuration for reactor was conducted using multivariable power least squares method (MPLSM). This alternative correlation method in the form of power function was applied in this study to determine the dominant factor affecting the ozone production using the multi-cylinder reactor. The regressed equation using MPLSM method indicated voltage as the dominant factor in the production of ozone compared to the effect of duty cycle. The correlations generated from MPLSM for both reactor configurations were able to predict most of the ozone concentration results within 25% deviation from the actual experimental data. As such, MPLSM could be considered as an alternative method to be used for correlations of non-polynomial results.

1. Introduction

With the current trend of intensified, clean and safe process [1, 2], ozonation is gaining attention as alternative for environmental remediation [3-5]. Ozone was also found to effectively decompose volatile organic compounds (VOC) and removing pollutant gases as well as odour treatment [6-9].

Recently, ozone is also studied for potential in combustion enhancement [10-13]. Ombrello *et al.* [10] identified that development of new technologies to enhance combustion should also cover beyond high speed propulsion devices. Stationary power generation and ultra-lean, ultra-low emission internal combustion engines are some of the areas which can be further improved through new combustion technologies such as plasma-assisted combustion technique [10]. Plasma activation offers the benefit of decreased ignition times and lower ignition temperatures, enhanced flame stabilization, increased flame propagation and increased flammability limit in combustion systems [11, 12, 14]. The improved combustion could be achieved via the presence of free electrons, ions, active radicals and excited molecules as well as thermal enhancement generated from the corona discharge [10, 12]. As such, modification of traditional combustion techniques by incorporating non-thermal plasma in the system is a promising area to be explored. Non-thermal plasma was found to be effective in producing ozone through excitation of energetic electrons [7].



This work is a continuation from our previous study on characterization of ozone production from multi-cylinder reactor in a non-thermal plasma device [15]. In our previous study, ozone production experiment was conducted, and the data collected was characterized using response surface methodology (RSM). However, it was found that the configuration was biased towards one of configuration. Consequently, the predicted results for another configuration was out of range.

MPLSM was selected as an alternative method for the characterization in this study because the trend of ozone generation is not always in polynomial form as it depends on the parameter or combination of parameters varied [8, 17, 18]. However, RSM usually analyses responses based on polynomial trend only. MPLSM is able to solve multivariable problems using power function, in which the indices of the parameters are indicated as real numbers. It is able to approximate the indices of the variables using simple matrix solution. The magnitude of the indices could also be used to indicate the variable dominance ranking.

In this study, the same data which was collected in our previous study was characterized for the ozone production using multivariable power least squares method (MPLSM) [16]. The accuracy of the regressed equation from the method would be compared with the regression from RSM.

2. Methodology

2.1 Regression using MPLSM

The experimental parameters from our previous study [15], as shown in Table 1, was used in this study. The data was obtained from variation of numerical factors, i.e. the range of voltage between of 12 kV to 16 kV and duty cycle from 10 to 30. The similar set of variation was conducted in categorical factor of multi-cylinder reactor configuration, i.e. 3 x 40 mm and 10 x 10 mm.

The evaluation on the effect of voltage and duty cycle to the ozone concentration produced from the multi-cylinder reactor was conducted for each configuration of cylinders using MPLSM [16]. The method considered the independent numerical variables, x_1, x_2, \dots, x_m , in which m is the total number of set in the independent variables, can be correlated with the dependent variable, y using the multiplication of respective power function of the independent variables as shown in Equation (1):

$$y \approx y^h = ax_1^{b_1} x_2^{b_2} \dots x_m^{b_m} \quad (1)$$

Equation (1) was then expanded in logarithmic form as shown in Equation (2) before the deployment of least squares method

$$\ln(y^h) = \ln(a) + b_1 \ln(x_1) + b_2 \ln(x_2) + \dots + b_m \ln(x_m) \quad (2)$$

By taking $A = \ln(a)$ and $B_j = b_j$, with the subscript j as the number of set of variables, the square of least squares residual was formulated as:

$$R^2 = \sum_{i=1}^n \left(\ln(y_i) - \ln(y_i^h) \right)^2 = \sum_{i=1}^n \left(\ln(y_i) - A - B_1 \ln(x_{1,i}) - B_2 \ln(x_{2,i}) - \dots - B_m \ln(x_{m,i}) \right)^2 \quad (3)$$

Upon expansion of Equation (3), solution for A was obtained by taking the minimization of R^2 with respect to A , in which:

$$A = \frac{1}{n} \left(\left(\sum_{i=1}^n \ln(y_i) \right) - \sum_{j=1}^m \left(B_j \sum_{i=1}^n \sum_{j=1}^m \ln(x_{j,i}) \right) \right) \quad (4)$$

where i is the i^{th} elements within the set of variables while n is the total number of elements within the set of variables. The minimization of R^2 with respect to B_1, B_2, \dots, B_m would yield the set of equations which was solved using matrix.

Table 1. Parameters varied in this study [15].

Run	Voltage (kV)	Duty cycle	Configuration (mm)
1	16	20	10x10
2	16	10	3x40
3	14	20	10x10
4	12	10	3x40
5	12	30	3x40
6	16	30	10x10
7	14	30	10x10
8	12	30	10x10
9	14	20	3x40
10	14	20	3x40
11	12	10	10x10
12	16	20	3x40
13	14	20	10x10
14	12	20	10x10
15	16	10	10x10
16	14	10	3x40
17	16	30	3x40
18	14	20	3x40
19	14	30	3x40
20	14	10	10x10
21	14	20	10x10
22	14	20	10x10
23	14	20	10x10
24	14	20	3x40
25	14	20	3x40
26	12	20	3x40

$$\begin{pmatrix} \gamma_1 & -\lambda_{12} & \cdots & -\lambda_{1m} \\ -\lambda_{21} & \gamma_2 & \cdots & -\lambda_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ -\lambda_{m1} & -\lambda_{m2} & \cdots & \gamma_m \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_m \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_n \end{pmatrix} \quad (5)$$

$$\gamma_j = n \left\{ \sum_{i=1}^n \sum_{j=1}^m [\ln(x_{j,i})]^2 \right\} - \left\{ \sum_{i=1}^n \sum_{j=1}^m [\ln(x_{j,i})] \right\}^2 \quad (6)$$

$$\xi_j = n \left[\sum_{i=1}^n \sum_{j=1}^m \ln(x_{j,i}) \ln(y_j) \right] - \left[\sum_{i=1}^n \sum_{j=1}^m \ln(x_{j,i}) \right] \left[\sum_{i=1}^n \ln(y_i) \right] \quad (7)$$

$$\lambda_{jk} = \left[\sum_{i=1}^n \sum_{j=1}^m \ln(x_{j,i}) \right] \left[\sum_{i=1}^n \sum_{j=1}^m \ln(x_{k,i}) \right] - n \left[\sum_{i=1}^n \sum_{j=1}^m \ln(x_{j,i}) \ln(x_{k,i}) \right] \quad (8)$$

The subscript k represents the value of second subscript of the term ρ . The matrix in Equation (5) was solved using Matlab R2013a software.

3. Results and discussion

3.1 Ozone production model based on MPLSM

Based on the method described in Section 2.1, the coefficients of the model with power based correlations generated from MPLSM for configuration of 3 x 40 mm and 10 x 10 mm are shown in Equation (9) and (10), respectively.

$$\text{Ozone concentration} = 0.01 \text{Voltage}^{1.84} \text{Duty cycle}^{0.0947} \quad (9)$$

$$\text{Ozone concentration} = 0.008 \text{Voltage}^{1.92} \text{Duty cycle}^{0.0451} \quad (10)$$

where unit for ozone concentration is ppm, unit for voltage is kV and duty cycle is unitless.

Based on the correlations, the predicted versus actual data for multi-cylinder reactor with configuration of 3 x 40 mm and 10 x 10 mm were plotted and presented in Figure 1 and Figure 2 respectively. The predicted data from our previous correlation based on RSM is also included in the graph for comparison [15].

It is observed that the correlations generated from MPLSM for both configurations was able to predict the response close within the 25% range of prediction target. Several points were slightly outside the targeted range. However, MPLSM managed to correct the range of the predicted ozone concentration for configuration of 3 x 40 mm closer to actual data.

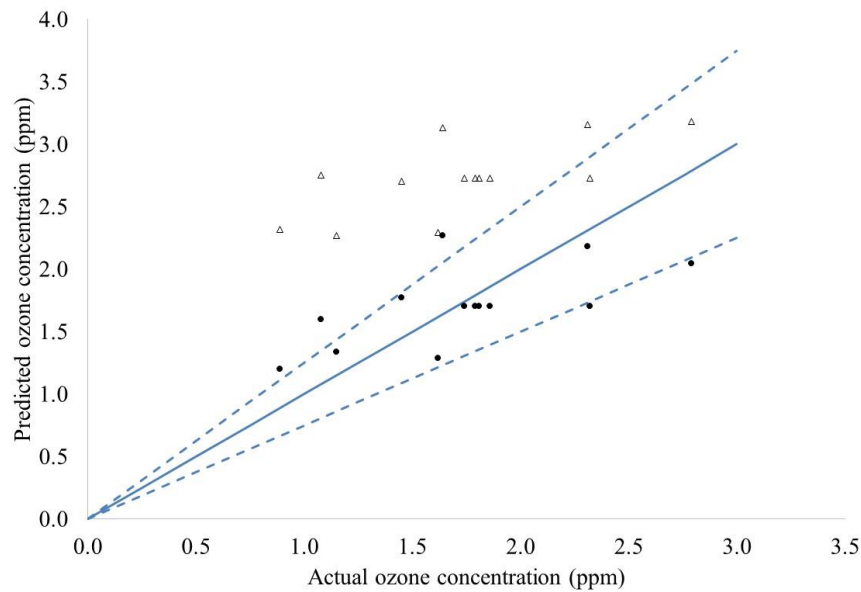


Figure 1. Comparison of predicted results using correlations based on MPLSM (•) and RSM (Δ) regression versus actual ozone concentration data generated from 3 x 40 mm electrode configuration. The solid line represents 100% accuracy while the dotted lines represent the 25% deviation from perfect accuracy.

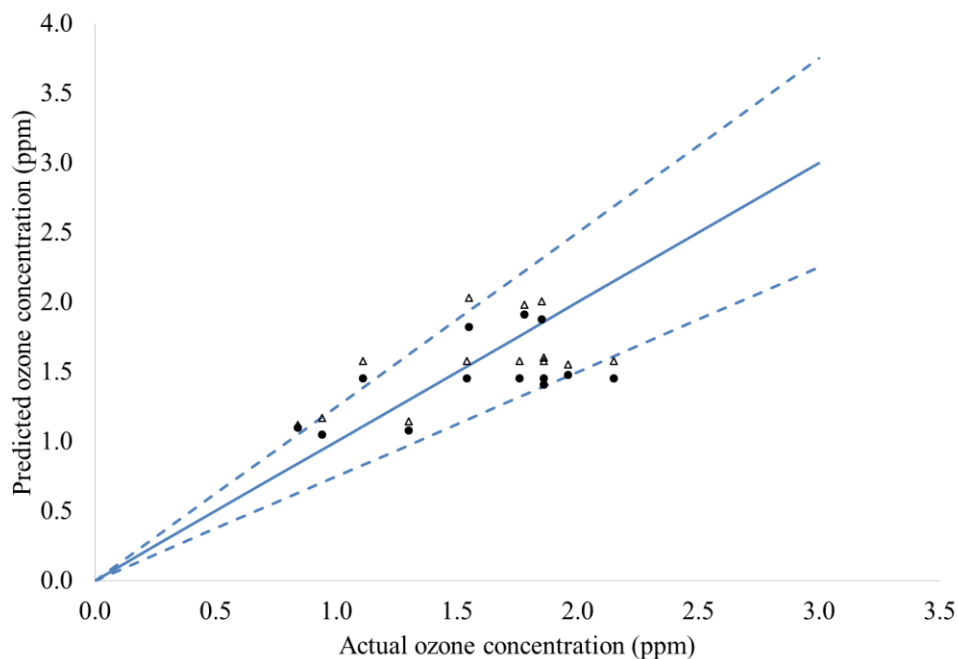


Figure 2. Comparison of predicted results using correlations based on MPLSM (•) and RSM (Δ) regression versus actual ozone concentration data generated from 10 x 10 mm electrode configuration. The solid line represents 100% accuracy while the dotted lines represent the 25% deviation from perfect accuracy.

From the indices of the variables in Equation (9) and (10), voltage was the dominant variable since it has the higher value of power compared to duty cycle. This is consistent with the ANOVA results from our previous RSM analysis [15].

Based on Figure 1 and Figure 2, it is also observed that cylinders configuration of 3 x 40 mm could produce higher ozone concentration compared to cylinders configuration of 10 x 10 mm. This was because stronger electric field was generated with the lower number of cylinders in the reactor as the same input power was divided across lesser cylinders. This led to increased electron number density which enhanced ionization and collisional excitation of plasma electrons [19].

3.2 Comparison of RSM and MPLSM for Characterization of Ozone Production

The advantage of RSM was that it could analyse the significance of both numerical and categorical factor at once. Hence, it would be beneficial to be used in analysis which required conformation of categorical factor based on statistical analysis. However, the resulting model from simultaneous numerical and categorical factor needs to be graphically verified based on set deviation target such as in Figure 1 and Figure 2. Otherwise, the biasness of model towards a certain categorical factor might be undetected.

As explained in Section 2.1, the trend of ozone production depends on the parameter or combination of parameters varied and it is not always in polynomial form. Under this circumstance, MPLSM is an alternative method to be used to correlate the variables with the response. The indices for each variable can also be used to determine the dominance of the factor in influencing the response. Based on the results obtained in this study, MPLSM appeared to be reliable in correlation of the data. However, MPLSM was unable to conduct numerical analysis for categorical and numerical factor simultaneously. As such, the significance of categorical factor would need to be analysed separately if MPLSM is employed.

4. Conclusion

The effect of voltage, duty cycle and different configuration on ozone production in multi-cylinders reactor in non-thermal plasma was characterized using MPLSM. Voltage was identified as dominant factor via analysis using MPLSM. The correlations generated from MPLSM for both configurations were able to predict the ozone concentration results close within the prediction target range. As such, MPLSM could be considered as an alternative method to be used for correlations of non-polynomial trend of results.

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