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Regression and Arima Residual Have High Accuracy to Estimate Percent Adsorption Spectral Based on Wavelength at Barium Titanate

Muhammad Nur Aidi[1], Budi Susetyo[1], Hendradi Hardhienata[2], Irzaman[2]
[1]Department of Statistics, Faculty of Mathematics and Sciences Natural (FMIPA), Bogor Agricultural University (IPB), Kampus IPB Dramaga Bogor Indonesia
[2]Department of Physics, Faculty of Mathematics and Sciences Natural (FMIPA), Bogor Agricultural University (IPB), Kampus IPB Dramaga Bogor Indonesia

ABSTRACT

Has successfully Reviewed Regression and Arima Residual Have High Accuracy To Estimate Percent adsorption Spectral-Based on Wavelength at Barium Titanate. Regression equations often produce errors that are not independent, especially in the regression of observational data. At wavelength from 400.06 to 463.77, the model combination between Arima and linear regression is Y_i=-1.115052+0.004X_i-0.98106 e_(i-1)+z_i. At wavelength from 464.13 to 724.85, The model combination between Arima and quadratic regression is Y_i=0.809462-0.001 X_i+8.82x 〖10〗^(-7) 〖X^2〗_i+ 〖1.000401 e〗_(i-1)+z_i. At wavelength 725.18 to 950.1, The model combination between Arima and quadratic regression (a convex form) is Y_i=-1.33887+0.005 X_i-2.82 x 〖10〗^(-6) 〖X^2〗_i+ 〖0.83931 e〗_(i-1)+0.1221 e_(i-2)+z_i. The absolute minimum of percent adsoption is 0.526015 % at x =566.893, local maximum of percent adsoption is 0.740028 % at x = 463.77, absolute maximum is 0.877442 % at x=886.525.

Keywords : Barium Titanate, Regression and ARIMA Residual, Percent Adsorption, Wavelength visible light, Maximum-Minimum Adsorption.

I. INTRODUCTION

Barium titanate is a dielectric ceramic for the capacitor. $BaTiO_3$ ceramics with perovskite structures are capable of producing 7,000 dielectric constants. BaTiO3 is a piezoelectric material for microphones with spontaneous polarization of single crystal barium titanate at room temperature between 0.15 C / m2 at and Curie temperature between 120 and 130 ° C. Barium Titanate can also result in non-linear optics with high beam coupling can also be operated at wavelength and near-infrared. Barium titanate filmization features electro-optical modulation to frequencies above 40 GHz. Barium titanate powder is also part of the new computer energy barium titanate for in electric vehicles (von Hippel, 1950; Shieh et al., 2009; Tang et al. 2004; Genchi et al., 2016).

Learning about the nature of Barium Titanate can be done by irradiation of light with wavelength of visible light in thin film Barium Titanate then measured percentage of visible light absorbed. Research with the Rietveld model and General Structure Analysis System (GSAS) developed to study the structure of atoms, one of which is Barium Titanate. The Rietveld Method (Rietveld, 1967, 1969) is a technique for improving the crystalline structure of X-rays and diffraction data of neutron powders. The ability to obtain detailed information about the crystal structure of the powder diffraction data is essential in the study of materials such as Barium Titanate which occur exclusively in the state of fine crystals (Walker, 1992).

The Barium Titanate irradiation process and other ferroelectric materials such as Barium Strontium Titanate, Lithium Niobate, Lithium Titanate are sequenced. This sequential illumination process results in the value of the rays diffracted on the current observations depending on the value of the previous observations. Therefore development of ARIMA model can be done. Excellence of Autoregressive Integrated Moving Average (ARIMA) Model Highly Predictable in Analyzing Spectral X-ray Diffraction (XRD) Data compared to Rietveld Model and General Structure Analysis System (GSAS), in 2010 ARIMA Model developed rapidly in Analyzing Spectral Data X-ray Diffraction (XRD) (Aidi et.al 2013; Mohan and Reddy, 2017; Wang et.al 2017; Zafra et.al 2017).

ARIMA can well model Fourier-transform infrared spectroscopy (FTIR) and X-ray powder diffraction (XRD) values in Barium Strontium Titanate (BST) powder. The results show that the first differencing model on ARIMA with AR order (2) and MA order (2) or less is very good to explain FTIR value in BST which is Lanthanum Oxide in some concentration. Similarly, the first differencing of AR (3) and MA (3) or less is very good for explaining the XRD value of the BST which is fed by Lanthanum Oxide at some concentration. The accuracy of ARIMA model on FTIR values in BST is more accurate than ARIMA model on XRD values in BST. (Aidi (a) et.al 2018). ARIMA model on FTIR and XRD values in Lithium Neobat which is Lanthanum Oxide at some concentration have high accuracy level, that is coefficient of determination more than 80%. The ARIMA model for FTIR data on Lithium Neobat is more accurate than ARIMA model for XRD data on Lithium Niobate (Aidi (b) et al. 2018).

The ARIMA model for FTIR data on Lithium Tantalate which was Lanthanum Oxide 0%, 5%, 10% were ARIMA (3.0,1), ARIMA (3,0,0) and ARIMA (3,0,1) each having coefficient of determination (R^2) 94%, 94%, and 97%). While ARIMA XRD data in Lithium Tantalate which is Lanthanum Oxide 0%, 5%, 10% are ARIMA (5.0,01), ARIMA (5.0,01) and ARIMA (7.0,0) each have coefficient of determination R^2) 91%, 92%, and 87%). ARIMA on FTIR data is simpler than ARIMA in XRD data, and the administration of Lanthanum Oxide will decrease the value of FTIR and XRD (Aidi (c) el.al 2018)

Furthermore, if We want to study the visible light adsorption properties in Barium Titanate related to the visible wavelength needs to be modelled between the independent variable that is the wavelength as well as the percentage of visible light adsorption on Barium Titanate as a dependent variable. Models are quite feasible to use is a regression model. The most powerful regression model is the non-linear spline regression model. This is due to the percentage of visible light adsorption by Barium Titanate due to the wavelength given its value fluctuates. With this model, we can predict what wave display value will have the maximum and minimum adsorption percentage of Barium Titanate. To improve the level of model accuracy, the remaining components of the regression are modelled again through the ARIMA model. This is due to the resulting regression model the possibility of residual components is not independent.

II. METHOD

2.1. Material Preparation

The chemical solution deposition (CSD) method is one of the methods of making thin films by using a solution placed on the substrate, then rotated at a certain speed with a spin coating device. Theoretical and experimental models for improving the quality of Barium Titanate thin films by chemical solution deposition (CSD) and spin coating methods are based on research done by Frutos et al. (1998), Lim et al.,

(2000) and Washo et al. (1977), Dahrul et al. (2010), Syafutra et al, (2010), Irzaman et al. (2013, 2014, 2016), Pamungkas et al. (2017), Mulyadi et al. (2017). Then modified by taking into account factors including surface tension, film viscosity, solution density, fluid flow rate, rotational speed, growth time, substrate form and solvent evaporation process (Meyerhofer, 1978, Daughton and Given, 1982, Scriven, 1988, Fitrilawati et al., 1999, Walsh and Franses, 1999). The next stage is to systematically investigate the symptoms of "Power Law" in the Barium Titanate material phase transition and its spectroscopic properties (Visible Light spectrum absorbance test).

2.2.Modeling

In the initial stage, there is data plotting between two variables, namely the dependent variable Y = Percentage of Adsorption by Barium Titanate, and the independent variable X = visible wavelength of light. From the plotting is done spline regression selection between variables Y with variable X. Determination of cutting nodes X region for each regression function, namely linear and quadratic regression.

When analyzing the relationship between the percentage of light adsorption, y, and the explanatory variable, i.e. the visible wavelength of visible light, the range x is different, the relationship can be either linear or nonlinear. In this case, a single linear model may not provide sufficient description and nonlinear models may not be appropriate. Therefore, the regression relationship pattern is a combination of linear and nonlinear regression. Spline regression is a regression form that allows multiple regression models to fit the data for different ranges of x. Breakpoints are values of x where the slope of the function is linear and nonlinear. The breakpoint value may or may not be known before the analysis, but it is usually unknown and should be estimated. The regression function on the breakpoint may be disconnected, but the model can be written in such a way that it functions continuously at all points including breakpoints. If there is one breakpoint, at x = c, the model can be written as follows:

$$y = a_1 + b_1x \text{ for } x \le c$$

$$y = a_2 + b_2x^2 \text{ for } x > c.$$

For the regression function to be sustainable at the breakpoint, the two equations for y must be the same at the breakpoint (when x = c):

$$a_1 + b_1c = a_2 + b_2c^2.$$

By substituting the value of c will be determined (Ryan and Porth, 2007; Poirier, D. J., 1973; McGee and Carleton, 2017).

The linear regression equation can be written as follows: $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$, Where y_i is the response variable and x_i is the independent variable. Next with the least sum squares of error method value

$$\widehat{\beta}_1 = \frac{\sum_i^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_i^n (x_i - \bar{x})^2},$$

And

$$\widehat{\beta_0} = \bar{y} - \widehat{\beta}_1 \bar{x}$$ (Fredman, 2009; Xin, 2009).

The percentage of light adsorption by Barium Titanate (Y) due to the visible light wavelength given (X) often has a concave or convex pattern. This means that the regression developed is a quadratic regression, by the formula, $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i$. To get an alleged value $\widehat{\beta_0}$, $\widehat{\beta_1}$, $\widehat{\beta_2}$, **β** by minimizing the sum square of error. The sum of these squares can be diminished if the first derivative of β is equal to zero or

$$SSE = \sum_{i=1}^{n} \left[y_i - f(x_i, \beta) \right]^2,$$

$$\frac{\delta SSE}{\delta \beta} = \sum_{i=1}^{n} \left[y_i - f(x_i, \beta) \right] \frac{\delta f(x_i, \beta)}{\delta \beta} = 0.$$

The first derivative of β is equal to zero forming a system of non-linear equations which can not be solved directly but can be approximated iteratively using numerical methods, one numerical method which can solve this is the Gauss-Newton method. Levenberg-Marquardt perfected the Gauss-Newton method by entering the β constant (the initial value of βi + 1 whose magnitude varies according to SSE changes, (Graubard and Grubard 1988; Gavin, 2017; Fan and Yuan, 2004).

Regression equations often produce errors that are not independent, especially in the regression of observational data. In the process of irradiation Barium Titanate by light with wavelength appears through a cascade process, i.e. visible light in the i taken after the visible light to i-1, i-2, i-3, ..., 1. Therefore, to optimize the result of regression equation and to overcome the error that is not independent done ARIMA modelling on error component. The combined model between regression and error can be written as $y_i = f(x_i, B) + Z_i$, Where $f(x_i, B)$ is the resulting regression model, and Zi is a non indepenent error. Zi which is not independent overcome with ARIMA model (p, q) is a model that based on terminology p autoregressive, and q moving average which can be written as follows

$$Z_i = c + e_i + \sum_{s=1}^{p} \vartheta_s Z_{i-s} + \sum_{r=1}^{q} e_{i-r}$$

(Box et al., 1994; Brockwell, and Davis. 2009; Tsay, 1984; Lin et.al., 1999)

III. RESULT AND DISCUSSION

3.1. Percent adsorption of light

Barium Titanate is exposed to a wavelength between 400.06 and 950.19. Percent of absorbed light is measured as percent adsorption. Plotting percent adsoption as dependent variable and wavelength as independent variable is presented at Figure 1. From Figure 1 can be said the line can be cut to 3 segments. Fist segment line is wavelength from 400,06 to 463,77, second segment line is wavelength from 464,13 to 724,85, and the last segment line is wavelength from 725,18 to 950,19. First segment is linear function with wavelength as independent variable (X) and percent adsorption as dependent variable (Y). Second and Third segments are quadratic functions with wavelength as independent variable (X) and percent adsorption as dependent variable (Y).

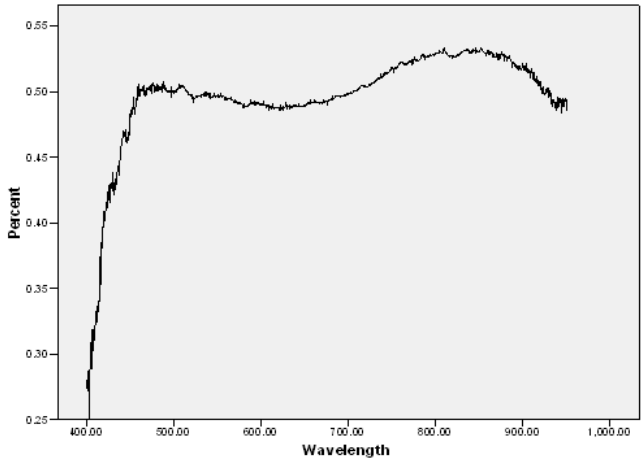

Figure 1. Plotting between wavelength as horizontal axis (Independent variable) and percent adsorption as vertical axis (Dependent variable)

3.1.1. Light segment with wavelength from 400,06 to 463,77

Function with first segment of wavelength as independent variable and percent adsorption as dependent variable is linear function. From Analisis of variance (Anova) could be concluded that linear function was accepted. H1 was accepted (Table 1). F-computed was 2106.79 with degrees of freedom (1, 173) and significant probability of 0.000.

Table 1. Anova of linear regression wavelength as independent and percent adsorption as dependent variables

Model	Sum of squares	Df	Means Square	F-compute	Sig
Regression	0.767	1	0.767	2106.79	0.000
Residual	0.063	173	0.000364		
Total	0.830	174			

a. Predictors: constant, wavelength
b. Dependent variable: Percent adsorption

The estimated regression function is

$$Y = -1.129 + 0.004\,X + e \qquad \text{(F.1)}$$

Y=percent of adsorbstion

X=wevelength

Where estimated **coefficients were reject H0 or accepted H1 with probabilty significant of 0.000 (Table 2). This regression has adjusted R Square of 92.4 %. From this regression we can say that** rays have a negative effect on percent of adsorbed light by barium titanate. Increasing wavelength of light one unit (in range 400,06 to 463,77) will decrease percent adsorbtion of 0.004 %. Ninety two percent of variation percent adsorbtion can be explained by this model. This linear regression has high accuration to estimate percent of adsorted light by barium titanate with wavelength as dependent variable.

Table 2. Estimated coefficient linear regresssion and significancy

Model	Coefficients	Standard error	t-compute	sig
Constant	-1.129	0.034	-33.489	0.000
Wavelenght	0.004	8.7146E-05	45.900	0.000

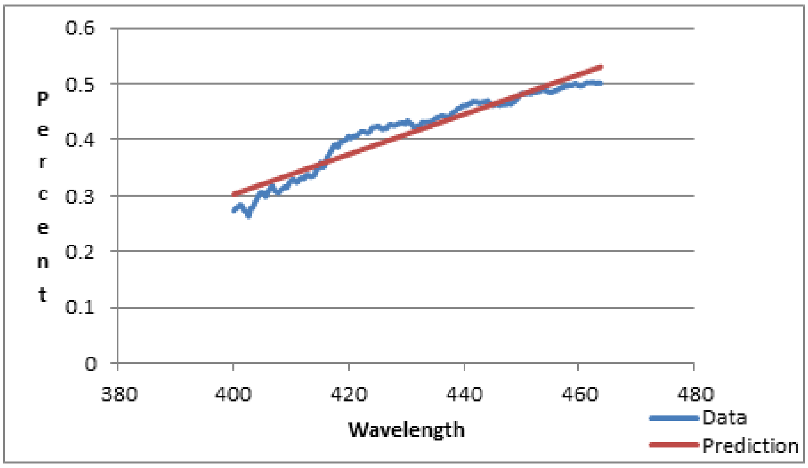

Figure 2. Plotting data and linear regression

Assumptions of this regression are residual has normal distribution and independent. Normal P-P Plot was used to evaluate normal distribution of residual and plot of residual was used to evaluate residual has independent distribution. From Figure 3 and 4, those can be concluded residual has normal distribution and not independent. Residual is not independent distribution has mean that residual has autocorrelation between observations. Behaviour of residual can be estimated by arima model.

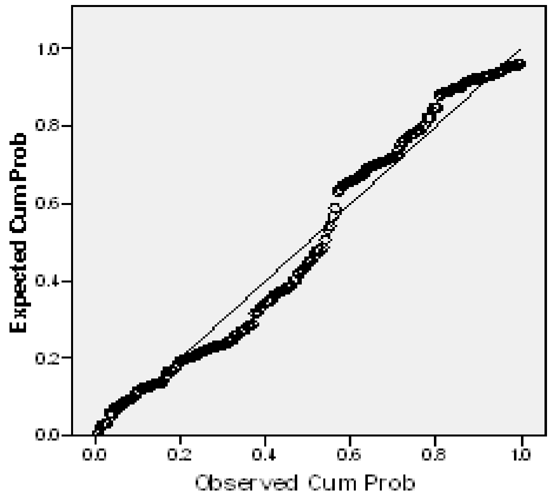

Figure 3. Normal P-P plot of residual regression

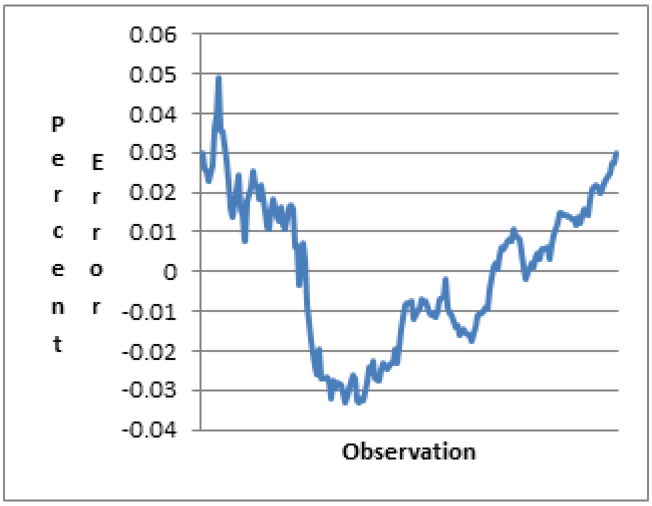

Figure 4. Plot of residual regression

First step of to estimate arima model of residual is to compute autocorrelation function (ACF) and partial autocorrelation function (PACF). Result of ACF and PACF residual. Based on Figure 5 and Figure 6, ARIMA (1,0,0) is may be good choice to estimate behaviour of residual.

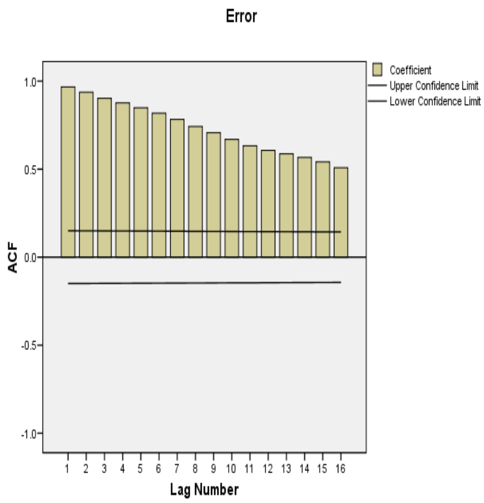

Figure 5. Plot ACF of residual

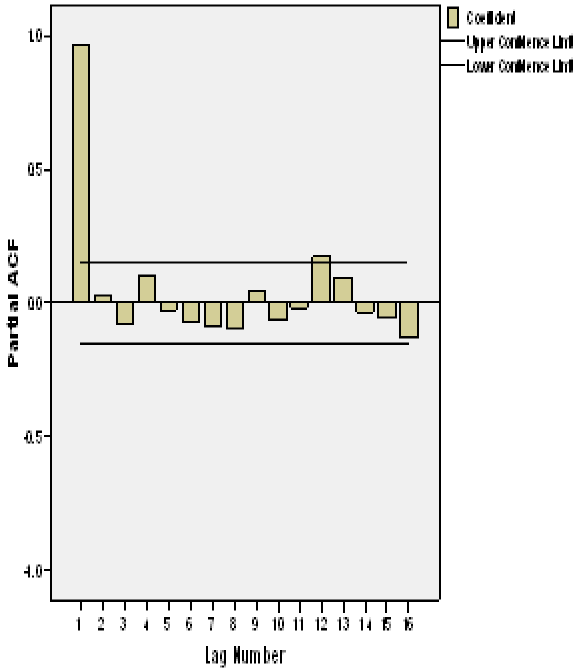

Figure 6. Plot PACF of residual

Arima model of residual is Arima (1,0,0) with function

$$e_i = -0.013 + 0.985\, e_{i-1} + u_i \qquad \text{(F.2)}$$

Then $\hat{e}_i = -0.013 + 0.985\, e_{i-1}$

Table 3. Arima (1,0,0) of residual

Model		Estimate	SE	T-compute	Sig.
Constant		-0.013	0.014	-0.884	0.378
AR	Lag1	0.985	0.012	81.504	0.000

Arima (1,0,0) has R^2 of 95.7% , this model has high accuration to estimate of residual at i based on residual at i-1. Plot data of residual and arima residual presented at Figure 7 where estimated from arima residual (1,0,0) can follow residual data.

Figure 7. Plot estimated of arima residual with residual data

Model of percent adsorbtion as dependent variable and wavelengt as independent variable can be constructed with two models above, linear regression and arima residual. Combination function is

$$Y_i = -1.128 + 0.004\, X_i - 0.996\; Estimated\ arrima\ residual + z_i \quad \text{(F.3)}$$

Where estimated arrima residual is $\widehat{e}_i = -0.013 + 0.985\, e_{i-1}$ and

$$e_{i-1} = (y_{i-1} - (-1.129 + 0.004\, X_{i-1}))$$

Anova of F.3. was presented at Table 4, which said H1 was accepted or H0 was rejected. Table 5 said Constant of -1,128 was accepted H1, parameter estimation of X of 0.004 was accepted H1, parameter of Estimate arima residual of -0.996 was accepted H1. F.3. has R^2 of 99.7% which mean prefectly accurate function to estimate percent adsorbtion based on wavelength.

Table 4. Anova of linear regression and arima residual

Model	Sum of square	df	Mean square	F-compute	Sig
Regression	0.807	2	0.403	29164.198	0.000
Residual2	0.002	171	0,000014		
Total	0.809	173			

Table 5. Estimation of regression parameters of linear regression and arima residual

Model	Coefficients	SE	t-compute	Sig
Constant	-1.128	0.007	-170.983	0.000
Wavelength (X)	0.004	1,7202E-05	232.525	0.000
Estimated arima residual ($\widehat{e}_i$)	-0.996	0.015	-66.057	0.000

F.3 can be changed as function below

$$Y_i = -1.128 + 0.004X_i - 0.996\,(-0.013 + 0.985\, e_{i-1}) + z_i \quad \text{(F.4)}$$

Then

$$Y_i = -1.115052 + 0.004X_i - 0.98106\, e_{i-1} + z_i \quad \text{(F.5)}$$

Where

Yi percent of adsorption at i, Xi wavelength at i (400,06 <= Xi <= 463,77), $e_{i-1} = (y_{i-1} - (-1.129 + 0.004\, X_{i-1}))$. F.5. has perfectly accurate function since has R^2 of 99.7% (Figure 8)

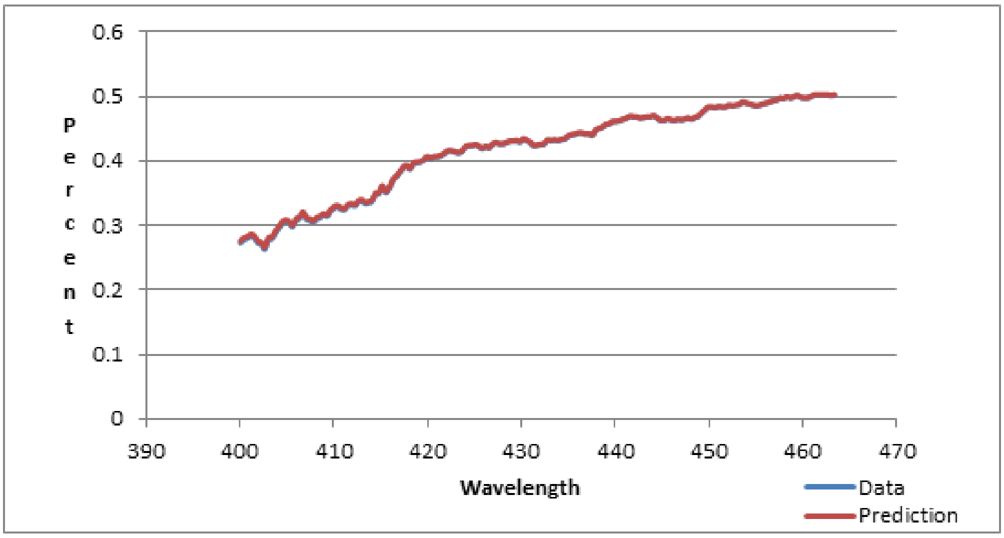

Figure 8. Plot Percent adsorbtion data with estimated function

3.1.2. Light segment with wavelength from 464.13 to 724.85.

Function with second segment of wavelength as independent variable and percent adsorption as dependent variable is qaudratic function. From Figure 9, the function is quadratic function with concave upward.

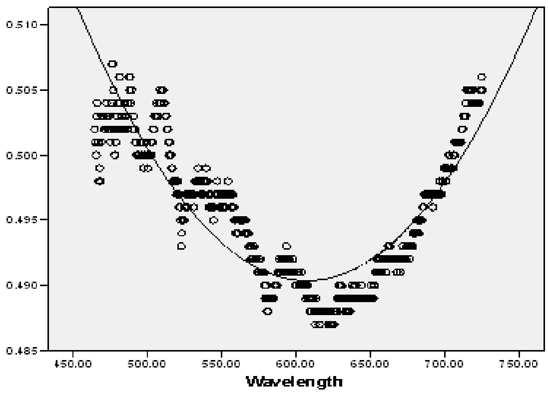

Figure 9. Plot between percent adsorbtion and wavelength

Analisis of variance (Anova) could be concluded that quadratic function was accepted. H1 was accepted (Table 6). F-computed was 1410.063 with degrees of freedom (2, 750) and significant probability of 0.000.

The function is

$$Y = 0.815 - 0.001\,X + 8.82x10^{-7}X^2 + e \quad \text{(F.6)}$$

Y=percent of adsorbstion

X=wevelength

Table 6. Anova of quadratic regression wavelength as independent and percent adsorption as dependent variables

Model	Sum of squares	Df	Means Square	F-compute	Sig
Regression	0.017	2	0.008	1410.063	0.000
Residual	0.004	750	5,67351E-06		
Total	0.021	152			

a. Predictors: constant, wavelength
b. Dependent variable:Percent adsorption

This quadratic regression has R Square of 79 %. This quadratic regression has significant intercept, significant coefficient of X and significant coefficient of X^2 (Table 7).

Table 7. Estimated coefficient quadratic regresssion and significancy

Model	Coefficients	Standard error	t-compute	sig
Wavelength	-0.001	1,9566E-05	-51.108	0.000
Wavelength**2	8.82E-007	1,5933E-08	50.211	
Constant	0.815	0.006	132.251	

Assumptions of this quadratic regression are residual has normal distribution and independent. Normal P-P Plot was used to evaluate normal distribution of residual and plot of residual was used to evaluate residual has independent distribution. From Figure 10 and 11, those can be concluded residual has normal distribution and not independent of residual. Residual is not independent distribution has mean that residual has autocorrelation between observations. Behaviour of residual can be estimated by arima model.

First step of to estimate arima model of residual is to compute autocorrelation function (ACF) and partial autocorrelation function (PACF). Result of ACF and PACF residual. Based on Figure 12 and Figure 13, ARIMA (1,0,0) is may be good choice to estimate behaviour of residual.

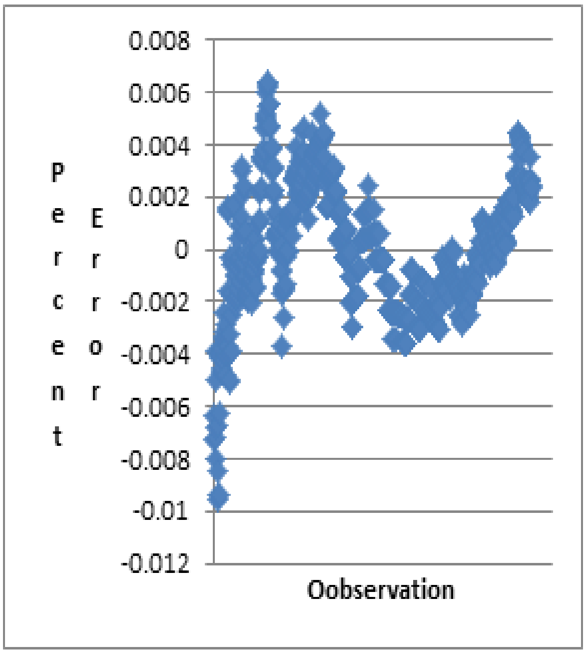

Figure 11. Plot of residual regression

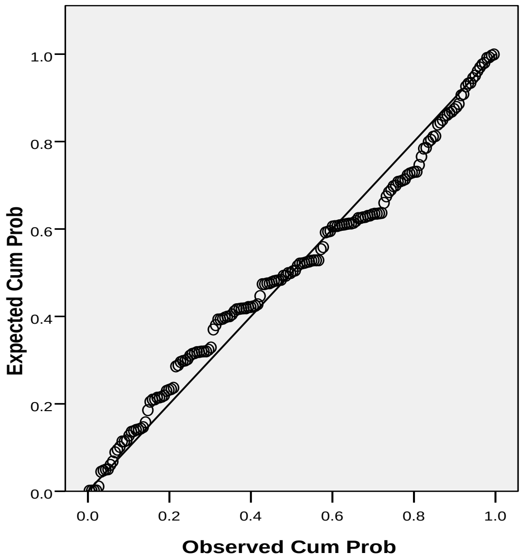

Figure 10. Normal P-P plot of residual regression

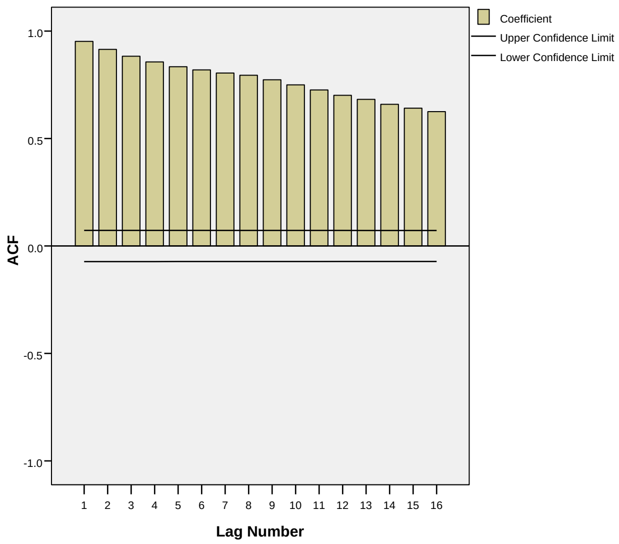

Figure 12. ACF of residual

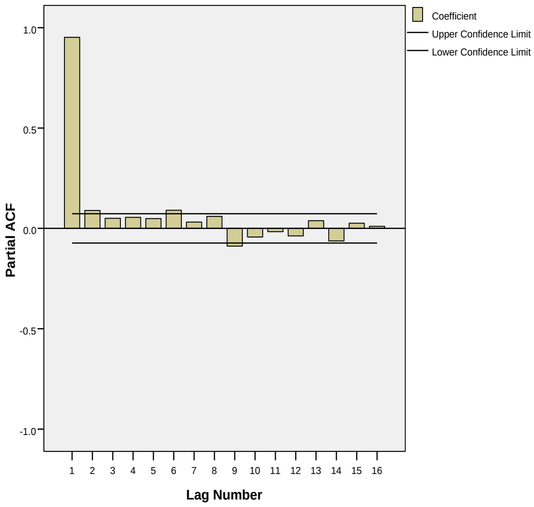

Figure 13. PACF of residual

Arima model of residual is Arima (1,0,0) with function

$$e_i = -0.00532 + 0.961\, e_{i-1} + u_i \qquad (F.7)$$

$$\text{Then } \hat{e}_i = -0.00532 + 0.961\, e_{i-1}$$

Table 8. Arima (1,0,0) of residual

Model		Estimate	SE	T-compute	Sig.
Constant		-0,00531915	0.001	-0.188	0.378
AR	Lag1	0.961	0.010	95.292	0.000

Arima (1,0,0) has R^2 of 91 % , this model has high accuration to estimate of residual at i based on residual at i-1. Plot data of residual and arima residual presented at Figure 14 where estimated from arima residual (1,0,0) can follow residual data.

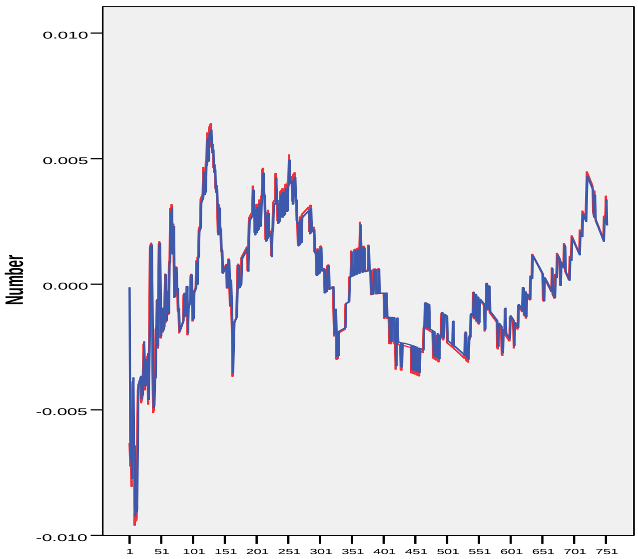

Figure 14. Plot estimated of arima residual with residual data

Model of percent adsorbtion as dependent variable and wavelenght as independent variable can be constructed with two models above, quadratic regression and arima residual. Combination function is

$$Y_i = 0.815 - 0.001\, X_i + 8.82x10^{-7} X^2{}_i + 1{,}041 \text{ Estimated arrima residual}_i + z_i \qquad (F.8)$$

Where estimated arrima residual is $\hat{e}_i = -0.00532 + 0.961\, e_{i-1}$
and

$$e_{i-1} = (y_{i-1} - (0.815 - 0.001\, X_{i-1} + 8.82x10^{-7} X^2{}_{i-1}))$$

Anova of F.8. was presented at Table 9, which said H1 was accepted or H0 was rejected. Table 10 said constant of 0.815 was accepted H1, parameter estimation of wavelength of -0.001 was accepted H1, parameter estimation of wavelength^2 of $8.82x10^{-7}$ was accepted H1, parameter of Estimate arima residual 1.041 was accepted H1. F.9. has R^2 of 99.99% which mean prefectly accurate function to estimate percent adsorbtion based on wavelenght.

Table 9. Anova of quadratic regression and arrima residual

Source	Sum of square	DF	Mean Square	F-compute	Sig.
Regression	0.0213	3	0.0071	867760985.70	0.000
Residual	6.119019×10^{-9}	748	8.1805×10^{-12}		
Total	0.0213	751			

Table 10. Estimated coefficient quadratic regresssion, estimated arima residual and significancy

Source	parameters	Standard Error	T-compute	Sig
Constant	0.815	7.221×10^{-6}	112871.28	0.000
Wavelenghth	-0.001	2.454×10^{-8}	-43606.50	0.000
Wavelenghth**2	8.82×10^{-7}	2.058×10^{-11}	42828.74	0.000
Estimated arima residual	1.041	4.443×10^{-5}	23420.75	0.000

F.8 can be changed as function below

$$Y_i = 0.815 - 0.001\, X_i + 8.82x10^{-7}X^2{}_i + 1{,}041\,(-0.00532 + 0.961\, e_{i-1}) + z_i$$

Then

$$Y_i = 0.809462 - 0.001\, X_i + 8.82x10^{-7}X^2{}_i + \; 1.000401\, e_{i-1} + z_i \quad \text{(F.9)}$$

Where

Yi percent of adsorption at i, Xi wavelength at i (464.13<= Xi <= 724.85), $e_{i-1} = (y_{i-1} - (0.815 - 0.001\, X_{i-1} + 8.82x10^{-7}X^2{}_{i-1}))$. F.9. has perfectly accurate function since has R^2 of 99.7% (Figure 15)

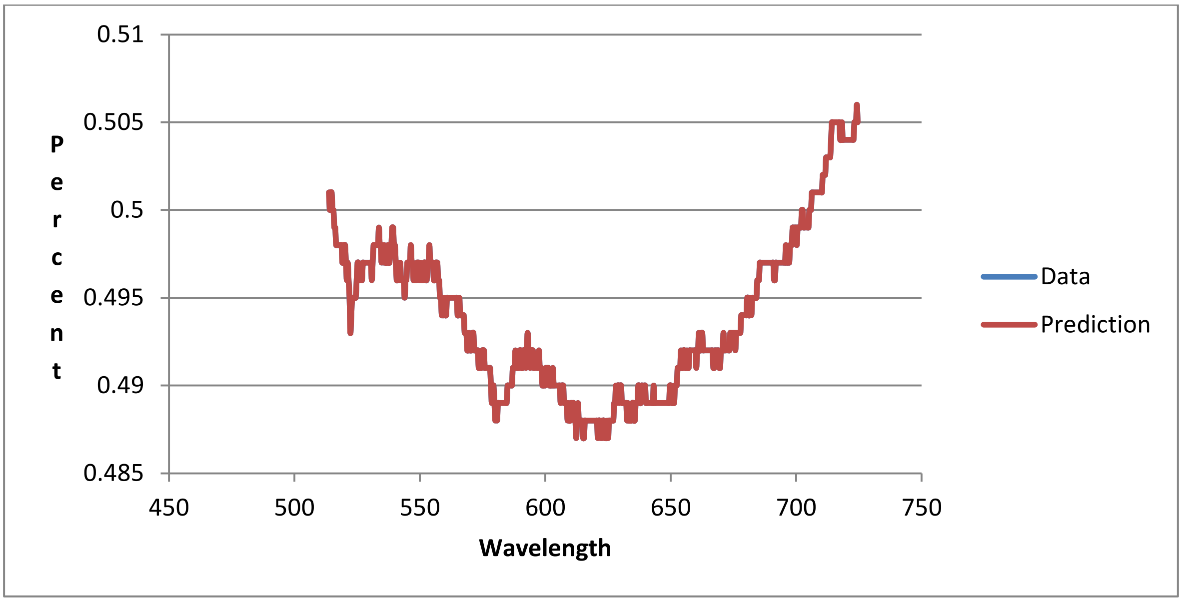

Figure 15. Ploting percent adsorption data and estimated function

3.1.3. Light segment with wavelength from 725.18 to 950.19

Function with second segment of wavelength as independent variable and percent adsorption as dependent variable is qaudratic function. From Figure 16, the function is quadratic function with concave down.

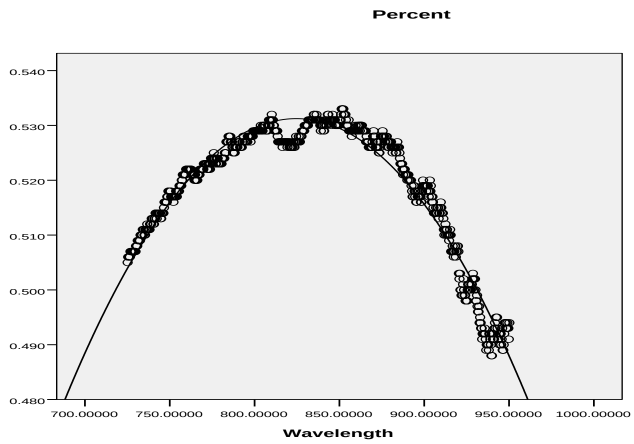

Figure 16. Plot between wavelength and percent adsorption at third segment

Analisis of variance (Anova) could be concluded that quadratic function was accepted. H1 was accepted (Table 11). F-computed was 766.925 with degrees of freedom (2, 750) and significant probability of 0.000.

The function is

$$Y = -1.341 + 0.005\,X - 2.80\,x10^{-6}X^2 + e \quad \text{(F.10)}$$

Y=percent of adsorbstion

X=wevelength

Table 11. Anova of quadratic regression wavelength as independent and percent adsorption as dependent variables

Source	Sum of square	df	Mean square	F-compute	Sig
Regression	0.095	2	0.047	766.925	0.000
Residual	0.004	710	$6{,}12837x\ 10^{-5}$		
Total	0.009	712			

This quadratic regression has R Square of 97 %. This quadratic regression has significant intercept, significant coefficient of X and significant coefficient of X^2 (Table 12).

Table 12. Estimated coefficient quadratic regresssion and significancy

Model	Coefficients	Standard error	t-compute	sig
Wavelength	0.005	0.00004	110.083	0.000
Wavelength**2	$-2.8x10^{-6}$	$2.45x\ 10^{-8}$	-11.984	0.000
Constant	-1.341	0.017	-77.873	0.000

Assumptions of this quadratic regression are residual has normal distribution and independent. Normal P-P Plot was used to evaluate normal distribution of residual and plot of residual was used to evaluate residual has independent distribution. From Figure 17 and 18, those can be concluded residual has normal distribution and not independent of residual. Residual is not independent distribution has mean that residual has autocorrelation between observations. Behaviour of residual can be estimated by arima model.

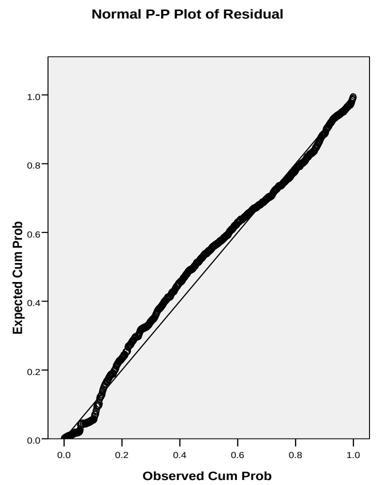

Figure 17. Normal P-P plot of residual regression

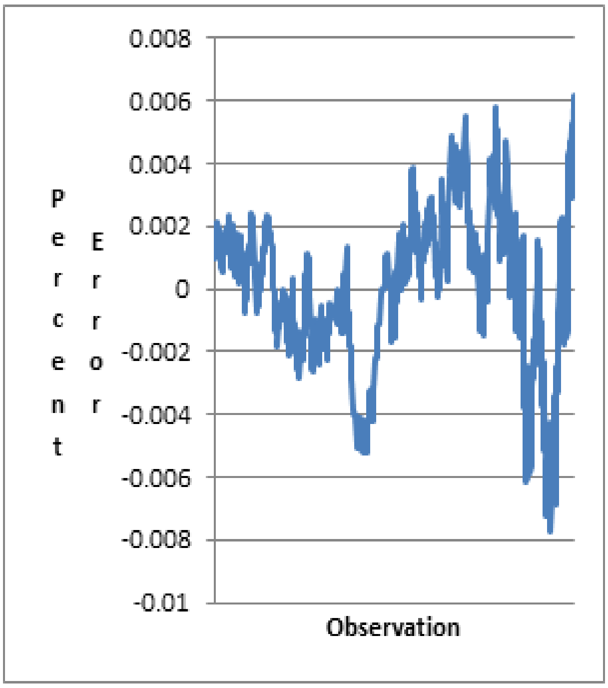

Figure 18. Plot of residual regression

First step of to estimate arima model of residual is to compute autocorrelation function (ACF) and partial autocorrelation function (PACF). Result of ACF and PACF residual. Based on Figure 19 and Figure 20, ARIMA (2,0,0) is may be good choice to estimate behaviour of residual

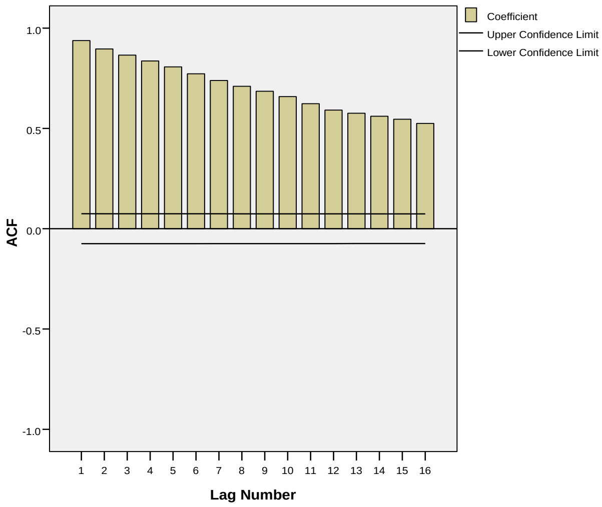

Figure 19. ACF of residual

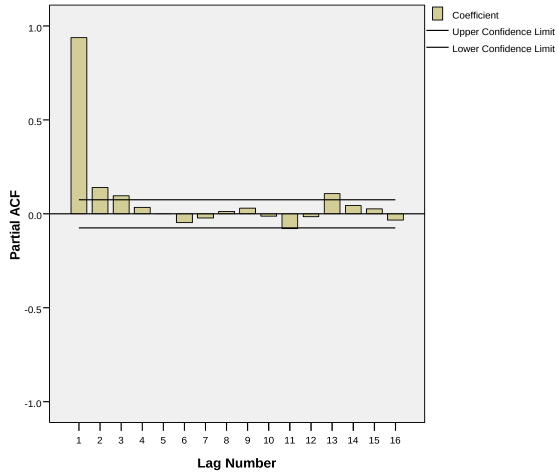

Figure 20. PACF of residual

Arima model of residual is Arima (2,0,0) with function

$$e_i = 0.003096 + 0.831\, e_{i-1} + 0.121\, e_{i-2} + u_i \quad \text{(F.11)}$$

Then $\widehat{e}_i = 0.003096 + 0.831\, e_{i-1} + 0.121\, e_{i-2}$

Table 13. Arima (1,0,0) of residual

Model		Estimate	SE	T-compute	Sig.
Constant		0,003096	0.001	0.323	0.747
AR	Lag1	0.831	0.038	22.040	0.000
	Lag2	0.121	0.038	3.202	0.001

Arima (2,0,0) has R^2 of 89 % , this model has high accuration to estimate of residual at i based on residual at i-1 and at i-2. Plot data of residual and arima residual presented at Figure 21 where estimated from arima residual (2,0,0) can follow residual data.

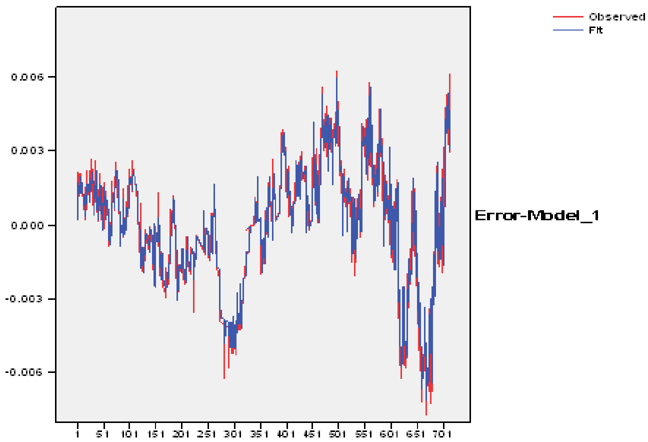

Figure 21. Plot estimated of arima residual with residual data

Model of percent adsorbtion as dependent variable and wavelenght as independent variable can be constructed with two models above, quadratic regression and arima residual. Combination function is

$$Y_i = -1.342 + 0.005\ X_i - 2.82x10^{-6}X^2{}_i + 1.010\ \text{Estimated arrima residual}_i + z_i\ (F.12)$$

Where estimated arima residual is $\widehat{e}_i = 0.003096 + 0.831\ e_{i-1} + 0.121\ e_{i-2}$
and
$e_{i-1} = (y_{i-1} - (-1.342 + 0.005\ X_{i-1} - 2.82x10^{-6}X^2{}_{i-1}))$

$$e_{i-2} = (y_{i-2} - (-1.342 + 0.005\ X_{i-2} - 2.82x10^{-6}X^2{}_{i-2}))$$

Anova of F.12. was presented at Table 14, which said H1 was accepted or H0 was rejected. Table 15 said constant of -1.342 was accepted H1, parameter estimation of wavelength of 0.005 was accepted H1, parameter estimation of wavelength² of $-2.82\ x\ 10^{-6}$ was accepted H1, parameter of Estimate arima residual 1.010 was accepted H1. F.12. has R^2 of 99.8 % which mean prefectly accurate function to estimate percent adsorbtion based on wavelenght.

Table 14. Anova of quadratic regression and arrima residual

Source	Sum of square	DF	Mean Square	F-compute	Sig.
Regression	0.097	3	0.032	61666.309	0.000
Residual	0,00037	707	$5.25x\ 10^{-7}$		
Total	0.098	710			

Table 15. Estimated coefficient quadratic regresssion, estimated arima residual and significancy

Source	Parameters	Standard Error	T-compute	Sig
Constant	-1.342	0.005	-265.446	0.000
Wavelenghth	0.005	$1,3334x\ 10^{-5}$	374.977	0.000
Wavelenghth**2	$-2.82x\ 10^{-6}$	$7,36914x\ 10^{-9}$	-381.320	0.000
Estimated arima residual	1.010	0.012	86.82	0.000

F.12 can be changed as function below

$$Y_i = -1.342 + 0.005\ X_i - 2.82x10^{-6}X^2{}_i + 1.010\ (0.003096 + 0.831\ e_{i-1} + 0.121\ e_{i-2}) + z_i$$

Then

$$Y_i = -1.33887 + 0.005\ X_i - 2.82\ x\ 10^{-6}X^2{}_i + 0.83931\ e_{i-1} + 0.1221\ e_{i-2} + z_i\ \ (F.13)$$

Where
Yi percent of adsorption at i, Xi wavelength at i (725.18 <= Xi <= 950.19), $e_{i-1} = (y_{i-1} - (-1.342 + 0.005\ X_{i-1} - 2.82x10^{-6}X^2{}_{i-1}))$, $e_{i-2} = (y_{i-2} - (-1.342 + 0.005\ X_{i-2} - 2.82x10^{-6}X^2{}_{i-2}))$. F.13. has perfectly accurate function since has R^2 of 99.8 % (Figure 22)

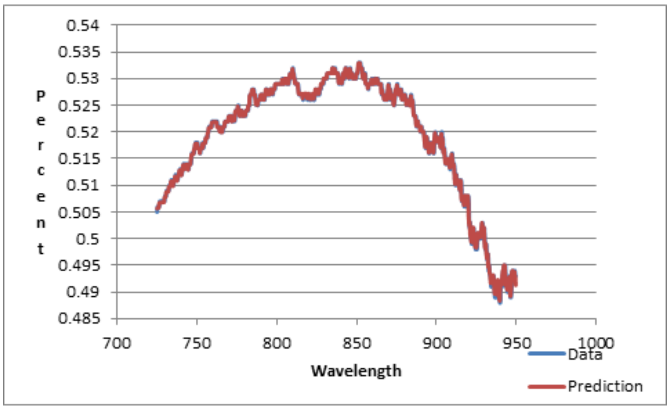

Figure 22. Plot Percent adsorbtion data with estimated function

3.2. Discussion

Linear regression between wavelength from 400,06 to 463,77 as independent variable with percent adsorption as dependent variable is $Y = -1.129 + 0.004\,X + e$. This model has coefficient determination of 92.4 %, which means 92.4% data can be explained by the model. Model combination between Arima and linear regression is $Y_i = -1.115052 + 0.004X_i - 0.98106\, e_{i-1} + z_i$ which has coefficient determination of 99.7 %. That model combination can explain 99.7 % data. The model combination between Arima and linear regression is better than linear regression, since there is increasing of coefficient determination.

Quadratic regression wavelength from 464.13 to 724.85 as independent variable with percent adsorption as dependent variable is $Y = 0.815 - 0.001\,X + 8.82x10^{-7}X^2 + e$ which has coefficient determination of 79 %. Model combination between quadratic regression and arima is $Y_i = 0.809462 - 0.001\,X_i + 8.82x10^{-7}{X^2}_i + 1.000401\, e_{i-1} + z_i$ which has coefficient determination of 99.7%. The model combination between Arima and quadratic regression is better than quadratic regression, since there is increasing of coefficient determination.

Quadratic regression wavelength from 725.18 to 950.19 as independent variable with percent adsorption as dependent variable is $Y = -1.341 + 0.005\,X - 2.80\,x10^{-6}X^2 + e$ which has coefficient determination of 97 %. Model combination between quadratic regression and arima is

$$Y_i = -1.33887 + 0.005\,X_i - 2.82\,x\,10^{-6}{X^2}_i + 0.83931\,e_{i-1} + 0.1221\,e_{i-2} + z_i$$

which has coefficient determination of 99.8 %. The model combination between Arima and quadratic regression is better than quadratic regression, since there is increasing of coefficient determination.

Model combination between Arima and regression for all range of wavelength from 400,06 to 950.19 is

$$Y_i = \begin{cases} -1.115052 + 0.004X_i - 0.98106\,e_{i-1} + z_i & for\ 400.06 \le x \le 463,77 \\ 0.809462 - 0.001\,X_i + 8.82x10^{-7}{X^2}_i + 1.000401\,e_{i-1} + z_i & for\ 464.13 \le x \le 724.85 \\ -1.33887 + 0.005\,X_i - 2.82\,x\,10^{-6}{X^2}_i + 0.83931\,e_{i-1} + 0.1221\,e_{i-2} + z_i & for\ 725.18 \le x \le 950.19 \end{cases}$$

At wavelength from 400.06 to 463.77, increasing of wavelength one unit of wavelength will a increasing of 0.004 percent adsorption. Maximum of adsoption is 0.740028 % at x = 463.77. At wavelength from 464.13 to 724.85, quadratic regression has a concave form. From this concave form we can find the minimum percent adsorption, by derived the function and equals zero. Df/dx= -0.001 + 0.000001764 x = 0, then x=566.893. Minimum percent adsorbtion is 0.526015 % at x =566.893. At wavelength from 725.18 to 950.19, quadratic regression has a convex form. From this convex form we can find the maximum percent adsorption, by derived the function and equals zero. Df/dx=0.005- 0,00000564 x=0, then x=886.525. Maximum percent adsorption is 0.877442 % at x=886.525. We can say the absolute minimum of percent adsoption is 0.526015 % at x =566.893, local maximum of percent adsoption is 0.740028 % at x = 463.77, absolute maximum is 0.877442 % at x=886.525.

IV. CONCLUSION

At wavelength from 400.06 to 463.77, the model combination between Arima and linear regression is better than linear regression, since there is increasing of coefficient determination. Model combination between Arima and linear regression is $Y_i = -1.115052 + 0.004X_i - 0.98106\,e_{i-1} + z_i$. At wavelength from 464.13 to 724.85, The model combination between Arima and quadratic regression is better than quadratic regression (a concave form), since there is increasing of coefficient determination. Model combination between quadratic regression and arima is $Y_i = 0.809462 - 0.001\,X_i + 8.82x10^{-7}{X^2}_i + 1.000401\,e_{i-1} + z_i$. At wavelength 725.18 to 950.1, The model combination between Arima and quadratic regression (a convex form) is better than quadratic regression, since there is increasing of coefficient determination. Model combination between quadratic regression (a convex form) and arima is

$$Y_i = -1.33887 + 0.005\,X_i - 2.82\,x\,10^{-6}X^2{}_i + 0.83931\,e_{i-1} + 0.1221\,e_{i-2} + z_i.$$

The absolute minimum of percent adsoption is 0.526015 % at x =566.893, local maximum of percent adsoption is 0.740028 % at x = 463.77, absolute maximum is 0.877442 % at x=886.525.

Has successfully Reviewed Regression and ARIMA Residual Have High Accuracy to Estimate Percent adsorption Spectral-Based on Wavelength at Barium Titanate. The results of regression analysis and ARIMA residual from Barium titanate material is very useful for processing advanced material data to develop nanoelectronics science and technology in the future.

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