BAREKENG: Journal of Mathematics and Its Applications
June 2023 Volume 17 Issue 2 Page 0659–0666
P-ISSN: 1978-7227 E-ISSN: 2615-3017
https://doi.org/10.30598/barekengvol17iss2pp0659-0666

G-OPTIMAL DESIGN OF NON-LINEAR MODEL TO INCREASE PURITY LEVELS OF SILICON DIOXIDE

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ABSTRACT

Article History:

Received: 29th September 2022
Revised: 8th April 2023
Accepted: 10th April 2023

Keywords:

G-optimal;
Non-linear model;
Optimal design;
Silicon dioxide.

Silicon Dioxide (SiO2) is one of the most abundant minerals found on earth. SiO2 is widely used in various fields, so its availability as a finite natural resource diminishes. A purity procedure can raise the purity of low-quality silica by altering the temperature and rate of temperature rise. This study aims to obtain the best design for increasing SiO2 levels—the G-optimal design on a non-linear model using the Variable Neighborhood Search (VNS) algorithm. The VNS algorithm employs two types of neighborhoods, one acquired by replacing one design point with a candidate set and the other by replacing two design points with two points in the candidate set. The model used to increase silicon dioxide's purity is a non-linear model that follows the exponential decay distribution. The best design points obtained from the G-optimal design on the relationship between temperature (oC) and the rate of temperature increase (oC/min) 800 oC to 900 oC is a pair of points 800 oC and 1,67 oC /min, 800 oC and 2,17 oC/min, 815 oC and 2,50 oC/min, 825 oC and 2,00 oC/min, 845 oC and 2,34 oC/min, 895 oC and 3,34 oC/min 900 oC and 3,50 oC/min with a G-efficiency of 96,41%.

How to cite this article:

N. Wulandari, Erfiani, Irzaman andU D. Syafitri., "G-OPTIMAL DESIGN OF NON-LINEAR MODEL TO INCREASE PURITY LEVELS OF SILICON DIOXIDE," *BAREKENG: J. Math. & App.*, vol. 17, iss. 2, pp. 0659-0666, June, 2023.

Journal homepage: *https://ojs3.unpatti.ac.id/index.php/barekeng/*
Journal e-mail: *barekeng.math@yahoo.com; barekeng.journal@mail.unpatti.ac.id*

Research Article • Open Access

1. INTRODUCTION

A series of statistical applications known as the experimental design is used to classify and quantify the correlation between the input and output variables in the process under research which aims to find the settings and conditions under which processes are optimized [1]. The experiment aims to obtain information or facts that follow the study's objectives by considering a minimum of time, cost, effort, and experimental materials [2]. The design of experiment (DOE) is a statistical method widely used in various scientific and industrial fields to support the design, development, and optimization of items and processes [3]. One use of the experimental design is the design for experiments on silicon dioxide.

Silica, often known as silicon dioxide ($SiO2$), is a mineral commonly found on Earth and obtained from mining materials. Silica is available as a naturally occurring resource that can be exhausted because of its many benefits in various fields. As a result, its selling price is extremely high. Efforts must be made to maintain the availability of silica and produce silica with a high purity level capable of providing opportunities in the business and industrial fields. Several studies have shown that it turns out that silica can be made from several materials that are around humans, such as rice husks, corn cobs, palm oil, bamboo leaves, and others for vegetable silica.

Based on previous research, the silica content in rice husk ash is 90-98% dry weight [4]. The second highest silica content is from bamboo leaf ash, which is 75.9% [5], while straw ash has a silica content of 75% [6]. The highest silica content is found in rice husks. Compared to mineral silica, silica made from rice husk has several advantages. It is more reactive, has more refined grains, is easier to produce, costs less, and is supported by the availability of abundant and renewable raw materials [7]. Complete combustion of rice husk ash produces silica as much as 90% to 98% dry weight. Silica with low purity can be increased through the purity process by adjusting the influencing factors.

The combination of these influencing factors will further increase silica purity. Research or experiments that want to know the effects of several experimental factors can be studied through a design that is processed using optimal design theory [8]. The optimal design is part of the design that estimates the parameters without bias with the smallest variance to produce accurate statistical inference [9]. An optimal design is needed to determine the points to be tested to optimize the design with the desired criteria.

Optimal design is part of the experimental design that allows parameter estimates without bias and has a minimum variance. The optimal design depends on the model used and the number of observations desired by estimating using optimal criteria. The G-optimal design minimizes the maximum mean squared prediction error in the experimental region by minimizing the maximum variance value of each predicted value [10].

A non-linear model is a relationship between the response variable and the explanatory variable that is not linear in the parameters. Taylor series is one approach that can be used to approach non-linear equations through linear equations. This research is a case study of silicon dioxide by using the temperature factor and the rate of temperature increase as factors that affect the rate of increase in the purity of silicon dioxide. The design used is the optimal design with G-optimal criteria on non-linear models. The optimal design leverages computational power and algorithms to generate a broad class of designs that can be used for many problems [12]. The VNS algorithm will be used to select the design point candidates. The VNS algorithm can be used to explore the neighborhood sequentially from the neighborhood with the fewest solutions to the neighborhood with the most solutions [13].

2. RESEARCH METHODS

2.1 Model Used

The model used in this study is a non-linear model with temperature (°C) and rate of temperature rise (°C /min) as factors and silica purity levels (percent) as a response. The higher the temperature at which silicon dioxide is burned, the higher the purity of silicon dioxide. However, the increase in silicon dioxide purity follows a non-linear trend, with the increase becoming smaller as it approaches 100 percent purity [11]. Exponential decay is a non-linear model in chemical kinetics that approximates an asymptote value [8]. This is the non-linear exponential decay model that was used:

$$f(t,r) = [A_0]\{1 - e^{-\theta_1 t + \theta_2 r}\} \tag{1}$$

where:

$f(t,r)$ = expected value of the response
A_0 = constant
θ_1, θ_2 = parameters
t = temperature
r = rate of temperature rise

The non-linear model is more complicated than the linear model, so it requires more analysis in the research process. One method for approaching non-linear equations through linear equations is the Taylor series. The multivariable Taylor method is written as follows:

$$f(t,r) = \sum_{i=0}^{n} \sum_{j=0}^{n-i} \frac{\frac{d^{(i+j)}}{\partial t^i \partial r^j} f(a,b)}{i!j!} (t-a)^i (r-b)^j \quad (2)$$

where $f(t,r)$ is a function of t and r, a and b are constants.

2.2 Steps of the Variable Neighborhood Search (VNS) Algorithm

The steps to choosing the optimal design point are as follows:

1. Make a list of candidate sets based on a combination of temperature points and rate of temperature rise. The temperature was raised from 800 to 900 °C, and the rate of temperature rise from 1.67 °C/min to 5 °C/min, with a 0.5 °C/min increase.
2. Make a starting design (initial design) with the following steps:
   a. To create the initial design, choose points randomly from candidate sets.
   b. Calculate and determine the estimated variance of the predicted value (SPV(x)). SPV can be calculated by [14]:

$$SPV(x) = N(\boldsymbol{x}_i' (\boldsymbol{X}'\boldsymbol{X})^{-1} \boldsymbol{x}_i) \quad (3)$$

   c. In the initial design, look at the highest predicted variance ($SPV(x)$) value as the best option.
3. Explore the neighborhood that has been set in the application of the Variable Neighborhood Search algorithm with the following steps:
   a. Neighborhood N_0
      1) Add a point at random from the list of candidate sets to the initial design.
      2) Using the same calculation as in step 2, calculate the expected variance of the predicted value of the current design.
      3) Review the maximum predictive variance ($SPV(x)$) value as the optimal solution in the current design.
      4) Compare the optimal design in the N_0 neighborhood to the initial design, choosing the one with the minimum and maximum variance. If the design in the N_0 neighborhood is not better than the first, the next neighborhood will be explored.
   b. Neighborhood N_1
      1) Replace two points from design N_1 with two points from the candidate sets.
      2) Using the same calculation as in step 2, calculate the variance of the predicted value of the current design.
      3) Review the maximum predictive variance ($SPV(x)$)value as the optimal solution in the current design.
      4) Compare the optimal design in the N_1 neighborhood with the N_0 design, and select the design with the minimum and maximum variance values.
4. Repeat steps 2 to 4 in the previous neighborhood. The third stage is repeated an infinite number of times.
5. Calculating the G-efficiency value in the chosen design. In the G-optimal design, the G-efficiency formula is [15]:

$$G - efisiensi = 100 \times \left(\frac{p}{max_{x_i \in R} SPV(x)} \right) \quad (4)$$

where p is the number of parameters in the model and p is a lower bound for $max_{x_i \in R} SPV(x)$.

3. RESULTS AND DISCUSSION

3.1. Non-linear Model Approach

A Taylor series approach with a k^{th} order polynomial will be used to approach the model employed in this study. The initial solution approach is used because it has the smallest mistake. The model's MSE (Mean Square Error) value is used to determine the order. The MSE values for the results of the SiO2 purity level given from the Taylor approximation simulation using θ_1= 0,005 and θ_2= 0,005 is as follows:

Table 1. Statistics descriptive

Order	MSE
1	7,83E-08
2	5,00E-10
3	1,86E-12

Based on the simulation in **Table 1**, the Taylor polynomial selected is in the second order. The second-order Taylor polynomial has a fairly small MSE and an uncomplicated model. Taylor's model uses **Equation (2)** with the second order as follows:

$$f(t,r) = 0{,}79413127 + 0{,}00037952\, t - 0{,}000379 r - 1{,}8130105.10^{-7} t^2 + 3{,}62602.10^{-7}\, tr - 1{,}8130105\ 10^{-7}\, r^2.$$

3.2. G-Optimal Design on Silicon Dioxide Purity Levels

n This study resulted in a design point for SiO_2 purity levels in the temperature range of 800 ºC to 900 ºC with a different number of points, namely the design of SiO_2 purity levels with seven design points, 12 design points, and 20 design points. The best design results are presented in the following table:

Table 2. G-optimal design with7 point design

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	2,17
3	815	2,50
4	825	2,00
5	845	2,34
6	895	3,34
7	900	3,50
G-efficiency		96,41%

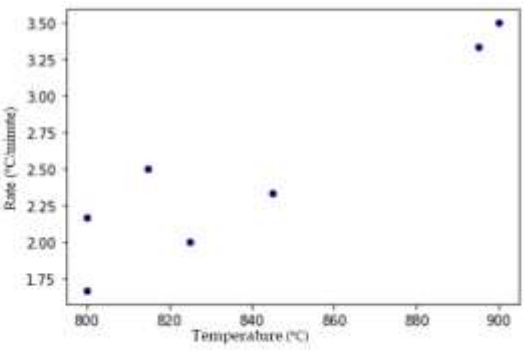


Figure 1. Visualization of SiO_2 design points with 7 points

The visualization of the design points obtained by design at a temperature of 800 ºC to 900 ºC with seven design points can be seen in **Figure 1**. The minor design point in the figure is at 800 ºC, and the rate of temperature increase is 1,67 ºC/minute, while the greatest is at 900 ºC, when the rate of temperature increase is 3,33 ºC/minute. The temperature points of 815 ºC and 825 ºC will then be changed to the lowest temperature point obtained, which is 800 ºC. The point of temperature rise rate of 3,34 ºC/minute and 2,50 ºC/minute is converted into the point of the maximum temperature rise rate obtained, which is 3,50 ºC/minute, to see if the design is better compared to the design obtained. The results are presented in **Table 3**.

The results from alternative 1, which replaced the temperature points of 815 ºC and 825 ºC for the lowest temperature point of 800 ºC, resulted in a lower G-efficiency value of 85,90%. Alternative two, which is obtained by replacing the point of the temperature rise rate of 3,34 ºC/minute and the rate of temperature increase of 2.50 ºC/minute to the point of the maximum temperature rise rate obtained is 3,50 ºC/minute, also obtains a smaller G-efficiency of 85,91%. That proved the G-optimal design at the level of SiO_2 purity levels with 7 points is the best design with a large enough G-efficiency value of 96.41%.

Table 3. Alternative G-optimal design with 7-point design

Alternative 1		Alternative 2	
Temperature (ºC)	**Rate (ºC/minute)**	**Temperature (ºC)**	**Rate (ºC/minute)**
800	1,67	800	1,67
800	2,17	800	2,17
800	2,50	815	2,50
800	2,00	825	2,00
845	2,34	845	3,50
895	3,34	895	3,50
900	3,50	900	3,50
G-efficiency	85,90%	G-efficiency	85.91%

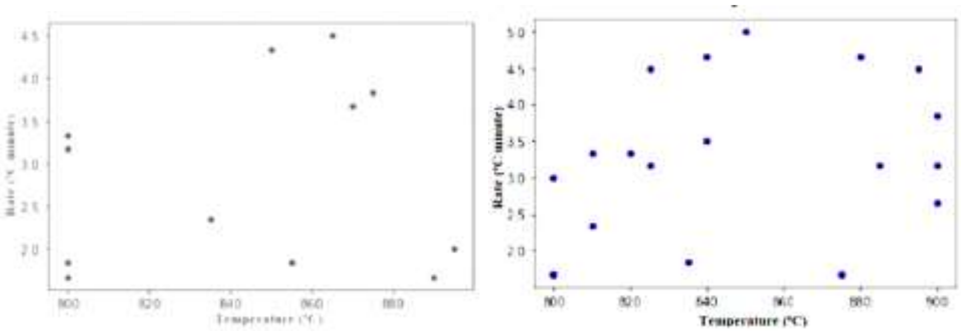
The design point for the level of purity of SiO_2 in the temperature range of 800 ºC to 900 ºC with 12 design points and 20 design points can be seen in Table 4 and Table 5 below.

Table 4. G-optimal design with 12 design points

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	1,84
3	800	3,17
4	800	3,33
5	835	2,67
6	850	4,33
7	855	1,84
8	865	4,50
9	870	3,67
10	875	3,84
11	890	1,67
12	895	2,00
G-efficiency		88,22%

Table 5. G-optimal design with 20 design points

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	1,67
3	800	1,67
4	800	3,00
5	810	2,33
6	810	3,33
7	825	3,17
8	825	4,50
9	835	1,87
10	840	3,17
11	840	4,67
12	850	5,00
13	875	1,67
14	880	1,67
15	875	2,67
16	875	3,17
17	880	4,67
18	895	5,50
19	900	2,67
20	900	3,17
G-efficiency		76,38%



(a) (b)

Figure 2. Visualization of SiO_2 design points with 12 points (a) and 20 points (b)

Table 4 shows the optimal design point for SiO_2 purity using a temperature range of 800 ºC to 900 ºC using 12 design points with a G-efficiency value of 88,22%. The best design point at the level of SiO2 purity using a temperature range of 800 ºC to 900 ºC with 20 design points is presented in **Table 5**. Based on **Table 5**, the G-efficiency value obtained is 76,38%. **Figure 2** shows the visualization results of the design points obtained by design at a temperature of 800 ºC to 900 ºC with 12 and 20 design points. The figure shows that the lowest temperature for the 12-point design is 800 ºC, while the highest is 895 ºC. The lowest temperature rise rate in the design with 12 points is 1,67 ºC/minute, and the largest temperature rise rate is 4.50 ºC/minute. The design with 20 points shows that the lowest temperature is 800 ºC, and the highest is 900 ºC. The lowest temperature rise rate in the design with 20 points is 1.67 oC/minute, and the largest temperature rise rate is 5 ºC/minute.

The DETMAX algorithm on the SAS program will be used to display the findings of this study's search for the best design utilizing the G-optimal criteria. The results of the VNS algorithm compared to the optimal design of the DETMAX algorithm to test whether the VNS design gives a better optimal design. The point exchange process is carried out by the DETMAX algorithm, namely, adding a design point from the initial design point, then reducing the current design point. The optimal design results using the DETMAX algorithm can be seen in **Tables 6** - **8**.

Table 6. G-optimal design using DETMAX with seven design points

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	5,00
3	825	3,67
4	855	1,67
5	890	5,00
6	900	1,67
7	900	3,50
G-efficiency		85.15%

Table 7. G-optimal design using DETMAX with 12 design points

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	4,33
3	800	5,00
4	805	2,00
5	840	2,84
6	845	3,34
7	860	5,00
8	870	2,00
9	895	1,67
10	900	2,17
11	900	4,00
12	900	5,00
G-efficiency		87,90%

Table 8. G-optimal design using DETMAX with 20 design points

No	Temperature (ºC)	Rate (ºC/minute)
1	800	1,67
2	800	2,50
3	800	3,34
4	800	3,34
5	800	4,17
6	810	4,67
7	810	5,00
8	835	2,00
9	835	2,00
10	855	5,00
11	875	3,34
12	880	3,34
13	880	3,34
14	880	3,34
15	885	3,34
16	890	1,67
17	895	1,84
18	900	1,67
19	900	5,00
20	900	5,00
G-efficiency		87,90%

Based on Tables 6 - 8, it can be concluded that the optimal design using the DETMAX algorithm has a lower G-efficiency value than the optimal design obtained using the VNS algorithm. Figure 2 and Figure 3 show the results of the G-optimal design points obtained using the DETMAX algorithm and the VNS algorithm in common; the design points obtained are very diverse and irregular.

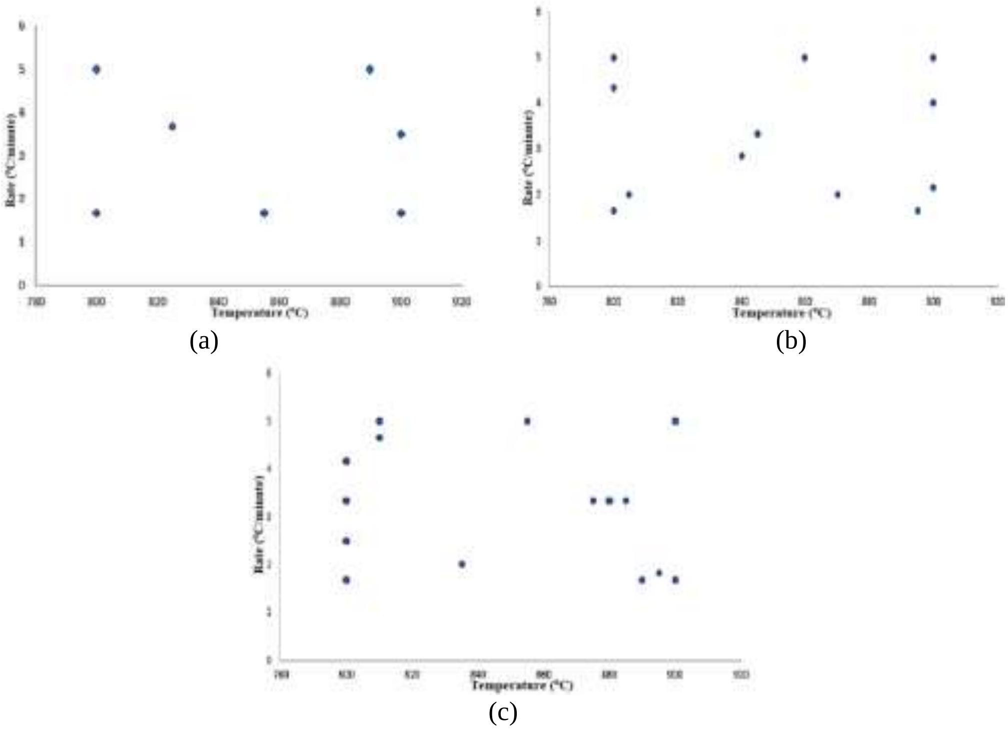


Figure 3. Visualization of SiO_2 design points with (a) 7 points, (b) 12 points, and (c) 20 points

Based on the results of this study, it can be concluded that the greater the number of points used, the greater the value of the maximum predictive variance, so that the value of G-efficiency obtained will be smaller. The best G-optimal design is the design using 7 points with a G-efficiency value of 96.41%.

4. CONCLUSIONS

The best design point obtained from the G-optimal design on the relationship between temperature (°C) and the rate of temperature increase (°C/min) on the response variable of the level of purity of SiO_2 with a temperature range of 800 °C to 900 °C is a pair of points 800 °C and 1,67 °C /min, 800 °C and 2,17 °C/min, 815 °C and 2,50 °C/min, 825 °C and 2,00 °C/min, 845 °C and 2,34 °C/min, 895 °C and 3,34 °C/min 900 °C and 3,50 °C/min with a G-efficiency of 96,41%.

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