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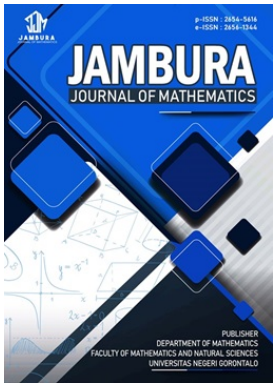

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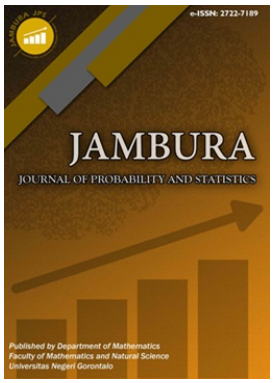

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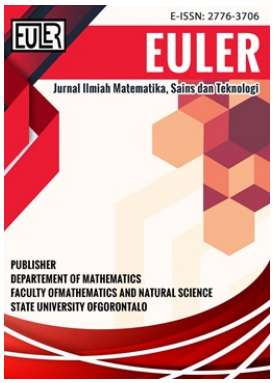

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Research Article

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The Comparison A-Optimal and I-Optimal Design in Non-Linear Models to Increase Purity Levels Silicon Dioxide

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ABSTRACT. *One of the obstacles that arise in optimal design is the non-linear model. The relationship between temperature factors and the temperature increase rates with the purity of silicon dioxide* (SiO_2) *forms a non-linear pattern. Determining the optimal design for a non-linear model is relatively more complex than a linear model because it requires additional information in its information matrix. Therefore, this issue necessitates further research on optimal design in non-linear models. This study uses the polynomial Taylor approach to approximate the non-linear equation through a linear equation using the appropriate optimal design methods, namely A-Optimal and I-Optimal criterion. The point search algorithm used was variable neighborhood search, this algorithm searches for design points by exploring several different neighborhood structures. These two methods were chosen to compare the characteristics and performance of the designs produced, aiming to obtain an optimal design to improve* (SiO_2) *purity (non-linear case) using the same algorithm, VNS. The research results showed that the design pattern produced by the A-Optimal design formed three temperature groups, namely the minimum temperature of* $800°C$ - $820°C$, *the middle temperature of* $850°C$, $860°C$, *and the maximum temperature of* $900°C$, *with varying temperature increase rates in the design area. The design pattern produced by the I-Optimal design formed a full quadratic pattern, namely the minimum temperature of* $800°C$ *and the maximum temperature of* $900°C$, *with varying temperature increase rates in the design area. The I-Optimal design demonstrated the best performance (most optimal) in the aspect of prediction variance compared to the A-Optimal design across all alternative points in this study to improve* (SiO_2) *purity.*

1. Introduction

An experimental design is a method for designing an experiment by arranging the possible factors used in the experiment. Experimental design is conducted to obtain information or facts that align with the research objectives, considering the time, cost, effort, and materials used in the experiment [1]. Experimental designs are widely utilized in various fields such as industry, agriculture, healthcare, and others. One of the benefits of experimental design is its application in the design of silicon dioxide (SiO_2).

Silicon dioxide, with the chemical formula SiO_2, is one of the most widely found minerals on earth, and it has a reasonably large utilization process. SiO_2 minerals are generally sold at relatively high prices. The raw materials used to obtain SiO_2 are relatively straight forward. SiO_2 can be produced from biomass, including rice straw, husks, and bagasse [2]. SiO_2 with a high level of purity (>95%) can be utilized in the industrial field, such as industrial raw materials, solar cells, microcomputer chips, electronics, semiconductors, and others [3, 4].

Low-purity SiO_2 can be improved through a purification process by adjusting the temperature factor (°C) and different rates of temperature increase (°C/minute), where the combination of these factors will affect the improvement of silica purity to varying degrees [5]. Therefore, experimental design can be applied to this issue. However, in the design of experiments, the combination of existing factors results in many experiments, so the cost, energy, and time spent is also quite large. Thus, optimal design is the solution to obtain the optimal combination of temperature and heating rate factors. Optimal design is an effort to find combinations of several factors to be tested with the aim of optimizing the design based on certain criteria according to statistical principles and considering the information contained in the design [6].

One of the obstacles that arise in optimal design is the non-linear model. A non-linear model is a relationship between response variables and explanatory variables that are not linear in parameters. Determining the optimal design in non-linear models is relatively more difficult than in linear models because it requires additional information in the information matrix. The relationship between temperature and temperature increase rates with the purity of silicon dioxide has a non-linear pattern, forming an exponential relationship [7]. The increase in purity decreases and becomes smaller as the purity value approaches 100 percent. Optimal designs in non-linear models are still rarely researched.

Research by Rivai et al. [7] and Wulandari et al. [8] pro-

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posed the Taylor series method using a *k*-th order polynomial to approximate nonlinear equations in optimal design criterion through linear equations. Thus, the information matrix used will approximate the information matrix in linear equations. Moreover, optimal design requires criterion in its analysis process. The criterion for optimal design is based on the variance of parameter estimates and the prediction variance values.

Previous research Jones et al. [9] compared the optimal design resulting from the A-Optimal criterion and the D-Optimal criterion, which are criterion based on the variance of parameter estimates in the case of screening experiments, where in this study, the A-Optimal design gave better results than the D-Optimal design. Another study for optimal design based on the prediction variance was conducted by Goos et al. [10] using the I-Optimal criterion and compared with the D-Optimal criterion in multidimensional non-linear cases in mixture experiments. The results showed that the optimal design performance resulting from the I-Optimal criterion resulted in a more minor prediction variance than the D-Optimal criterion.

In addition, optimal design also requires a point search algorithm to obtain optimal design results. Previous research Wulandari et al. [8] conducted optimal design research by comparing a point search algorithm using variable neighborhood search (VNS) with one of the algorithms often used in optimal design, namely the Detmax algorithm, which is part of the point exchange algorithm, where this research provides point search results using the VNS algorithm more efficiently than the Detmax algorithm in non-linear cases.

Based on the above explanation, this study utilizes the *k*-th order Taylor polynomial model as a non-linear approach in optimal design. The design criterion used are A-Optimal and I-Optimal, with a design point search algorithm using VNS and using the range of temperature factors (°C) and the temperature increase rates (°C/minute) from the research of [7, 8] alternative nine design points and alternative 12 design points with the aim of comparing the characteristics and performance of the design produced by the A-Optimal and I-Optimal criterion in non-linear models in order to obtain the best design to increase the purity of silicon dioxide.

2. Methods

2.1. Case study

This study uses factors that can increase the purity of silicon dioxide (SiO_2), namely combustion temperature (°C) and the temperature increase rates (°C/minute). The data used is simulation data for design. The design case formed in this study will use a temperature range of 800°C - 900°C with a temperature increase rates factor range of 1.67°C/minute - 5°C/minute from research [8]. Then, two alternative points are tried, namely one alternative choosing nine design points, and two alternative choosing 12 design points.

2.2. Non-Linear Models

This study explores how the factors of combustion temperature (°C) and temperature increase rates (°C/minute) can affect the improvement of the purity of silicon dioxide (SiO_2). The optimal design will use these two factors, and the model used in the optimal design is non-linear. The higher the combustion temperature of silicon dioxide, the higher the purity of silicon dioxide produced. However, increasing purity is non-linear, where the increase in purity decreases and becomes smaller as the purity value approaches 100 percent [7]. The non-linear model used is exponential decay, which is a model that is often used in chemical kinetics research. The non-linear exponential decay model is as follows [8]:

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

where $f(t,r)$ is the silica purity grade, A_0 is a constant, θ_1, θ_2 are parameters, t is the temperature factor, and r is the temperature increase rates. Estimating parameters in non-linear models usually cannot be solved analytically, so this study uses the Taylor approach. A model is approximated using the Taylor approach to get results closer to the initial solution [11]. Here is the Taylor Polynomial formula:

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

(t,r) is a function of the variables t (temperature) and r (temperature increase rates), a and b are constants obtained from the average value of each factor.

2.3. Design and Analysis Steps

The steps taken to develop the optimal design point for silicon dioxide (SiO_2) purity are as follows:

A. Form a non-linear model with a *k*th-order Taylor Polynomial approach and determine the best model selected based on Mean Square Error (MSE).
B. Develop the Variable Neighborhood Search (VNS) algorithm to form the optimal design point for each criterion as follows:
   (a) VNS steps on the A-Optimal criterion
      1. Create a candidate point set (*N*) containing all the possibilities. The process of forming candidate points is done by changing the value of the temperature factor and temperature increase rates to a scale of -1 to 1. Then, 11 candidate points are obtained so that there are 121 combinations of candidate points to be tested.
      2. Create a design point as the starting design by randomly selecting points from the set of candidate sets to form the initial design. Then, as the optimal solution to the initial design. Calculate and review the value of $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$, the optimal solution to the initial design.
      3. Exploring neighborhoods using the Variable Neighborhood Search algorithm with the following steps:
         - Neighborhood N_0
         a. Replace one randomly drawn point from the candidate set to the initial design.
         b. Calculating and reviewing the $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ value as the optimal design solution in this neighborhood.
         c. Comparing the optimal plan in the neighborhood N_0 with the initial design. Select the

design in a neighborhood with the minimum $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ value. If the $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ value obtained in neighborhood N_0 is greater than the initial design, then explore the next neighborhood.

- Neighborhood N_1

a. Replace two randomly drawn points from the candidate set to the initial design.
b. Calculating and reviewing the $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ value as the optimal design solution in this neighborhood.
c. Comparing the optimal plan in the neighborhood N_1 with the neighborhood N_1. Select the design in a neighborhood with the minimum $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ value.

4. Steps 2 through 3 are repeated 1000 times to select the design that is the most optimal solution as the best design for this criterion.

(b) VNS steps on the I-Optimal criterion

1. Create a candidate point set (*N*) containing all the possibilities. The process of forming candidate points is done by changing the value of the temperature factor and the temperature increase rates to a scale of -1 to 1. Then, 11 candidate points are obtained so that there are 121 combinations of candidate points to be tested.
2. Create a design point as the starting design by randomly selecting points from the set of candidate sets to form the initial design. Then, as the optimal solution to the initial design. Calculate and review the value of $AV(x)$, the optimal solution to the initial design.
3. Exploring neighborhoods using the Variable Neighborhood Search algorithm with the following steps:
   - Neighborhood N_0

   a. Replace one randomly drawn point from the candidate set to the initial design.
   b. Calculating and reviewing the average prediction variance $AV(x)$ value as the optimal design solution in this neighborhood.
   c. Comparing the optimal plan in the neighborhood N_0 with the initial design. Select the design in a neighborhood with the minimum $AV\left(x\right)$ value. If the $AV(x)$ value obtained in neighborhood N_0 is greater than the initial design, then explore the next neighborhood.
   - Neighborhood N_1

   a. Replace two randomly drawn points from the candidate set to the initial design.
   b. Calculating and reviewing the average of prediction variance $AV\left(x\right)$ value as the optimal design solution in this neighborhood.
   c. Comparing the optimal plan in the neighborhood N_1 with the neighborhood N_1. Select the design in a neighborhood with the minimum $AV\left(x\right)$ value.
4. Steps 2 through 3 are repeated 1000 times to select the design that is the most optimal solution as the best design for this criterion.

C. Examining the characteristics of the design obtained from each criterion by observing the design patterns at each alternative point.
D. Evaluating the best design from each criterion using A-efficiency and I-efficiency values.
E. Comparing the performance of A-Optimal and I-Optimal designs using Fraction of Design Space (FDS).

2.3.1. A-Optimal Criterion

The A-Optimal criterion is an optimal design criterion based on parameter estimation that focuses on minimizing the variance of parameter estimates by minimizing the sum of the main diagonal elements of the inverse of the information matrix $\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ [9]. This sum of the main diagonal elements is also referred to as the trace (tr) of the inverse of the information matrix. In other words, the A-Optimal criterion aims to minimize $tr\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}$ among all possible designs, where $\boldsymbol{X}$ is the $n \times p$ model matrix, n is the number of design points, and p is the number of parameters in the model [12].

2.3.2. I-Optimal Criterion

The I-Optimal criterion is a criterion based on predicted values constructed to minimize the average prediction variance $AV\left(x\right)$ in the design space [13]. The formula for the average prediction variance is as follows:

$$AV\left(x\right) = tr\left[\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\mathbf{M}\right] \tag{3}$$

where $\boldsymbol{X}$ is the $n \times p$ model matrix, n is the number of design points, and p is the number of parameters in the model. $\boldsymbol{M}$ is the moment matrix, which is calculated using the following formula:

$$\mathbf{M} = \int_{\boldsymbol{X} \in [-1,\,+1]^k} f\left(\boldsymbol{x}\right) f'\left(\boldsymbol{x}\right) dx \tag{4}$$

In the context where the integral is applied to a matrix of single-term polynomials (monomials), this notation should be interpreted as a matrix of single-term polynomial integrals (monomials). The experimental region is defined as $[-1,\,+1]^k$, where k represents the number of factors [10].

2.3.3. Evaluating Designs

Suppose $\boldsymbol{X}_1$ is the first design and $\boldsymbol{X}_2$ is the second design. Then, the A-efficiency and I-efficiency formulas are as follows:

$$A - efisiensi = \frac{tr\left(\boldsymbol{X}_2'\boldsymbol{X}_2\right)^{-1}}{tr\left(\boldsymbol{X}_1'\boldsymbol{X}_1\right)^{-1}}. \tag{5}$$

Whereas if the A-efficiency value is greater than 1, then the first design is considered better than the second design in terms of the A-Optimal criterion [12].

$$I - efisiensi = \frac{AV\left(x_2\right)}{AV\left(x_1\right)}. \tag{6}$$

Whereas if the I-efficiency value is greater than 1, then the first design is considered better than the second design in terms of the I-Optimal criterion [14].

2.3.4. Variable Neighborhood Search Algorithm

The Variable Neighborhood Search (VNS) algorithm is a metaheuristic method for solving combinatorial optimization and global optimization problems [15]. VNS enhances local search-based algorithms by exploring several neighborhood structures to achieve optimal criteria. This is done to obtain optimal solutions within a specific neighborhood structure (local optimal) and optimal across different neighborhoods, thus achieving global optimal solutions [16]. One strategy of the VNS algorithm involves exploring neighborhoods sequentially, from the one with the fewest solutions to the one with the most solutions [10]. Larger neighborhoods are only explored when other neighborhoods fail to produce a better solution than the initial one.

The initial stage of the VNS algorithm involves creating a candidate design point set of size N. Then, an initial design (nc) is created, and several different neighborhoods are explored to generate an optimal design. The VNS algorithm improves the initial design by making small changes iteratively. The changes from the neighborhoods used are as follows: the first neighborhood is denoted as N0 generated by exchanging one design point with one point from the candidate point set. The last neighborhood in this study is N1, generated by replacing two design points with two points from the candidate point set [8].

2.3.5. Fraction of Design Space Plot

The fraction of Design Space (FDS) plot compares the prediction variance between two designs. The FDS plot is employed to visualize the minimum and maximum prediction variance. It shows the cumulative distribution of prediction variance across the entire design space or experimental region.

$$\mathrm{f}'(x)\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} f(x). \tag{7}$$

FDS plot consists of vertical and horizontal lines. The vertical line represents the prediction variance values, while the horizontal line indicates the fraction of the experimental region ranging from 0 to 1. A good design will exhibit the smallest prediction variability compared to other designs across the experimental region [17].

3. Results and Discussion

3.1. *Taylor Polynomial Approach for Non-linear Model*

The Taylor approach is illustrated to determine the order that will be used in this study, with the selection of the order based on the model's Mean Square Error (MSE) value. Based on the combination of Equation (1) and Equation (2), the illustration of the Taylor approach for the model of SiO_2 purity level is as follows:
First-order Taylor polynomial

$$f(t,r) = 1 - E + \theta_1 E(t-a) - \theta_2 E(r-b), \tag{8}$$

with

$$E = e^{-\theta_1 a + \theta_2 b}.$$

Second-order Taylor polynomial

$$\begin{aligned} f(t,r) = {} & 1 - E + \theta_1 E(t-a) - \theta_2 E(r-b) \\ & + \frac{1}{2!}[-\theta_1^2 E^2 (t-a)^2 + 2\theta_1\theta_2 E(t-a)(r-b) \\ & - \theta_2^2 E (r-b)^2]. \end{aligned} \tag{9}$$

This study conducted a simulation to determine the order to be used in the Taylor polynomial approach. The following are the MSE values from the Taylor approach simulation on the SiO_2 purity level model using parameters $\theta_1 = 0.01$ and $\theta_2 = 0.005$.

Table 1. MSE Values for Taylor Polynomial of Silica Purity Level

Taylor Polynomial	MSE
First Order	2.67e-10
Second order	**6.70e-12**

Based on the MSE values in table 1, the chosen Taylor polynomial is of order two because it has the smallest MSE value. The resulting model is then expanded to form a full quadratic model as follows:

$$\begin{aligned} f(t,r) = {} & 0.79413 + 0.00038t - 0.00038r \\ & - 1.81301 \cdot 10^{-7} t^2 - 1.81301 \cdot 10^{-7} r^2 \\ & + 3.62602 \cdot 10^{-7} tr \end{aligned} \tag{10}$$

Equation (10) is the model that will be used in this study to produce the optimal design. Figure 1 and Equation (10) show that the positive coefficient of the temperature factor indicates that each temperature increase increases SiO_2 purity [18]. Negative coefficient for the temperature increase rates explains that the higher the temperature increase rates, the lower the SiO_2 purity.

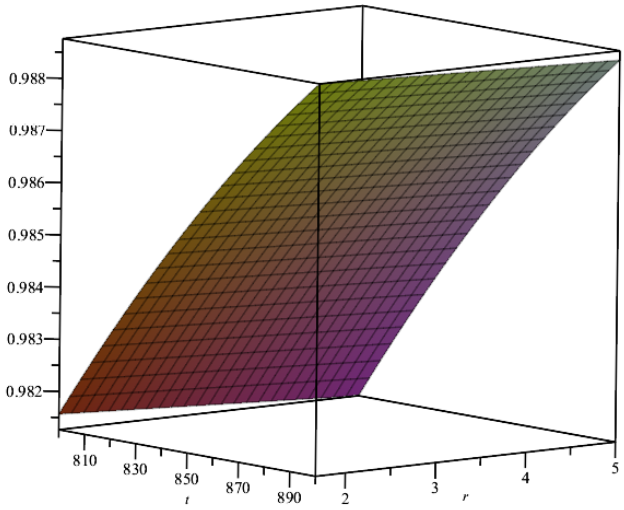


Figure 1. Relationship between temperature and temperature increase rates on silica purity at temperatures ranging from 800°C to 900°C, with temperature increase rates ranging from 1.67°C/minute to 5°C/minute.

Table 2. A-Optimal and I-Optimal Design Points for Alternative One

No	A-Optimal Design		I-Optimal Design	
	Temperature (°C)	Temperature increase rates (°C/minute)	Temperature (°C)	Temperature increase rates (°C/minute)
1.	800	3.34	800	1.67
2.	800	1.67	800	3.67
3.	800	5.00	810	2.67
4.	850	4.67	830	4.67
5.	850	3.67	840	3.34
6.	850	1.67	860	5.00
7.	900	4.67	860	2.67
8.	900	1.67	890	2.00
9.	900	1.67	900	3.67
A-Opt criterion value = 2.7660			I-Opt criterion value = 0.5446	

Table 3. A-Optimal and I-Optimal Design Points for Alternative Two

No	A-Optimal Design		I-Optimal Design	
	Temperature (°C)	Temperature increase rates (°C/minute)	Temperature (°C)	Temperature increase rates (°C/minute)
1.	800	1.67	800	4.33
2.	810	4.67	800	3.00
3.	810	3.67	800	1.67
4.	820	5.00	820	1.67
5.	850	1.67	830	3.00
6.	860	4.00	840	5.00
7.	860	4.00	850	3.67
8.	860	5.00	850	3.67
9.	900	1.67	860	3.67
10.	900	3.34	880	2.00
11.	900	4.33	900	2.34
12.	900	5.00	900	4.67
A-Opt criterion value = 2.0723			I-Opt criterion value = 0.3763	

3.2. A-Optimal and I-Optimal Designs for SiO_2 Purity Level

The initial step to obtaining the moment matrix for calculating the I-Optimal design involves utilizing the second-order Taylor polynomial approach after expanding the model formed in this design into a full quadratic model. This result forms the basis of this research to find the moment matrix for the I-Optimal design that will be used. Using Equation (4) to calculate the moment matrix for the full quadratic model with two continuous factors that can take values in the interval $[-1, +1]$, is as follows:

$$f'(x) = f'(x_1, x_2) = \begin{bmatrix} 1 & x_1 & x_2 & x_1x_2 & x_1^2 & x_2^2 \end{bmatrix}.$$

So, the moment matrix is

$$\begin{aligned} \mathbf{M} &= \int_{x\epsilon[-1,+1]^2} f(x) f'(x)\, dx \\ &= \int_{-1}^{+1}\int_{-1}^{+1} f(x_1, x_2) f'(x_1, x_2)\, dx_1 dx_2 \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 & 1/3 & 1/3 \\ 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/9 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/5 & 1/9 \\ 1/3 & 0 & 0 & 0 & 1/9 & 1/5 \end{bmatrix}. \end{aligned}$$

The best design results from the A-Optimal and I-Optimal designs in non-linear models using the VNS algorithm with the help of Phyton Google Colaboratory version 3.10 to increase the purity level of silicon dioxide in alternative one based on the A-Optimal criterion formula and Equation (3) are presented in Table 2.

The best design for alternative one ($n = 9$ points) resulted in an A-Optimal criterion value of 2.7660 and an I-Optimal criterion value of 0.5446. These criterion values are the optimal values from the results of the VNS algorithm on each design. Subsequently, the design points were expanded to 12 points for alternative two to achieve improved results, as presented in Table 3.

The best design for alternative two ($n = 12$ points) resulted in an A-Optimal criterion value of 2.0723 and an I-Optimal criterion value of 0.3763. These criterion values are the optimal values from the results of the VNS algorithm on each design. The A-Optimal design and I-Optimal design points for each alternative are then visualized in a scatter plot to observe the pattern of the resulting design points. The patterns of A-Optimal and I-Optimal designs in the non-linear models exhibit distinct characteristics, as shown in Figure 2. The A-Optimal designs for alternative one and alternative two are divided into three temperature groups: minimum, middle, and maximum. In Alternative one, Group 1 consists of a minimum temperature of 800°C, Group 2 comprises a middle temperature of 850°C, and Group 3 includes a maximum temperature of 900°C. Each temperature group has varying temperature increase rates in its design area. In Alternative two, Group 1 ranges from the minimum temperature of 800°C to 820°C, Group 2 includes temperatures of 850°C and 860°C, and Group 3 consists of the maximum temperature of 900°C. Each temperature group has varying temperature increase rates vari-

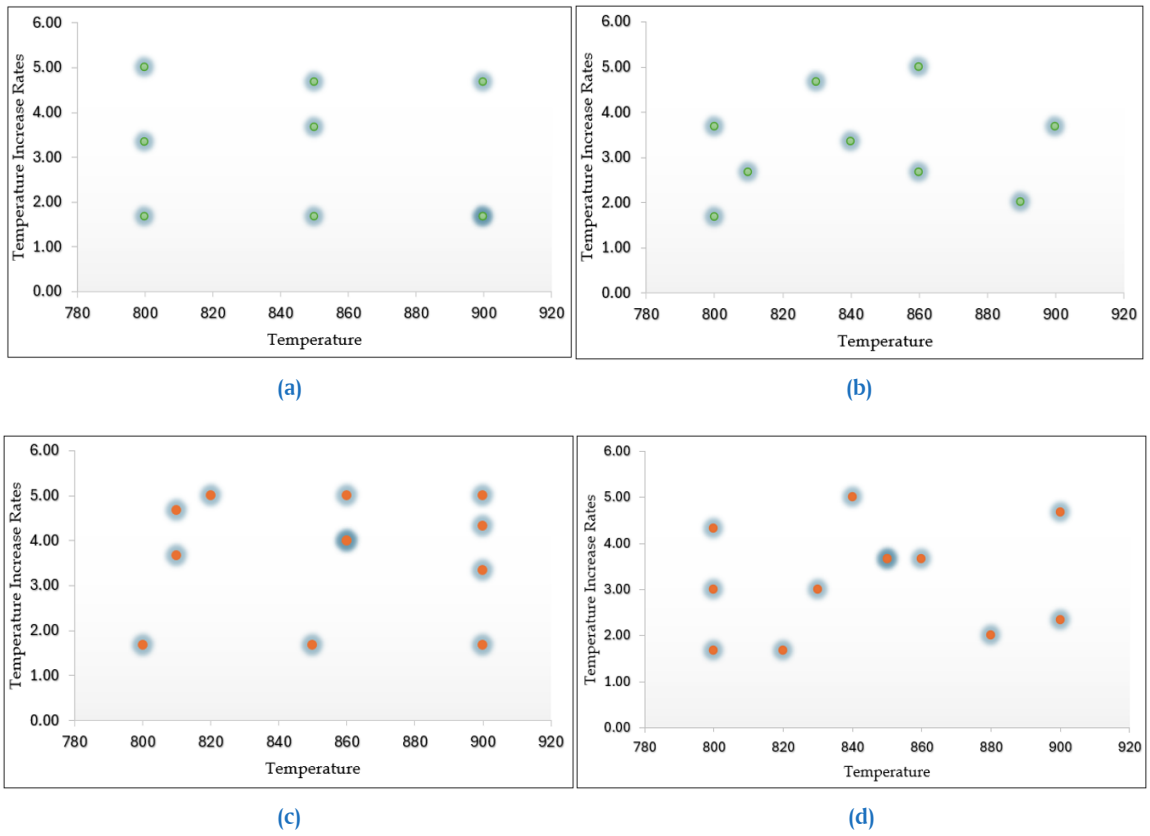


Figure 2. Design points for: (a) A-Optimal Alternative one, (b) I-Optimal Alternative one, (c) A-Optimal Alternative two, (d) I-Optimal Alternative two

ation in its design area. There is a repetition of points in alternative two, namely at a temperature of 860°C and a temperature increase rate of 4°C/minute.

The I-Optimal design in alternative one and alternative two design points form a quadratic pattern in the design area, this pattern has a relationship with the model used, namely the full quadratic model. Alternative one and alternative two obtained the same design point results, namely the lowest temperature for the resulting design is 800°C, while the highest is 900°C with the highest temperature increase rates of 5°C/minute and the lowest temperature increase rates of 1.67°C/minute. There is a repetition of points in alternative two, namely a temperature of 850°C and a temperature increase rates of 3.67°C/minute. Based on alternative one and alternative two in each design provide information that the larger the design point produced, the more repetition of points occurs in the design area.

3.3. Comparison of A-Optimal and I-Optimal Designs for SiO_2 Purity Level

The comparison of designs begins with evaluating each design using A-efficiency and I-efficiency values. The purpose is to determine whether the A-Optimal and I-Optimal designs are efficient for improving the silicon dioxide purity level at each alternative design point used in this study.

In evaluating A-efficiency, an illustration is provided by finding the A-Optimal criterion value for the I-Optimal design and then comparing it with the A-Optimal design. If the A-efficiency value is greater than 1, the A-Optimal design is considered more efficient than the I-Optimal design from terms of the A-Optimal criterion. In evaluating I-efficiency, an illustration is provided by finding the I-Optimal criterion value for the A-Optimal design and then comparing it with the I-Optimal design. If the I-efficiency value is greater than 1, the I-Optimal design is considered more efficient than the A-Optimal design in terms of the I-Optimal criterion. The results of A-efficiency and I-efficiency in alternative one and alternative two, which are calculated based on Equation (5) and Equation (6), can be seen in Table 4 and Table 5.

Table 4. Evaluation of A-Optimal and I-Optimal Designs in terms of A-Optimal Criterion

	Comparison of Designs	A-efficiency
Alternative One	A-Optimal vs I-Optimal	1.3247
Alternative Two	A-Optimal vs I-Optimal	1.1977

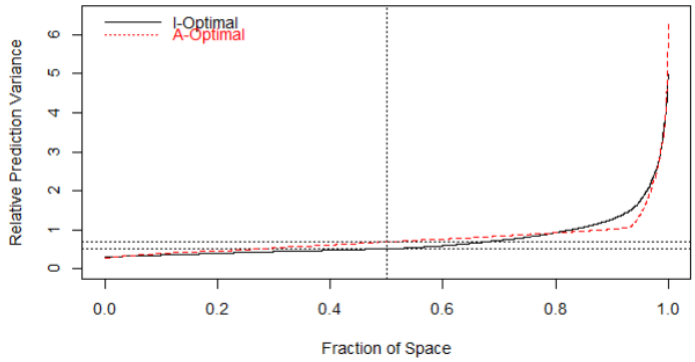
Table 5. Evaluation of A-Optimal and I-Optimal Designs in terms of I-Optimal Criterion

	Comparison of Designs	I-efficiency
Alternative One	I-Optimal vs A-Optimal	1.0143
Alternative Two	I-Optimal vs A-Optimal	1.0571

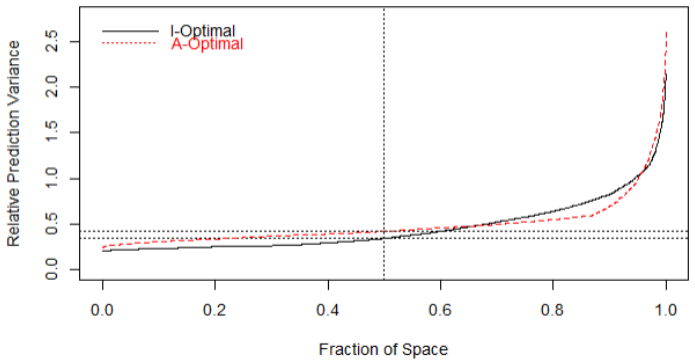
Table 5 shows that alternative one and alternative two in the A-Optimal design are more efficient than the I-Optimal design in terms of the A-Optimal criterion, as the A-efficiency values obtained are all greater than (>) 1. Table 6 shows that alternative

one and alternative 2 in the I-Optimal design are more efficient than the A-Optimal design in terms of the I-Optimal criterion, as the I-efficiency values obtained are all greater than (>) 1. From these results, both designs are efficient for improving the purity level of silicon dioxide (SiO_2).

Next, the performance of the designs generated by both methods is compared across 100% of the experimental region in the aspect of prediction variance using an FDS plot. The goal is to observe the variance prediction of the two designs, which is calculated based on Equation (7). This analysis aims to conclude which design is the best for improving silicon dioxide purity in this study.



(a) I-Optimal and A-Optimal for alternative one



(b) I-Optimal and A-Optimal for alternative two

Figure 3. Comparison of FDS plots for designs

Figure 3a shows that for Alternative 1, approximately 78% of the experimental region indicates that the prediction variance of the I-Optimal design is lower than that of the A-Optimal design. This suggests that the performance of the I-Optimal design is significantly more optimal than the A-Optimal design, except at the extreme right side of the graph. Figure 3b demonstrates that for Alternative 2, around 70% of the experimental region indicates that the prediction variance of the I-Optimal design is lower than that of the A-Optimal design. This implies that the I-Optimal design provides more optimal results than the A-Optimal design, except at the extreme right side of the graph. Overall, across 74% of the experimental region, the I-Optimal design outperforms the A-Optimal design in all alternatives in this study.

4. Conclusion

The best design points from the non-linear model using the VNS algorithm on temperature and temperature increase rates (°C/minute) for SiO_2 purity in the A-Optimal design form three temperature groups. These groups include minimum temperatures ranging from 800°C to 820°C, middle temperatures at 850°C and 860°C, and maximum temperatures at 900°C, with varying temperature increase rates within the design region on Alternatives one and two. The resulting criterion values are 2.7660 and 2.0723, respectively. The I-Optimal design patterns form a full quadratic pattern, with a minimum temperature of 800°C and temperature increase rates of 1.67°C/minute, and a maximum temperature of 900°C with temperature increase rates of 5°C/minute. The resulting criterion values on Alternatives one and two are 0.5446 and 0.3763, respectively. The I-Optimal design demonstrates superior performance compared to the A-Optimal design in in the aspect of prediction variance for enhancing silicon dioxide purity. Future research is expected to employ more neighborhood exploration in the VNS algorithm to achieve even more optimal results.

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