Data Article

Data on the enzymatic conversion of alkaline peroxide oxidative pretreated sugarcane bagasse for the production of fermentable sugars

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Abstract

Central composite design (CCD) approach of the response surface methodology design of experiment was adopted to determine the production of fermentable sugars after enzymatic conversion of alkaline peroxide oxidative pretreated sugarcane bagasse lignocellulose. MINITAB 16 statistical software was used to design the experiments, evaluate and interpret data generated during the process. The effects of factors such as time, hydrogen peroxide concentration, and temperature on treated biomass for reducing sugars (RS) production were investigated. Operating pretreatment conditions (low—high design levels) were reaction time (6–10 h), hydrogen peroxide concentrations (1–3%v/v), and reaction temperature (60–90 °C). With the desirability of optimization of 1.000, optimal reducing sugar yield after enzymatic hydrolysis was validated to be at 100.2 °C, reaction time of 4.6 h, and hydrogen peroxide concentration of 0.3% with optimum RS yield of 153.74 mg equivalent glucose/g biomass.

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1. Data

The compositional distribution of the raw biomass samples estimated by gravimetric method [1,2] (Table 1) has total polysaccharide content of 62.56% (w/w) indicating sugarcane bagasse as a potential feedstock for the production of fuels and chemicals. Table 2 shows the pretreatment operating parameters for the duplicated experimental runs and the corresponding fermentable (reducing) sugars production.

Figs. 1–3 show the interactions of pretreatment operating parameters on reducing sugars (RS) yields. The surface plots showed effective range prediction for the optimum production of fermentable sugars. Fig. 4 shows the experimental data and the predicted values having minimal deviations.

Table 3 shows the analysis of variance (ANOVA) description of generated regression model (Eqs. 1 and 2) used for the adequate prediction of reducing sugars with the operating pretreatment parameters values.

Fig. 5 shows the validated optimum pretreatment conditions (Time: 4.63 h, \(H_2O_2\): 0.32%v/v, and Temperature: 100.23 °C) and the optimum value of RS (153.75 mg/g).

| Table 1 |
| Dried raw sugarcane bagasse compositional analysis. |
| --- |
| Composition (%w/w) |
| Extractive | 3.40 |
| Hemicellulose | 25.61 |
| Lignin | 29.84 |
| Cellulose | 36.95 |
| Ash | 4.20 |
Table 2
Design matrix and compositional estimation of biomass after pretreatment and enzymatic hydrolysis.

| Run Order | Time (h) | H₂O₂ (%v/v) | Temperature (°C) | Observed RS yield (mg/g) | Predicted RS yield (mg/g) | Residual |
|-----------|----------|--------------|------------------|--------------------------|--------------------------|----------|
| 1         | 8        | 0.32         | 75               | 78.23                    | 80.64                    | −2.4     |
| 2         | 10       | 3            | 90               | 71.08                    | 72.66                    | −1.6     |
| 3         | 4.64     | 2            | 75               | 93.07                    | 99.04                    | −6.0     |
| 4         | 6        | 1            | 60               | 73.74                    | 71.65                    | 2.1      |
| 5         | 6        | 1            | 90               | 113.35                   | 108.48                   | 4.9      |
| 6         | 8        | 2            | 75               | 62.36                    | 76.26                    | −13.9    |
| 7         | 8        | 2            | 49.77            | 68.90                    | 69.40                    | −0.5     |
| 8         | 11.36    | 2            | 75               | 85.63                    | 80.37                    | 5.3      |
| 9         | 10       | 1            | 90               | 82.83                    | 85.58                    | −2.8     |
| 10        | 6        | 3            | 60               | 87.22                    | 83.96                    | 3.3      |
| 11        | 6        | 3            | 90               | 93.29                    | 93.05                    | 0.2      |
| 12        | 8        | 2            | 75               | 78.43                    | 76.26                    | 2.2      |
| 13        | 8        | 2            | 75               | 81.27                    | 76.26                    | 5.0      |
| 14        | 8        | 3.68         | 75               | 81.83                    | 80.13                    | 1.7      |
| 15        | 10       | 1            | 60               | 70.11                    | 69.84                    | 0.3      |
| 16        | 8        | 2            | 100.23           | 90.07                    | 90.28                    | −0.2     |
| 17        | 8        | 2            | 75               | 82.61                    | 76.26                    | 6.3      |
| 18        | 10       | 3            | 60               | 80.31                    | 84.67                    | −4.4     |
| 19        | 8        | 2            | 75               | 78.00                    | 76.26                    | 1.7      |
| 20        | 8        | 2            | 75               | 75.03                    | 76.26                    | −1.2     |

Fig. 1. Surface plot for reducing sugar yield against %H₂O₂ and Temperature.

Fig. 2. Surface plot for reducing sugar yield against Time and Temperature.
**Fig. 3.** Surface plot for reducing sugar yield against %H₂O₂ and Time.

**Fig. 4.** Diagnosis for the regression model fit for the experimental and predicted values.

**Table 3**

Analysis of Variance (ANOVA) for the regression model obtained from the central composite design.

| Source           | DF | Seq SS  | Adj SS  | Adj MS  | F     | P     |
|------------------|----|---------|---------|---------|-------|-------|
| Regression       | 9  | 3808.65 | 3808.65 | 423.18  | 15.56 | 0.000 |
| Linear           | 3  | 1894.18 | 582.85  | 194.28  | 7.14  | 0.001 |
| X₁               | 1  | 841.18  | 83.73   | 83.72   | 3.08  | 0.090 |
| X₂               | 1  | 0.63    | 217.13  | 217.13  | 7.98  | 0.008 |
| X₃               | 1  | 1052.36 | 170.93  | 170.93  | 6.28  | 0.018 |
| Square           | 3  | 693.74  | 693.74  | 231.25  | 8.50  | 0.000 |
| X₁²              | 1  | 595.85  | 595.85  | 231.25  | 8.50  | 0.000 |
| X₂²              | 1  | 51.73   | 51.73   | 23.86   | 0.93  | 0.344 |
| X₃²              | 1  | 46.17   | 46.17   | 46.17   | 1.70  | 0.203 |
| Interaction      | 3  | 1220.73 | 1220.73 | 406.91  | 14.96 | 0.000 |
| X₁X₂             | 1  | 6.34    | 6.34    | 6.34    | 0.23  | 0.633 |
| X₁X₃             | 1  | 444.85  | 444.85  | 444.85  | 16.35 | 0.000 |
| X₂X₃             | 1  | 769.54  | 769.54  | 769.54  | 28.29 | 0.000 |
| Residual error   | 30 | 816.10  | 816.10  | 27.20   |       |       |
| Lack-of-fit      | 5  | 280.16  | 280.16  | 56.03   | 2.61  | 0.049 |
| Pure error       | 25 | 535.94  | 535.94  | 21.43   |       |       |
| Total            | 39 | 4624.75 |         |         |       |       |
2. Experimental design, materials, and methods

2.1. Enzymatic conversion of treated biomass to fermentable sugars

Experimental data generated after enzymatic hydrolysis of treated biomass were used to develop a regression model for predicting the reducing sugar yields for different operating parameters. After each pretreatment, mass loss was estimated for required mass balances for enzymatic hydrolysis step. The cellulase enzyme complex (Trichoderma reesei) having an activity of 57.8 FPU/ml was used on 2% biomass loading and 25 FPU/g biomass enzyme dose. A cost effective method for hydrolyzing cellulose and hemicellulose to valuable products such as fermentable sugars is through the enzymatic hydrolysis process [3].

2.2. Model development, optimization, and validation of the optimum conditions

A model equation was generated from the experimental data by considering reducing sugar (Y) yield as the predicted response associated with factor combinations of time (X1), %H2O2 (X2), and temperature (X3).

\[ Y = \alpha_1 + \alpha_1 X_1 + \alpha_2 X_2 + \alpha_3 X_3 + \alpha_{1,1} X_1^2 + \alpha_{2,2} X_2^2 + \alpha_{3,3} X_3^2 + \alpha_{1,2} X_1 X_2 + \alpha_{1,3} X_1 X_3 + \alpha_{2,3} X_2 X_3 \] (1)

Substituting the values of the operating parameters into Eq. 2 gives the predicted values for the RS yields (Table 2). Fig. 4 shows the accuracy of symmetry of the residuals (absolute difference between experimental and predicted values) versus the fitted values indicating the reliability of Eq. 2 for adequate prediction.

![Fig. 5. RS yield at optimized operating pretreatment conditions.](image-url)
Data obtained using the analysis of variance (Table 3) validate the reliability of regression model by interpreting with the F-statistics and the probability values (P-values) of the linear, quadratic, and interactive effects on RS yields. The desirability of optimization was 1.000, optimal reducing sugar yield of 153.74 mg/g after pretreatment was validated to be at 100.2 °C, reaction time of 4.6 h, and hydrogen peroxide concentration of 0.3% (Fig. 5). Factors that affect the yield of reducing sugar from lignocelluloses include accessibility and adsorption characteristics of the cellulose, reactivity of the cellulose and adsorption characteristics of the lignin present [4,5].

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Transparency document

Transparency document associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2019.103867.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.103867.

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