Prediction of Kappa number and carbohydrate degradation in oxygen delignification of Abaca fiber

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Abstract. Abaca banana fiber (Musa textilis) is a source of non-wood fiber that can be used as material in the manufacture of pulp. Oxygen delignification is a process to reduce lignin content in pulp with Kappa numbers as parameters. In addition, carbohydrate degradation also occurs which is indicated by the value of viscosity. The purpose of this study is to predict the decrease in Kappa number, to predict carbohydrate degradation, and to determine the best operating condition based on prediction data obtained from the kinetic reaction model. Comparison between experimental data and prediction data was also analyzed. The prediction of Kappa number was started by developing kinetic model of oxygen delignification from experimental data, in which the rate of Kappa number reduction is dependent to temperature, hydroxy ion concentration, and oxygen pressure with specific reaction order of each species. Similar steps were done for predicting carbohydrate degradation. Prediction of Kappa number and carbohydrate degradation was done at various operating conditions, which are: oxygen pressures (2–5 bar), temperatures (70–100 °C), sodium hydroxide concentrations (NaOH) (1–5%), and heating times (0–120 min). The prediction results showed that the best operating conditions were at pressure of 2 bar, temperature of 85°C, 1% of NaOH for 56.6 min with a viscosity of 878.52 ml/g. This study also performed that the experimental data were fitted well with the prediction data.

1. Introduction

Abaca banana fiber (Musa textilis) is one of the natural fibers which has great potential as a substitute for wood because it has good mechanical and chemical properties. Abaca fiber has good tensile and flexural strength and is resistant to rot. Abaca fiber can be used as an organic raw material for textiles and paper because it contains 63% of cellulose, 21% of hemicellulose, 14% of lignin, and 2% of impurity. Abaca fiber is one of the non-wood fiber-producing plants that have long fibers [1].

The oxygen delignification process is a pre-bleaching process that is useful for reducing the lignin content of brown pulp. In addition, the function of oxygen delignification is to save expensive chemicals in the bleaching stage and at the same time reduce the impact on the environment. The oxygen delignification process takes place in a medium consistency of pulp with high temperature and pressure, while the chemicals used are oxygen and alkali. One of the alkalis used is NaOH or oxidized white liquor. Delignification takes place in the flow at the top of the reactor, where the retention time
for delignification is 50-60 minutes, this is in accordance with the most common process conditions applied in industry [2].

Lignin reduction occurs during oxygen delignification. The oxygen delignification kinetics are influenced by the reaction temperature, oxygen pressure, and the concentration of alkali as well as the mixing of oxygen and alkalis with fiber. Most of the kinetic models are empirical and ignore the effect of mass transfer in the mathematical representation data. The degree of delignification is usually measured by determining the amount of Kappa pulp (Kappa number) which is an indirect measure of lignin content of the pulp.

In industrial practice, delignification is usually stopped when the kappa number in oxygen delignified pulp is reduced by about 50%. This is due to the carbohydrate degradation reaction which also occurs during oxygen delignification, which causes the decrease in pulp strength (viscosity). The carbohydrate degradation reaction is described in terms of the reduction of intrinsic viscosity, "Δη", of the pulp. The reactions of cellulose and hemicellulose polymers have been studied by many researchers [3,4]. A decrease in the cellulose chain length leads to the decrease in the viscosity of the pulp, which results in the loss of pulp strength [3]. In this work, we studied how to determine the best operating conditions for the oxygen delignification process by predicting the kappa number and carbohydrate degradation in oxygen delignification of Abaca fiber at various operating conditions. Therefore, it is expected that conducting experiment will be more efficient and effective because we already know the best operating conditions for the oxygen delignification process.

2. Materials and Methods

2.1. Materials

The Abaca banana fiber (Musa textilis) was supplied from Aceh, Indonesia. The fiber was screened (SCAN-CM 40:94), dried and stored at 25% water content. The concentration standard of NaOH and Na₂S for pulping was set to 97.0 g/L and 32.4 g/L, respectively. The Abaca fiber was cooked in Kraft pulping process prior to oxygen delignification.

2.2. Methods

The research was conducted by predicting the kappa number and viscosity value obtained from kinetic model of oxygen delignification process. The kinetic reaction models of oxygen delignification consist of kinetic models of kappa number reduction and viscosity change as described in equation (1) and equation (2), respectively [6].

\[ \frac{dK}{dt} = k[OH^-]^m[O_2]^nK^q \] (1)

\[ \frac{d\eta}{dt} = k[OH^-]^x[O_2]^\beta\eta^\lambda \] (2)

where: K is Kappa number and η is intrinsic viscosity.

The reaction rate constant (k) is dependent on temperature and shown by Arrhenius equation, as described in equation (3) and (4) for kinetic models of kappa number reduction and viscosity change, respectively [6].

\[ k = Aexp \left( -\frac{E_A}{RT} \right) \] (3)

\[ k = A_mexp \left( -\frac{E_m}{RT} \right) \] (4)

where: E_A and E_m are activation energy, A and A_m are frequency factor.

The value of constants of m, n, q, A, E_A from kinetic models of kappa number reduction and constants of x, β, λ, A_m, E_m from kinetic models of viscosity reduction were determined empirically by using experiment data from Darmawan et.al [5]. The operating condition of oxygen delignification was varied experimentally as shown in table 1.
The prediction data were obtained at various operating condition of oxygen delignification, as following: heating time spans of 0-120 minutes with an interval of 20 minutes, pressures from 2 to 5 bars with an interval of 1 bar at constant temperature of 85°C and NaOH concentration of 2%, temperatures of 70-100°C with interval of 5°C at constant pressure of 2 bar and NaOH concentration of 2%, and NaOH concentrations from 1 to 5% with interval of 1% at a constant temperature of 85°C and pressure of 2 bar.

Table 1. Experiment variable in oxygen delignification process done by Darmawan et. al [5].

| Constant Variable | Changing Variable |
|-------------------|-------------------|
| Material: *Musa textilis* fiber | Pressures: 2 bar, 3 bar, dan 4 bar |
| Pulp Process: Kraft pulping | Temperatures: 75°C, 85°C, 95°C dan 100°C |
|                   | NaOH Concentrations: 1%, 2%, dan 4% |
|                   | Heating times: 20, 40, and 60 min |

2.3. Analysis

The analysis was done by evaluating the prediction data of Kappa number and viscosity reduction at various condition of oxygen delignification. Then, the prediction data were compared with the experimental results. From the Kappa number analysis, the reduction level of Kappa number at each variable was observed. This indicates the level of delignification of the fibers, especially lignin part in the fibers. From the viscosity analysis, the level of carbohydrate degradation, which is proportional to the viscosity reduction, at each variation of operating condition was also examined. The decrease in viscosity value indicates the level of fiber or carbohydrate degradation and describes the yield of pulp obtained in the delignification process. The best operating condition of oxygen delignification based on prediction data was chosen from the value of Kappa number and viscosity which comply to the standard quality value of pulp.

3. Result and Discussion

From experimental data, the prediction of carbohydrate degradation and lignin reduction was carried out on the oxygen delignification of kraft pulp. The parameters for analyzing the pulp quality resulted from oxygen delignification process were kappa number and viscosity. The Kappa number shows the level of delignification. The lower of Kappa number, the higher amount of lignin dissolved after the oxygen delignification process. The higher amount of lignin lost, the higher value of the degree of delignification in the oxygen delignification process. The viscosity value indicates the cellulose degradation value or the degree of polymerization. The lower of viscosity value, the higher level of cellulose degradation. Table 2, table 3, and table 4 show the prediction data of Kappa number and viscosity of Abaca fiber kraft pulp at various operating condition of oxygen delignification.

Table 2. Prediction results of Kappa number and viscosity at various pressures.

| Oxygen Pressure [bar] | Heating Time [minutes] | 20 | 40 | 60 | 80 | 100 | 120 |
|-----------------------|------------------------|----|----|----|----|-----|-----|
| 2                     | Kappa Number           | 7.89 | 6.11 | 5.11 | 4.46 | 3.99 | 3.63 |
|                       | Viscosity [ml/g]       | 916.70 | 885.71 | 861.52 | 841.77 | 825.15 | 810.83 |
| 3                     | Kappa Number           | 6.33 | 4.65 | 3.8 | 3.26 | 2.89 | 2.62 |
|                       | Viscosity [ml/g]       | 898.49 | 859.19 | 830.46 | 807.97 | 789.59 | 774.1 |
| 4                     | Kappa Number           | 5.26 | 3.75 | 3.02 | 2.58 | 2.28 | 2.06 |
|                       | Viscosity [ml/g]       | 882.37 | 837.35 | 805.93 | 782 | 762.8 | 746.81 |
| 5                     | Kappa Number           | 4.49 | 3.14 | 2.52 | 2.14 | 1.89 | 1.7 |
|                       | Viscosity [ml/g]       | 868.02 | 818.91 | 785.82 | 761.09 | 741.48 | 725.29 |
Table 3. Prediction results of Kappa number and viscosity at various NaOH concentrations.

| Alkali Charge [%] | Heating Time [minutes] | 20 | 40 | 60 | 80 | 100 | 120 |
|-------------------|-------------------------|----|----|----|----|-----|-----|
| 1                 | Kappa Number            | 8.84 | 7.12 | 6.08 | 5.37 | 4.84 | 4.43 |
|                   | Viscosity [ml/g]        | 923.92 | 896.89 | 875.11 | 856.96 | 841.44 | 827.92 |
| 2                 | Kappa Number            | 6.88 | 5.14 | 4.23 | 3.65 | 3.25 | 2.94 |
|                   | Viscosity [ml/g]        | 908.31 | 873.22 | 846.7 | 825.5 | 807.92 | 792.95 |
| 3                 | Kappa Number            | 7.3 | 5.53 | 4.58 | 3.97 | 3.54 | 3.21 |
|                   | Viscosity [ml/g]        | 911.94 | 878.57 | 852.99 | 823.37 | 815.17 | 800.46 |
| 4                 | Kappa Number            | 7.89 | 6.11 | 5.11 | 4.46 | 3.99 | 3.63 |
|                   | Viscosity [ml/g]        | 916.7 | 885.71 | 861.52 | 841.77 | 825.15 | 810.83 |
| 5                 | Kappa Number            | 6.55 | 4.84 | 3.97 | 3.42 | 3.03 | 2.74 |
|                   | Viscosity [ml/g]        | 905.35 | 868.93 | 841.68 | 820.05 | 802.2 | 787.05 |

Table 4. Prediction results of Kappa number and viscosity at various temperatures.

| Temperature [°C] | Heating Time [minutes] | 20 | 40 | 60 | 80 | 100 | 120 |
|------------------|-------------------------|----|----|----|----|-----|-----|
| 70               | Kappa Number            | 7.89 | 6.11 | 5.11 | 4.46 | 3.99 | 3.63 |
|                  | Viscosity [ml/g]        | 916.70 | 885.71 | 861.52 | 841.77 | 825.15 | 810.83 |
| 75               | Kappa Number            | 8.29 | 6.52 | 5.5 | 4.82 | 4.32 | 3.94 |
|                  | Viscosity [ml/g]        | 925.3 | 899.1 | 877.84 | 860.06 | 844.78 | 831.44 |
| 80               | Kappa Number            | 8.1 | 6.33 | 5.31 | 4.64 | 4.16 | 3.79 |
|                  | Viscosity [ml/g]        | 921.28 | 892.75 | 870.04 | 851.26 | 835.3 | 821.46 |
| 85               | Kappa Number            | 7.88 | 6.11 | 5.11 | 4.45 | 3.98 | 3.62 |
|                  | Viscosity [ml/g]        | 916.7 | 885.7 | 861.5 | 841.76 | 825.14 | 810.83 |
| 90               | Kappa Number            | 7.65 | 5.87 | 4.89 | 4.26 | 3.79 | 3.45 |
|                  | Viscosity [ml/g]        | 914.6 | 882.6 | 852.26 | 831.57 | 814.33 | 799.58 |
| 95               | Kappa Number            | 7.39 | 5.62 | 4.66 | 4.04 | 3.605 | 3.27 |
|                  | Viscosity [ml/g]        | 905.7 | 869.44 | 842.28 | 820.7 | 802.88 | 787.75 |
| 100              | Kappa Number            | 7.09 | 5.34 | 4.41 | 3.81 | 3.39 | 3.08 |
|                  | Viscosity [ml/g]        | 899.9 | 859.86 | 831.23 | 808.79 | 790.44 | 774.97 |

3.1. Oxygen Delignification Kinetic Analysis

In order to obtain the kinetic equation of oxygen delignification reaction, it is necessary to correlate several parameters, such as: q, m, n, $E_A$, and $A_e$ as shown in equation (1) and (3). The experimental data collected were correlated using the kinetic model given by equation (1).

Kinetic of oxygen delignification is dependent to temperature, hydroxy ion concentration, and oxygen pressure with specific reaction order of each species. Assuming a constant alkaline concentration and oxygen solubility during oxygen delignification reaction, the kinetic model can be written as general kinetic model, as shown in the equation (5) below [6]:

$$\frac{-dK}{dt} = k_q K^q$$  \hspace{1cm} (5)

The constants m, n and q are determined empirically from experimental data [7]. In kinetic studies, the reaction rate constant ($k_q$) was correlated to the initial alkali concentration [OH⁻, g/L], temperature
(T, K), activation energy (E\_A, kJ/mole) and oxygen solubility (O\_2, g/L), as described in equation (6) [2].

\[ k_q = A_q \exp \left( -\frac{E_A}{R_T} \right) (OH^-)^m (O_2)^n \]  

(6)

Integration of equation (5) under conditions of constant oxygen partial pressure and initial alkali concentration gives the equation for the Kappa number as a function of time [2].

\[ \frac{1}{\ln K} - \frac{1}{\ln K_0} = kt \]  

(7)

With q is unequal to 1, the parameter q, which indicates the reaction rate order with correlation to the Kappa number cannot be found explicitly from equation (7), so a trial and error solution was conducted following the integral analysis method. Reaction rate order (q) was obtained by choosing the highest value of regression from trial and error. The other parameters were determined by linear regression of the experimental data. The value of q was found to be 2.675. Therefore, the Kappa number reduction reaction rate equation for Abaca fiber (Musa textilis) is displayed below:

\[ -\frac{dK}{dt} = 33.11 \exp \left[ -\frac{24.76}{R_T} \right] [OH^-]^{0.568} [O_2]^{1.494} K^{-2.675} \]  

(8)

Table 5 shows the comparison of kinetic parameters of Kappa number reduction obtained in this study and from literatures. As seen in Table 5, it can be concluded that for the oxygen delignification process, the reaction orders obtained in this study are not significantly different from that obtained from literatures, even tough, others are significantly different. The significant difference occurs because of the difference in the experimental variables used in the oxygen delignification. The initial Kappa number and the change in the Kappa number value with time are also different in each study, so that the value of activation energy, m, n, A, and q obtained for each material are also different.

**Table 5.** Comparison of kinetic parameters of Kappa number reduction.

| Reference                        | [OH\^-] exponent (m) | [O\_2] exponent (n) | Kappa Number exponent (q) | Activation Energy (kJ/mol) | Frequency Factor (A) |
|----------------------------------|----------------------|---------------------|---------------------------|----------------------------|----------------------|
| Pine [8]                         | 0.47                 | 0.47                | 3.5                       | 47                         | 2.5                  |
| Pine [9]                         | 0.7                  | 0.7                 | 2.0                       | 51                         | 3 x 10^6             |
| This study (Abaca banana fiber)  | 0.568                | 1.494               | 2.675                     | 24.979                     | 33.11                |

Figure 1, figure 2, and figure 3 show the decrease in predicted and experimental Kappa number with heating time of Abaca fiber at various concentrations of NaOH, oxygen pressures, and temperatures, respectively. The longer time of oxygen delignification is carried out, the Kappa number decreases at condition of different NaOH concentrations, oxygen pressures and temperatures. In addition, the predicted Kappa numbers are close to the value of experimental Kappa numbers (dotted).

Figure 1, figure 2, and figure 3 also show that the Kappa number reduction increases with the increase of NaOH concentration, as well as oxygen pressure and temperature. The lowest Kappa number was reached at the highest temperature, oxygen pressure, alkali concentration, and at the longest of oxygen delignification reaction. The reduction of Kappa number of the pulp after oxygen delignification is indeed expected. However, it does not mean that the lowest Kappa number is the best condition. The decrease of Kappa number is associated with the decrease of viscosity, which shows the carbohydrate degradation. Carbohydrate degradation influences the physical properties of the pulp. Therefore, to choose the best condition, the value of Kappa number in associated with viscosity need to be considered based on the standard value of Kappa number and viscosity for good quality of the pulp, as discussed in the next section.
Figure 1. The decrease in predicted and experimental Kappa number with heating time of *Musa textilis* at various concentrations of NaOH and constant temperature of 85°C and oxygen pressure of 2 bar.

Figure 2. The decrease in predicted and experimental Kappa number with heating time of *Musa textilis* at various oxygen pressures and constant temperature of 85°C and NaOH concentration of 2%.

Figure 3. The decrease in predicted and experimental Kappa number with heating time of *Musa textilis* at various temperatures and constant oxygen pressure of 2 bar and NaOH concentration of 2%.
3.2. Carbohydrate Degradation Kinetic Analysis

In order to determine the kinetic equation for viscosity reduction, which represents the carbohydrate degradation, after oxygen delignification, it is necessary to calculate several parameters, such as: $\lambda$, $\beta$, $E_m$, and $A_m$, as described in equation (2) and (4). The general rate equation of carbohydrate degradation in terms of viscosity is shown in equation (9) below: [7]

$$\frac{-d\eta}{dt} = k_2\eta^\lambda$$

(9)

and

$$k_2 = A_2\exp\left(-\frac{E_A}{RT}\right) (OH^-)^x(O_2)^\beta$$

(10)

where, $\eta$ is intrinsic viscosity (ml/g), [OH$^-$] is NaOH concentration (g/L), [O$_2$] is oxygen solubility (g/L), and $t$ is time (min). Integration of equation (9) under conditions of constant oxygen concentration and alkali concentration give the equation for the $\eta$ as a function of time [7].

$$\left(\frac{1}{\eta - 1}\right) - \left(\frac{1}{\eta_0 - 1}\right) = kt = y$$

(11)

With $\lambda$ is unequal to 1, the parameter $\lambda$, which indicates the rate order with correlation to the viscosity cannot be found explicitly from equation (11), so a trial and error solution was conducted following the integral analysis method. Reaction rate order ($\lambda$) was obtained by choosing the highest value of regression from trial and error. The other parameters were determined by linear regression of the experimental data. The value of $\lambda$ was found to be 8. The carbohydrate degradation reaction rate equation for *Musa textilis* is shown below:

$$\frac{-d\eta}{dt} = 2.5 \times 10^{-18}\exp\left(-\frac{33.25}{RT}\right)[OH^-]^{0.315}[O_2]^{1.087}\eta^8$$

(12)

| Reference       | [OH$^-$] exponent ($x$) | [O$_2$] exponent ($\beta$) | Viscosity exponent ($\lambda$) | Activation Energy [kJ/mol] | Frequency Factor ($A_m$) |
|-----------------|------------------------|-----------------------------|-------------------------------|---------------------------|------------------------|
| Eucalyptus [7]  | 0.43                   | 0.35                        | 11                            | 30.23                     | 8.75x10$^{-8}$         |
| This study (Abaca fiber) | 0.315                   | 1.087                       | 8                             | 33.25                     | 2.5x10$^{-18}$         |

Table 6 shows the comparison of kinetic parameters of carbohydrate degradation obtained in this study and literatures. It shows that various values of kinetic parameters are obtained for different raw materials. The difference occurs because of the difference in the experimental variables used in the oxygen delignification reaction. The initial viscosity and its change with time are also different in each study, so that the value of activation energy, $x$, $\beta$, $A_m$, and $\lambda$ obtained for each material are also different.

Figure 4, figure 5, and figure 6 show the decrease in predicted and experimental viscosity with heating time of Abaca fiber at various NaOH concentrations, oxygen pressures, and temperatures, respectively. The longer time of oxygen delignification is carried out, the viscosity decreases at condition of different NaOH concentrations, oxygen pressures and temperatures. In addition, the predicted viscosity data are almost the same as the viscosity obtained experimentally (dotted). The decrease in viscosity represent the cellulose degradation or carbohydrate degradation. Therefore, it can be stated that the carbohydrate degradation increases with the increasing of NaOH concentration, as well as oxygen pressure and temperature.
Figure 4. The decrease in predicted and experimental viscosity with heating time of *Musa textilis* at various concentrations of NaOH and constant temperature of 85°C and oxygen pressure of 2 bar.

Figure 5. The decrease in predicted and experimental viscosity with heating time of *Musa textilis* at various oxygen pressures and constant temperature of 85°C and NaOH concentration of 2%.

Figure 6. The decrease in predicted and experimental viscosity with heating time of *Musa textilis* at various temperatures and constant oxygen pressure of 2 bar and NaOH concentration of 2%.
3.3. Degree of Polymerization
The degree of polymerization on the fiber is related to the viscosity of the pulp [10]. The long reaction time will produce pulp with low viscosity. The bond between fibers, especially cellulose, is degraded by the liquor leading to low fiber strength and increased pulp solubility. Delignification and degradation processes occur during the oxygen delignification process. The degree of polymerization depends on the type of material used, the processing technology, and the method of cellulose insulation. Oxygen delignification prediction is carried out, so that the best operating conditions for a certain material are known and then the oxygen delignified kraft pulp specifications are maintained. The relationship between the degree of polymerization of cellulose and viscosity is stated in equation 13 [11].

\[
dp = 0.75 \eta^{1/0.905}
\]  

(13)

Table 7. The time to achieve a 50% reduction of lignin content at various concentrations of NaOH.

| Alkali Charge [%] | 1   | 2   | 3   | 4   | 5   |
|------------------|-----|-----|-----|-----|-----|
| Heating time [min] | 56.6 | 38.2 | 30.3 | 25.7 | 22.7 |
| Viscosity [ml/g]     | 878.52 | 888.18 | 893.52 | 897.14 | 899.68 |

Table 8. The time to achieve a 50% reduction of lignin content at various oxygen pressures.

| Oxygen [bar] | 2   | 3   | 4   | 5   |
|-------------|-----|-----|-----|-----|
| Heating time [min] | 38.2 | 20.8 | 13.5 | 9.7 |
| Viscosity [ml/g]     | 888.18 | 896.6 | 902.18 | 906.03 |

Table 9. The time to achieve a 50% reduction of lignin content at various temperatures.

| Temperature [°C] | 70   | 75   | 80   | 85   | 90   | 95   | 100  |
|------------------|------|------|------|------|------|------|------|
| Heating time [min] | 48   | 44.9 | 41.6 | 38.2 | 34.8 | 31.4 | 28   |
| Viscosity [ml/g]     | 896.41 | 893.5 | 890.76 | 888.18 | 885.76 | 883.6 | 881.63 |

Table 7, table 8, and table 9 show the time to achieve a 50% reduction of lignin content at various NaOH concentrations, oxygen pressures, and temperatures, respectively. Table 7 shows the time to achieve a 50% reduction of lignin content at various NaOH concentrations and constant oxygen pressure of 2 bar and temperature of 85°C. Table 8 shows the time to achieve a 50% reduction of lignin content at various oxygen pressures and constant NaOH concentration of 2% and temperature of 85°C. Table 9 shows the time to achieve a 50% reduction of lignin content at various temperatures and constant NaOH concentration of 2% and oxygen pressure of 2 bar. The oxygen delignification process should be stopped when the decrease in lignin content has reached 50%. If the decrease in lignin is more than 50%, it will result on the degradation of carbohydrates [2]. The time needed (retention time) for delignification is around 50-60 minutes because the pulp consistency used is medium consistency [2]. The minimum viscosity value for pulp according to the standard of degree of polymerization is 846 ml/g [12,13]. From the table above, it can be concluded that the best process conditions for Musa textilis are at a pressure of 2 bar, temperature of 85°C and 1% of NaOH for 56.6 minutes with a viscosity of 878.52 ml/g.

4. Conclusion
The prediction of Kappa number reduction and carbohydrate degradation in oxygen delignification of Abaca banana fiber was accomplished to obtain best operating condition for the efficient and effective
process. The decrease in Kappa number indicates the lignin content reduction. The carbohydrate degradation is revealed by the decrease in viscosity value. The prediction was completed by obtaining reaction kinetic model derived from experimental data. The decrease in lignin content can be predicted by knowing the values of kinetics parameters, which are q, m, n, E_A, and A for predicting kappa number. The degradation of carbohydrates can be predicted by knowing the values of λ, x, β, E_m, and A_m for predicting viscosity value. Based on the prediction results, the best process conditions for oxygen delignification of Abaca fiber (*Musa textilis*) are at a pressure of 2 bar, temperature of 85°C and 1% of NaOH for 56.6 minutes with a viscosity of 878.52 ml/g. This prediction result can be used as consideration for conducting oxygen delignification experimentally, especially for selecting the process condition.

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