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SIMULATION OF DELIGNIFICATION PROCESS IN DIGESTER WITH TWO INLETS WHITE LIQUOR USING CFD ANSYS 19.2FOR PREDICTING LIGNIN RESIDUE

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ABSTRACT

Based on the pulp refinery data on October 2020, the total average of lignin content in the digester was about 20.5%. This high amount of lignin during the pulping process was due to the non-uniformity mixing between white liquor and lignin. Therefore, the objective of this research was to simulate delignification process in digester with two inlets white liquor using CFD Ansys 19.2. The various NaOH concentrations (16%-22%) and operating temperatures (151°C-160°C) were also investigated. The simulation results using CFD Ansys Fluent 19.2 showed the optimum condition of the remaining lignin of 16.7% obtained at NaOH 14 g/l and the temperature of 151°C, which was lower than the actual data (20.7%)Data obtained from the simulation results can be used to analyze several aspects such as mass fraction of each compound, temperature distributions, velocity profile, and vector. CFD simulations can be used by researchers as a guide for experiment.

Keywords:Ansys Fluent 19.2, Delignification, Digester, Lignin

I. INTRODUCTION

Based on data of the Indonesian Pulp and Paper Association in 2015, the capacity of the pulp industry in Indonesia is 7.9 million tons per year and the paper industry is 13.9 million tons per year. According to this association, the pulp productionwill still grow of about 5% in future, due to the increasing global and domestic demand. One of these pulp companies has produced 4,596.5 tons of pulp (ADT) per day using a digester with a G2 compact cooking system where the kraft process continuously and impregnation was carried out at low temperature.The conversion of wood chips into pulp mainly took place in a long, upright, tubular vessel known as the pulp digester (Rahman et al., 2020). The type of wood used as a raw material is acacia crassicarpa and mangium. Based on the refinery data, a lignin level during pulp cooking process exceeds the standard range of 16% - 22%. The effect of NaOH and temperature treatments on lignin content of varied wood or other plant materials have been studied by several researchers. Previous researchers found that NaOH had a significant effect on lignin removal with delignification ranging from 42.3% to 84.6% depending on the severity of pretreatment (Jung et al., 2018). Other authors added 5% NaOH to grass sillage at 100 °C. Their results showed that the removal of lignin was about 21.2% (Xie et al., 2011). The lignin degradation of sunflower straw was achieved at 20% NaOH and 80 °C for 24 hours according to (Antonopoulou et al., 2015). Previous study report that more severe NaOH pretreatments resulted lower lignin in the insoluble residues lignin in sugar cane bagasse (Martínez et al., 2016). Meanwhile other work, added 8% of NaOH and 1% of H_2O_2 to rice husk at temperature of 20 °C which had removed 71.78% of lignin (Bazargan et al., 2020). Treated Acacia mangium with 5.50% w/v (NaOH concentration) at 70 °C for 3 hours (reaction time) and removed 12.66% lignin content . However, it needs higher temperature in a digester proccess compares to a small scale treatment or research. Previous study in digester where liquor inlet position only one at the top of digester (actual), result showed 20.5% lignin residue at temperature of 151°C, which was still high. This was due to the contours of the Na-Lignate mass fraction formed too quickly on the above side of the digester and high concentration on this side and did not mix thoroughly inside digester and not uniform (Sudrajat et al., 2020).

This research was done in order to decrease the amount of lignine residue by simulating a digester with two white liquor inlets at above on right and left design using CFD Simulation (Ansys Fluent 19.2). A CFD model for the physical structure of a pulp digester and prediction of the continuous chemical reactions inside the digester had been reported by (Pourian & Dahlquist, 2011), (Rahman et al., 2018) and (Sudrajat et al., 2020) which one inlet white liquor.The aims of study were to simulate delignification process in digester with two inlets white liquor using CFD Ansys 19.2, and the various NaOH concentrations (14%-22%) and operating temperatures (151°C-154°C) were also predicted.

II. CFD MODELLING OF DELIGNIFICATION PROCESS IN DIGESTER

1.1 Modelling Algorithm

Algoritm of CFD modelling of delignification process in digester using Ansys Fluent 19.2 software is served in Figure 1.

1.2 Numerical Procedure

The first step of CFD Modeling using Ansys Fluent 19.2 is the constructing of geometry using Ansys DesignModeler, then create the reactor according to the actual design. The scematic of three dimensional digester was described in figure 2. Furthermore, the geometry was devided to several volume elements as referred as meshing stage. Then, the boundary conditions were determined. It can be seen in figure 3. After that, the setup menu was chosento insert the governing equations such as: mass transfer, momentum displacement, heat transfer, and turbulence (viscosity). The physical and chemical characteristics of raw materials and products and reaction mechanisms were determined. In addition, it is also investigated the boundary condition of the inlet (raw materials, white liquor), and its outlets.Operating conditions of digester in Table 1.

The various operating temperatures used in this study were 151°C, 152°C, 153°C, and 154°C. NaOH concentrations of 14 gl^{-1}, 16 gl^{-1}, 18 gl^{-1}, 20 gl^{-1}, and 22 gl^{-1} were applied. The mass flow rate of raw material supplied into the digester was about 4,596.5 $tonsday^{-1}$. The process of pulp delignification in the digester, was simulated using the CFD application Ansys Fluent 19.2 to take into account the lignin level. Simulation using Ansys Fluent 19.2 is also using the equation of conservation of mass balance or continuity equation, it can be seen in equation (1)(2). To know energy transfer due to temperature difference or determine velocity of transfer energy at certain condition, this delignification process using the equation of heat transfer balance that showed up in equation (3)(4). And for kinetic turbulance energy and viscosity of dissipation included the heat of chemical reaction, it also can be figured in equation (4)(5)(6).

III. RESULTS AND DISCUSSION

This CFD model with two inlets liquor has succeeded in following lignin mass fraction, NaOH, Na-Lignate and temperature based on contour colors which are in accordance to the paper by(Ahsan & Hussain, 2017).

1.3 Contour of Lignin Mass Fraction in Digester

Lignin mass fraction resulting from simulation with various concentrations of NaOH of (14, 16, 18, 20, 22) gl^{-1} and temperatures of 151°C, 152°C, 153°C, and 154°C can be seen in Figure 4. Only the distinguished contour mass fractions were showed in all Figures. The red color indicates the highest mass fraction of lignin, while the blue color is the lowest mass fraction. The red color dominates at the upper center of the inlet lignin or feed digester, while the blue color dominates on the right and left sides of the NaOH inlet digester. This is in accordance with the actual conditions of the limits that have been set. According to this contour of lignin (green), a low lignin concentration is showed by treatment of 14 gl^{-1} NaOH and 151°C temperature.

From Figure 4, it can be seen that the presence of two inlets made the mass fraction of Na-Lignate formed more uniform and thoroughly inside the digester. Otherwise, from the previous studied by (Rahman et al., 2019)and (Sudrajat et al., 2020)with only one inlet showed that the contour of Na-Lignate were only formed on the topside of the digester which still have higher residual lignin than with two inlets. Lignin here acted as reactant, and it is seen that the mass fraction of lignin reduced throughout the digester because it was converted into a Na-Lignate product and water, as shown in the equation of the degradations reaction between lignin and NaOH using the following equation:

$$(C_{10}H_{12}O_4)_n \; + \; NaOH \quad \rightarrow \quad n\, C_{10}H_{11}\, NO_4 - Na \; + \; H_2O$$

Thus 2 inlet model can decrease lignin residue which is in permitted lignin levels between 16% - 22%with consideration not less than 15%. The remaining levels of lignin can be seen varied from the contours above, this is similar to the results by (Fan, 2005), (Fearon et al., 2020) and (Sudrajat et al., 2020).

1.4 Contour of NaOH Mass Fraction in Digester

From Figure 5 it can be seen that the presence of two inlet made the reaction between mass fraction of Lignin and NaOH more uniform thoroughly inside the digester. Otherwise, from the previous studied by (Sudrajat et al., 2020) with only one inlet showed that the reaction only started from the middle through the bottom of the digester. NaOH here acts as a reactan, and it appears that the mass fraction of the NaOH decreased throughout the digester. The red color in the contour image above shows the highest Mass Fraction of NaOH, while dark blue indicates the lowest fraction.

The red color dominates the NaOH inlet side on the right and left side of the digester, while the dark blue color lignin enters from the upper center of the digester. The further down the digester the more visible the gradation of red and dark blue turn into light blue. This indicates that the reducing mass fraction of the NaOH as it reacted with lignin to become Na-Lignate and H_2O.

1.5 Contour of Natrium Lignate Mass Fraction in Digester

Contour of the mass fraction of Na-Lignate increased along the digester due to the process of pulp delignification. In figure 6 it can be seen that the difference in contour of the Mass Fraction of Na-Lignate. Orange indicates the highest mass fraction of Na-Lignate and light blue indicates the lowest mass fraction of Na-Lignate. At the beginning of inlet entry, the contours are blue and green are lignin and NaOH as reactan. This means that the Na-Lignate product has not yet formed, then there is a red color in the middle to the bottom of the digester which is the most reactive zone where in the delignification process begins to form Na-Lignate. The more Na-Lignate products that are formed, the more lignin is converted so the less lignin there is left.

1.6 Contour of Velocity Profile in Digester

Data obtained from the simulation results can be used to analyze several aspects such as mass fraction of each compound, temperature distributions, velocity profile, and vector. CFD simulations can be used by researchers as a guide for experiment. In addition, CFD also being able to save on the use of certain chemicals and heat energy. As well as the results of heat distribution that occurred inside the reactor can also be seen with this simulation of CFD Ansys Fluent 19.2.

Figure 7 described the gradation of velocity contour along the digester were attained after 50 iterations. It can be seen that the cyan color displays the highest velocity and blue color displays the lowest velocity. The highest velocity gradient occurs in the middle of the digester, due to friction between the reactan and the product with the digester wall.

A velocity contour indicated the turbulence condition. It can be described that there is irregularity in the fluid trajectory and indicated by the formation of vortexes in the flow (Welty et al., 2000). From the figure it appears that the uneven velocity distribution along the column illustrated the possibility that what happened in turbulent flow. It can be seen from figure 8 that there is a turbulent flow in the digester at the time of delignification process.

1.7 Effect of NaOH Concentrations on Lignin Levels at Varied Temperatures

As shown in Figure 9 and Table 2, lignin levels after CFD simulation of digester data were validated with actual data (after considering the actual and simulated white liquor inlets position). From the simulated data, it showed that the levels of lignin formed decreased with the higher concentrations of NaOH and temperatures. This results were similar with researches done by (Martínez et al., 2016), (Jung et al., 2018) and(Bazargan et al., 2020) where more NaOH addition produced less lignin residue.

This was because the kinetics of the reaction was getting faster, more uniform and mixed thorougly by using the 2 inlets position than one inlet. While in one inlet digester, Na-lignate was formed mostly on above side of digester caused by instant and quick reaction in above part of digester(Sudrajat et al., 2020).

The simulation result of CFD Ansys Fluent 19.2, shows lignin levels after pulp delignification process (after adding the amount of white liquor (NaOH) at temperature of 151to 154^{o}C (Figure 9). It showed that the remaining lignin produced wererather similar, but lower than the actual results. As discussed above, the lowest lignin level of the simulations results was obtain of about 17.1% at 14 gl^{-1} of NaOH concentration which was lower than the actual data (20.7%). This simulation results was better comparedto previous work (Sudrajat et al., 2020), which produced the remaining lignin by 20.5%. This result is also better than the other simulations (Fan, 2005) with lignin levels about 23.93%. Actually, lignin residue can be used for other source of energy such as bioplastics, coatings, fuels and chemicals (Demuner et al., 2019).

In general, it might be concluded that the simulation digester with 2 liquor inlet position at the top of digester is very effective in determining the remaining lignin at range temperatures of 151^{o}C to 154^{o}C.

1.8 Mass Fraction of Reactan (NaOH and lignin) and Products (Na-Lignat) Along Digester Height

Figure 10. showed the profile of reactan and products along digester height.It has been described that mass fraction of reactan reduced along the digester height. On the other hand, product mass fraction increased with the height of digester. This is due to conversion of lignin and NaOH to become Na-Lignate. The highest Na-Lignate achieved at 27 m of digester height.

IV. CONCLUSION

This CFD model with two inlets liquor has succeeded in following lignin mass fraction, NaOH, Na-Lignate and temperature based on contour colors. The simulation results using CFD Ansys Fluent 19.2 showed the optimum condition of the remaining lignin of 16.7% obtained at NaOH 14 g/l and the temperature of 151^{o}C,which was lower than the actual data (20.7%)Data obtained from the simulation results can be used to analyze several aspects such as mass fraction of each compound, temperature distributions, velocity profile, and vector. CFD simulations can be used by researchers as a guide for experiment.

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FIGURES

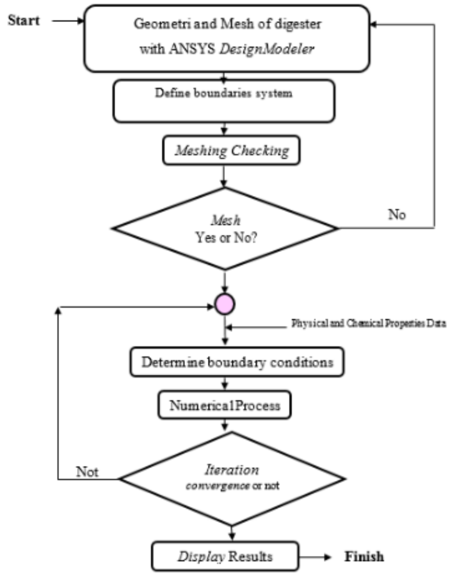

Figure 1. Algorithm of CFD modelling of delignification process in digester using Ansys Fluent 19.2 software

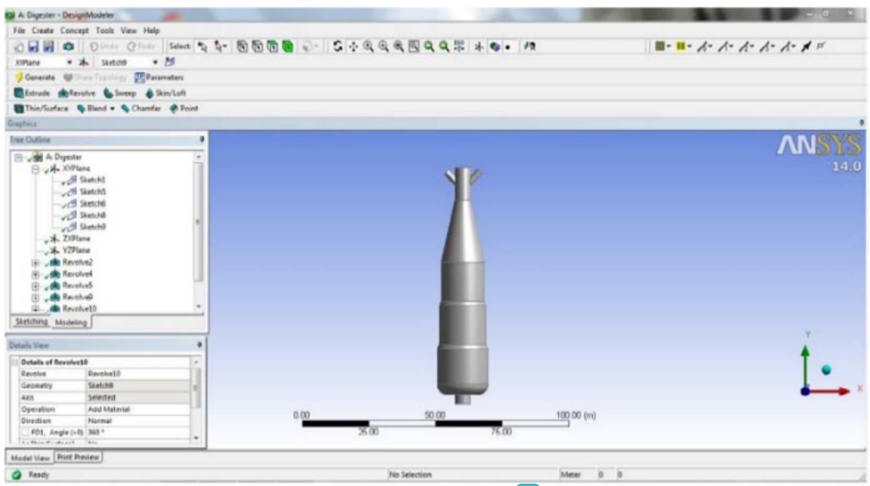

Figure 2. Geometry design of pulp-making digester using Ansys Fluent 19.2 software

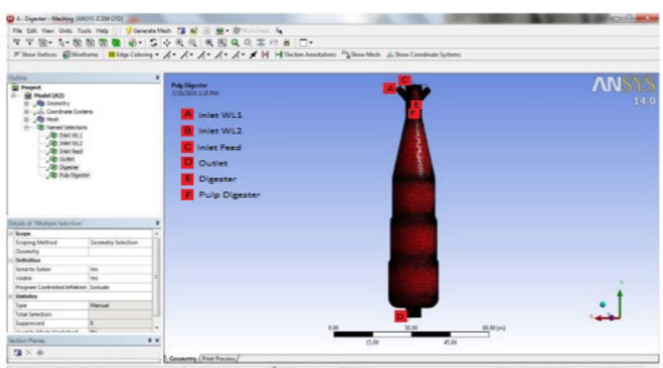

Figure 3. Pulp-making digester boundary conditions using Ansys Fluent 19.2 software

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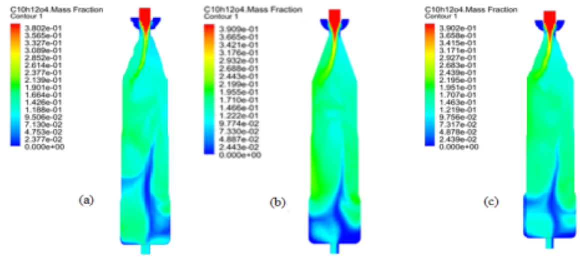

Figure 4. Contour of Lignin Mass Fraction in digester (a). C NaOH 14g/l, T 151°C, (b). NaOH 22g/l, T 152°C, (c). NaOH 18g/l, T 153°C,

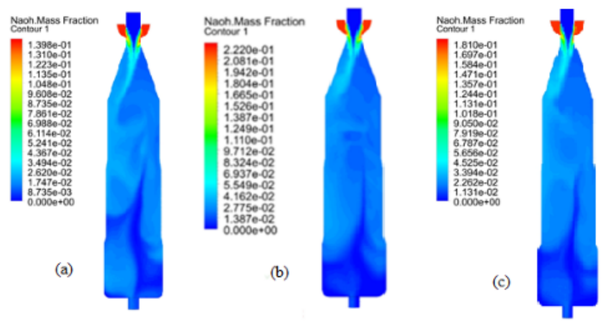

Figure 5. Contour of NaOH Mass Fraction with Ansys 19.2 CFD Simulation (a). C NaOH 14g/l, T 151°C, (b). C NaOH 22g/l, T 152°C, (c). C NaOH 18g/l, T 153°C

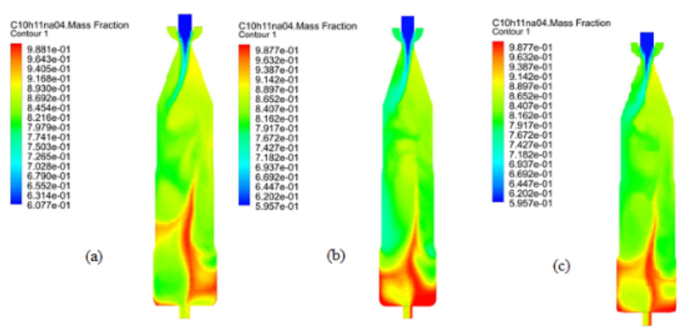

Figure 6. Contour of Na-Lignate Mass Fraction with Ansys 19.2 CFD Simulation (a). C NaOH 14g/l, T 151°C, (b). C NaOH 22g/L, T 152°C, (c). C NaOH 18g/l, T 153°

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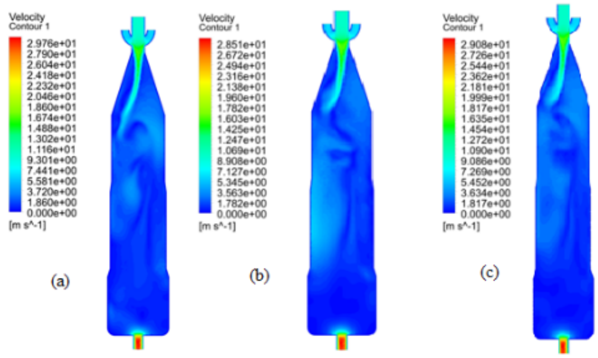

Figure 7. Velocity Contour of Delignification process in digester (a). C NaOH 14g/l, T 151^{o}C, (b). C NaOH 22g/l, T 152^{o}C, (c). C NaOH 18g/l, T 153^{o}C.

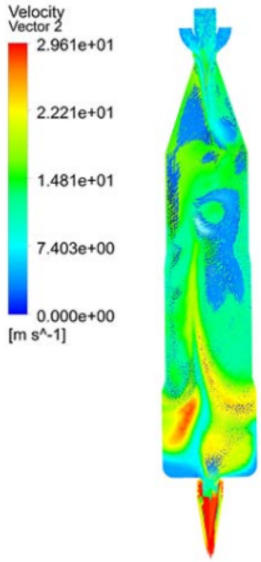

Figure 8. Velocity Vector of delignification process in digester C NaOH 20 g/l; T: 153^{o}C

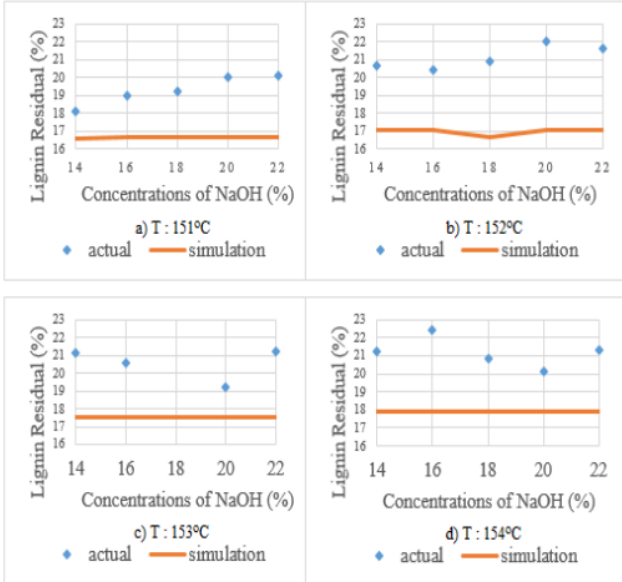

Figure 9. The Effect of NaOH Concentrations on Lignin Levels at Temperature 151°C, 152°C, 153°C, and 154°C (Actual and Simulated Results)

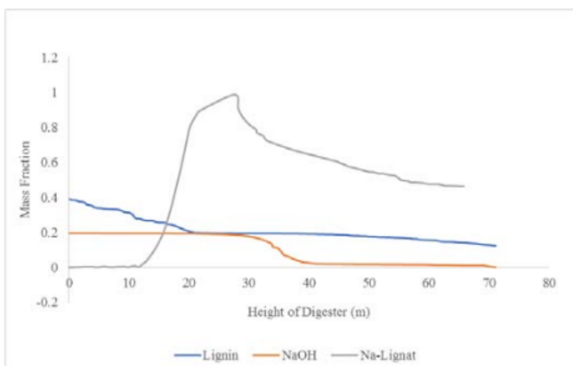

Figure 10. Mass Fraction of Reactan and Products Along the Digester results of CFD Simulation Ansys Fluent 19.2

TABLES

Table 1. Residual Lignin Simulated and Actual Data

Digester volume	4,930 m^3
Digester height	71.460 m
Digester diameter	12.5 m x 70 m
Digester widht	100 mm
Desain capacity	4,596.5 $ADTday^{-1}$
Desain temperature	100°C – 160°C

Table 2. Residual Lignin Simulated and Actual Data

C NaOH (g/l)	T (°C)	Simulated Data (%)	Actual Data (%)
14	151	16,6	18,1
14	152	17,1	20,7
14	153	17,5	21,1

14	154	17,9	21,2
16	151	16,7	21

C NaOH (g/l)	T (^{o}C)	Simulated Data (%)	Actual Data (%)
16	153	17,5	20,6
16	154	17,9	22,4
18	151	16,7	20,5
18	152	16,7	20,9
18	153	17,5	19
18	154	17,9	20,8
20	151	16,7	20,9
20	152	17,1	22
20	153	17,5	19,2
20	154	17,9	20,1
22	151	16,7	22,5
22	152	17,1	21,6
22	153	17,5	21,2
22	154	17,9	21,3

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