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Phenol Concentration in Liquid Smoke Production from Rubberwood by Experiment and Simulation with CFD Modeling

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ABSTRACT

Liquid smoke is produced through condensation resulting from the pyrolysis process of rubberwood, without the presence of oxygen. One of the dominant contents of liquid smoke products is phenol. Therefore, this study aimed to examine the molar concentration of simulated liquid smoke and the comparison between the experimental and simulated molar concentrations. The simulation used Ansys Fluent 19.2, a Computational Fluid Dynamics (CFD) program using the finite volume method in its solution. The several stages in completing Ansys simulation include pre-processing, meshing, processing, and post-processing. The geometry depicted in this study was a 2-dimensional pyrolysis reactor. Assumptions made for the simulation comprised using lignin as raw material, along with specified flowrate, and pyrolysis time. The results showed that based on the reaction mechanism, lignin in the pyrolysis process produced a phenol yield of 4.52%. In the final stage, quantitative data simulation results were obtained in the form of molar concentrations produced from liquid smoke products. The molar concentrations in the simulation during pyrolysis for 1, 2, 3, 4, and 5 hours were 0.00183512, 0.0017854, 0.00170856, 0.0017628, and 0.00166788 kmol/m^3, respectively. The experimental molar concentration results also showed the same pattern as the simulation data. At 4 hours of pyrolysis, the molar concentration of phenol increased, resulting in liquid smoke with the best quality. A comparison of liquid smoke molar concentration for the simulation and experiment indicated a minimal difference of 0.005%.

1. Introduction

Indonesia is ranked top globally in terms of rubberwood plantation area [1], with Sumatra and Kalimantan serving as suitable areas for cultivating rubber due to the favorable land conditions. The size of rubber plantations on Sumatra Island reaches 2,570,000 hectares, while Kalimantan Island ranks second at 963,300 hectares [2]. This prominence underscores the significance of rubberwood

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as one of the essential natural resources for development and profitability, capable of bolstering the economy.

The production value of rubberwood is obtained through the development of downstream industries and its use as raw material in the woodworking sector. However, rapid development could be negatively impacted when the waste generated is not considered. This waste may be in the form of old rubberwood that does not emit sap. The amount of waste in Indonesia is estimated at 1.782.456-2.638.238 m^3, obtained from public farms, private companies, or government [3]. Furthermore, the utilization of rubberwood waste in the pyrolysis process produced 2.7 liters of liquid smoke out of 5 kg feedstock [4], suggesting the potential to be used as feedstock for added-value products.

Effective management of rubberwood waste is crucial to avoid causing other environmental problems. The content can be reused in the form of a more valuable product with a higher selling value. One way to develop rubberwood waste is to process into liquid smoke using the pyrolysis method, thereby converting biomass waste into a valuable resource [5]. The resulting liquid smoke contains phenolics, acids, carbonyls, tar compounds, water, and benzopyrene.

The components of rubberwood include hemicellulose, cellulose, and lignin, which decompose into more than 300 compounds at high temperatures. Liquid smoke is produced using the pyrolysis method, yielding charcoal and smoke [5]. The purpose of using the method is to remove volatile matter components contained in rubberwood, resulting in a product with a high calorific value.

Liquid smoke can be used in food preservation, environmentally friendly pest control, and organic herbicides. Due to the numerous benefits, the production process using the pyrolysis method is considered the most effective [4] and the associated stages include pyrolysis, condensation, and distillation. Pyrolysis is defined as a thermochemical decomposition process of biomass occurring between 400-650 ^oC in the absence of O_2.

The thermochemical conversion includes three main processes, namely direct combustion, pyrolysis, and gasification. The pyrolysis process is carried out in an inert atmosphere to convert biomass into bio-oil, biochar, and fuel gas. The majority of previous studies focused more on liquid and syngas products than biochar because oil and syngas are more valuable. Additionally, the yields and composition of pyrolysis oil and syngas change with temperature [6].

Pyrolysis is divided into two groups, namely slow and fast, specifically, slow pyrolysis uses temperatures ranging from 400-600 ^oC. Meanwhile, fast pyrolysis characterized by rapid heating between 10 to 1000 $^oC/s$ produces high liquid within a short duration of less than 2 seconds. The temperature range is between 400-650 ^oC with rapid cooling attributed to the steam [7]. Fast pyrolysis uses biomass or waste to produce products suitable as both energy sources and raw materials for chemical production. High heating rates increase bio-oil yields, while low heating rates favor bio-char formation [8]. Pyrolysis equipment is typically sizable and operates on an industrial scale.

Previous studies often use a 1D model, with variables such as temperature, volatile release, shrinkage, and swelling. The model is simplified into four layers, increasing efficiency compared to the number of cells, but the parameters cannot be calculated for each layer. Other studies state that 2D models are used to analyze the pyrolysis of dry and wet logs. These models can predict important parameters, namely surface temperature, mass loss, and gas fraction [9].

Several innovative efforts have been undertaken to produce more straightforward pyrolysis equipment, as evidenced in the study conducted by [4]. The design process uses Fusion 360 software to support the fabrication of liquid smoke production equipment for maximum results. The liquid smoke produced in this study will be analyzed using the software. Analysis of the content contained in the liquid smoke product was carried out using a Computational Fluid Dynamics (CFD) simulation.

This study also analyzed liquid smoke content resulting from previous investigations using CFD with 2D geometry. Simulation using CFD can be utilized to further study a process without the need for physical equipment and experiments [10].

The utilization of CFD in this study enabled the provision of detailed information about the molar concentration, as well as mass and molar fraction. The modeling software used was Ansys fluent 19.2 with a working process divided into three, namely, pre-processing, processing, and post-processing [11]. The pre-processing stage includes geometry and mesh creation, while the processing stage determines boundary conditions and selects the initiation method. Finally, the post-processing stage displays the results of the calculations on the boundary conditions and graphs that depict mesh, contour, vector, and pathline. This study aimed to explore rubberwood pyrolysis through simulation, with a particular focus on ascertaining its optimal potential and subsequently contrasting the results with existing experiments conducted using modest equipment.

2. Methodology

In this study, experiments were carried out by referring to previous studies, which included pyrolysis and condensation processes to produce liquid smoke [12]. Figure 1 shows the process of liquid smoke production on experimental methods. This process was then modeled in CFD simulation to find the best results using the same operating conditions and compared with existing experiments.

The geometry in the simulation process referred to the tools used in field experiments to produce liquid smoke. Figure 2 shows a series of tools used for the pyrolysis process, with a major focus on the pyrolysis reactor designed in two dimensions using Ansys Fluent 19.2.

Figure 3 shows the flow diagram of the Ansys Fluent 19.2 simulation process to obtain the molar concentration of phenol. Analysis of problems in the simulation process was used to determine the results of the modeling and computation in selecting the suitable model. The geometry stage was carried out with a 2-dimensional method using general modeling. Afterward, the meshing step was performed to divide the geometry into smaller elements and produce a more accurate analysis. The mesh method was set to automatic generation [13].

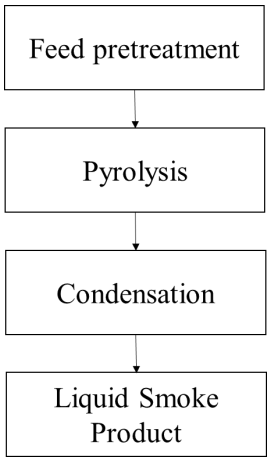

Fig. 1. Flowchart of experimental process

Fig. 2. Pyrolysis equipment sets [3]

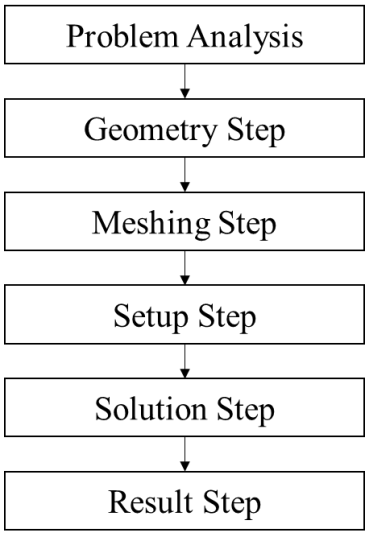

Fig. 3. Flowchart of simulation Process

Figure 4 shows the pyrolysis reactor geometry simulated using Ansys Fluent 19.2. The simulation process started from pre-processing, meshing, processing, and post-processing. The pre-processing stage included the process of creating geometry and the parameters used. The geometry of the pyrolysis reactor used Ansys fluent 19.2 with a 2D design, where the dimensions of the reactor were 79 cm long and 100 cm high. The dimensions of the reactor were obtained from the size of the experimental reactor.

After the geometry was completed, meshing divided the geometric structure into smaller ones. Optimal meshing also aims to achieve faster convergent results during analysis. The geometry was mapped to define the inlet, outlet, and reactor walls. Figure 5 shows the results of the meshing performed.

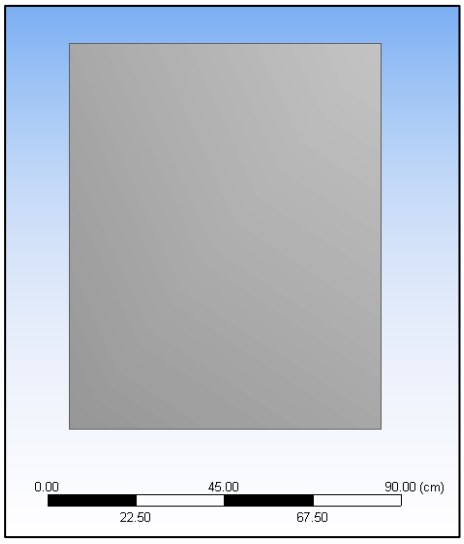

Fig. 4. Pyrolysis reactor geometric

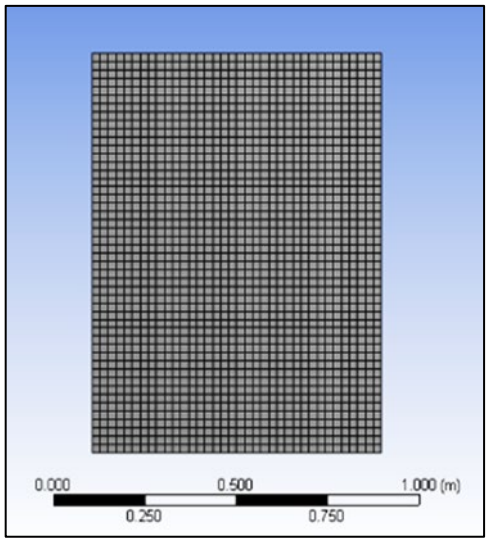

Fig. 5. Pyrolysis reactor mesh

After the meshing process, the processing stage commenced by setting the variables to be entered and calculated. The variables entered were boundary conditions and others, then a trial-and-error process was carried out for several methods followed by an iteration process. The success of a simulation process is determined by the steps. During the trial-and-error process in this study, Ansys

Fluent software was used. Errors occur when drawing geometry or inputting data which cause the results to be unreadable by the system. When the data entered is incorrect, the results of the iteration in the system do not converge. The solution is to check for boundary conditions, poor-quality mesh, inaccurate geometry, and numerical instability.

The final stage of the Ansys Fluent 19.2 simulation process is post-processing. The simulation results obtained were quantitative data in the form of molar concentrations of phenol produced from liquid smoke products. This stage compared the calculation results obtained with existing experiments.

3. Results

3.1 Ansys Fluent 19.2 Simulation Stages

After carrying out the geometry stages, the meshing results were found to significantly influence the next processes. The meshing process was considered excellent because the skewness aspect reached a value of 1.3057×10^{-10}, consistent with the standard. When the skewness reaches >0-0.25 it is considered excellent for the meshing process. In a 2D context, all cells should ideally be good or better. The presence of cells rated fair or worse indicates sub-optimal boundary node placement, and in such cases, efforts should be made to improve the boundary mesh, because the quality of the overall mesh cannot exceed that of the boundary [14].

The processing steps include selecting the 2D space and time type using transient, determination of models, materials, boundary conditions, operation conditions, solution method, as well as control and iteration. Transient analysis was conducted for polymer pipes under pressure using a 2D approach [15]. Before carrying out the calculation run, the time step size was set to 59 (s) with the number of time steps to 100 and the max iteration/time step at 20.

The use of the turbulence model, in this case, k-epsilon, can provide consistent results [16]. The P1 radiation model was used in this study because the results were quite equivalent in predicting the temperature and gas composition [17]. For combustion determined by stoichiometric reactions such as pyrolysis, a species transport model is preferable.Finite-rate eddy dissipation was used in the reaction model due to its renowned accuracy [18]. This model was selected based on its avoidance of reliance solely on mixing using one global reaction step, such as the eddy dissipation model.

The material used in this study was ($C_9H_{10}O_2$) containing components such as phenol (C_6H_5OH), water (H_2O), and cyclopropenylidene (C_3H_2). Boundary conditions in Ansys selected mass flow inlet and outlet pressure on each component that has been defined.

The parameters related to the conditions in the operating model were set when entering the data. In this study, the force of gravity did not affect the calculation, while the parameters used in the solution methods and controls included SIMPLE, Least Square Cell Based, Second Order Upwind, and First Order Upwind. The SIMPLE algorithm was used for the pressure-velocity coupling scheme [19]. Initializing conditions is a method used to facilitate the simulation process to achieve convergence, with the variables being variations in flow rate and pyrolysis time. Figure 6 shows the iteration calculations that have reached convergence.

The accuracy of a model in the simulation is reflected in the convergence test. Convergence, which aims to provide convergent modeling results is the determination of how many iterations and the limit of the Root Mean Square (RMS) before the calculation. Furthermore, the overall balances were monitored, along with the maximum value of the velocity at the outlet [20]. Simulation time affects the number of iteration calculations [21] and the iteration obtained in the study was 153. Figure 7 shows the phenol concentration profile inside the pyrolysis reactor after the simulation for

4 hours. Based on the results, most of the phenol was formed on the reactor wall, marked with a red color on the contour.

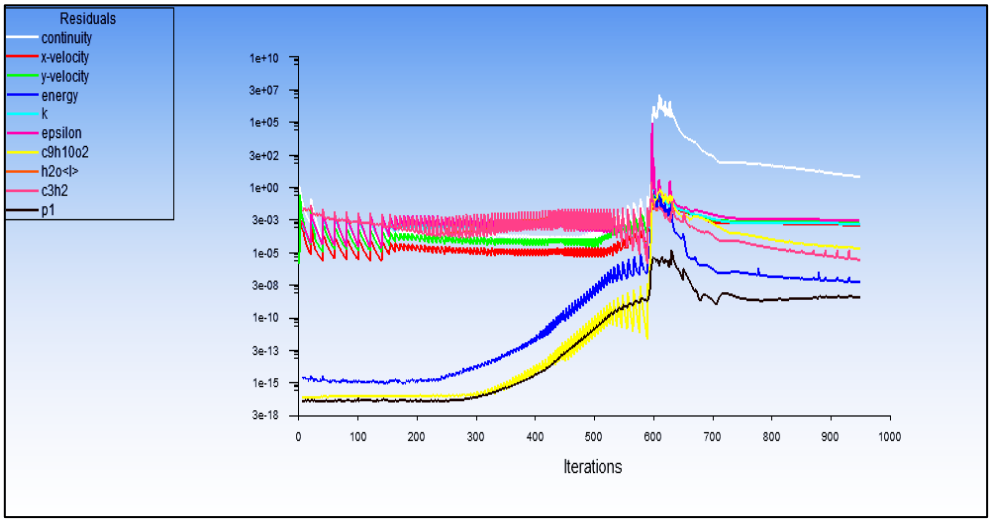

Fig. 6. Convergence iteration temperature at 400 °C and flow rate of 0.000358 kg/s

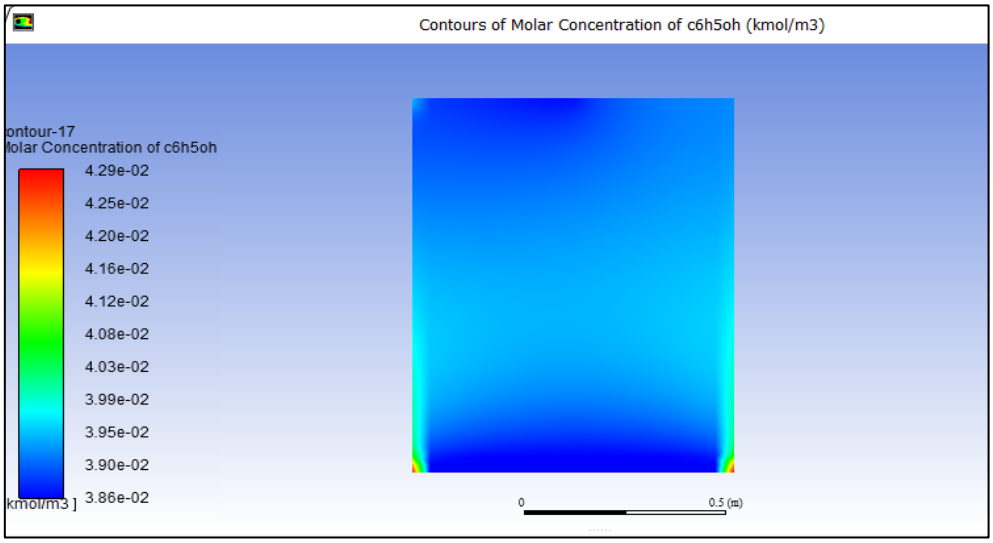

Fig. 7. Display of contours molar concentration of phenol with a mass flow rate of 4 hours

3.2 Phenol Molar Concentration of Liquid Smoke from Experimental and Simulation

This study compared the simulated and experimental molar concentrations. During the simulation process, several assumptions were used. Firstly, the raw material input into the reactor was assumed to be lignin, with phenol as the resulting product. These assumptions were based on the dominant percentage of raw materials and products. Secondly, the flow rate was estimated hourly by comparing the mass of raw materials and the pyrolysis time. The process of lignin decomposition into phenol is described in Figure 8 below.

Based on the mechanism (Figure 8), lignin decomposes immediately during pyrolysis to form monomeric phenolics with a yield of 8.54%. These monomeric phenolics were heated further, leading to vapor-phase reactions that generated several products including simple phenol, methanol methanethiol, unconverted monomeric phenolics, and others. The simple phenol produced

amounted to 4.52% and was used as a reference for product assumptions when calculating the experimental phenol molar concentration [22].

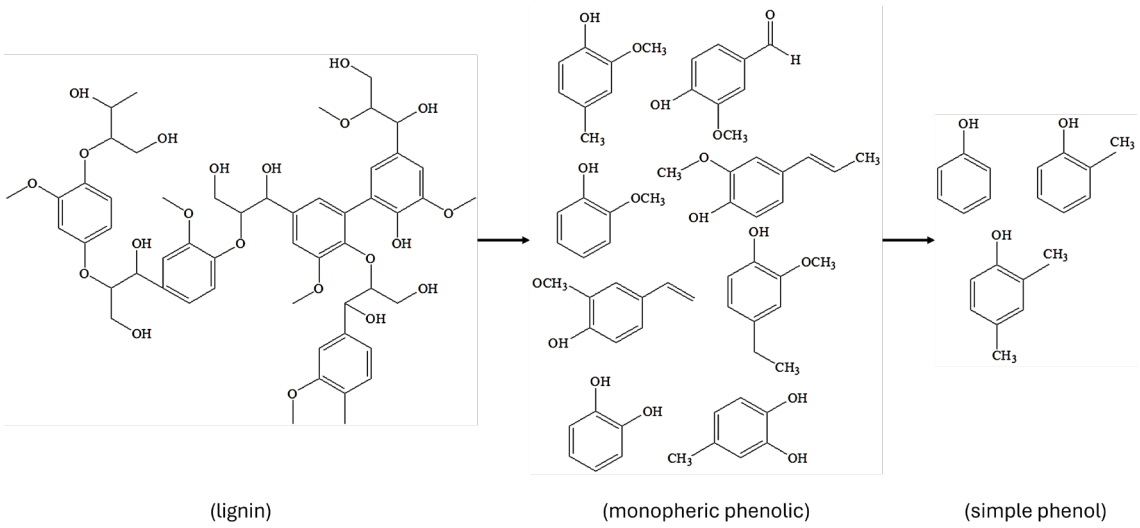

Fig. 8. Lignin decomposition mechanism

The lignin content used during the experiment had different ranges. The simulation required exact data for the assumption of raw materials and a lignin content of 33.54% was used based on a previous study [23]. Figure 9 shows the results of the phenol molar concentration at the time of simulation and experiment.

Validation is conducted to determine the simulation results, ensuring similarity with existing experiments of modeled cases with the slightest possible error. Figure 6 compares the results of the molar concentration for phenol at the pyrolysis time of 1, 2, 3, 4, and 5 hours using various flow rates. The similarity between experimental and simulation results can be caused by the heating conditions in the tool which were not continuously controlled during the operating time and the use of simple equipment. This observation underscores the need for modifications and optimization of pyrolysis equipment for the production of phenol from rubberwood.

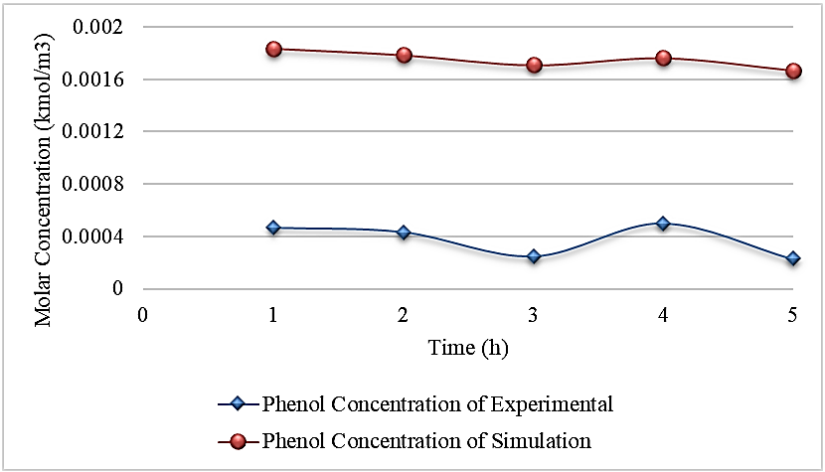

Fig. 9. Phenol molar concentration on the liquid smoke product

Several factors contributed to the difference between the experiment and the simulation results. For example, the instability of the temperature in the pyrolysis reactor, attributed to the use of firewood as the heat source, hinders optimal pyrolysis products. Since the pyrolysis reactor had no

temperature control, the alternative was to use a thermogun. However, the use of thermogun was not effective in this study. The flow rate of the pyrolysis reactor was not measured, relying instead on assumptions during the simulation. When the phenol analysis was carried out, the resistance of the liquid smoke product was reduced due to prolonged storage, decreasing yield. Validation error between simulation and experimental results was calculated using Eq. (1).

$$\text{Error} = \sum \left(\frac{(\text{Tcal-Tmeas})^2}{\text{Tmeas}} \right) \quad (1)$$

where Tmeas represents the total molar concentration of phenol from the experimental results and Tcal represents the total molar concentration of phenol from the simulation results. Although there were differences in the simulation data, the experimental and simulation patterns were close at 4 hours of operation time, and the molar concentration of phenol increased. Therefore, the liquid smoke with the best quality was obtained at a pyrolysis time of 4 hours. The validation error value between the experimental and the simulation was 0.005 %.

4. Conclusions

In conclusion, based on the reaction mechanism of lignin in the pyrolysis process, it produced phenol estimated at 4.52% of the supposed molar concentration. The study documented phenol molar concentrations at sequential intervals from 1 to 5 hours, yielding values of 0.00183512; 0.0017854; 0.00170856; 0.0017628; and 0.00166788 kmol/m^3, respectively. The comparison between simulated and experimentally derived liquid smoke presented a negligible discrepancy in molar concentration, estimated at around 0.005%. Notably, the simulation conducted using Ansys Fluent 19.2 indicated that the flow rate significantly influences the molar concentration of phenol. Based on the analysis, liquid smoke with the best quality was obtained at a pyrolysis time of 4 hours with experimental and simulation concentrations of 0.0017628 kmol/m^3 and 0.000499203 kmol/m^3.

Acknowledgment

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