Process Modelling and Economic Evaluation for NanoLignin Production

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Abstract. Lignin nanoparticles (nanolignin, NL) are sustainable, green material which can be derived from industrial and agricultural waste. NL has enhanced properties compared to standard lignin due to a larger surface to volume ratio. Hence, it’s suitable for a wide range of applications including drug delivery, stabilising agent, substitute for silver nanoparticles and reinforcement material. This study analyses the commercial feasibility of NL production from high pressure homogenization. The production process was simulated based on the basic laboratory results using commercial simulation software, SuperPro Designer. Manufacturing cost and minimum selling price for NL was estimated to be 5.1 USD/kg and 6.1 USD/kg for a continuous plant with 15t/day production rate. The sensitivity of three factors; Lignin concentration to the homogenizer, production rate and lignin price on process economics was analysed and results shown lignin concentration has a severe impact on manufacturing cost and selling price. The production cost reduces to 2.46 USD/kg when the lignin concentration increases to 6%.

1. Introduction
Lignin is the second most abundant polymer from biomass and the primary source for aromatic polymers. The presence of different organic functional groups such as phenolic, aliphatic hydroxyl, methoxy and terminat aldehyde make lignin a potential component to synthesize environmentally friendly polymer based materials [1]. However, lignin is still hugely underutilised, and most of the industrial lignin use as a low cost fuel for energy generation. A small fraction of Lignin has been used as carbon black substitute, rubber reinforcer, phenolic resin component and pre-cursor for carbon fiber [2]. Lignin is a complex heterogeneous polymer whose structure and characteristics highly depend on the source and the pulping method. Also, poor reactivity, hydrophobicity and difficult processability (due to high branched and hydrogen bonded three-dimensional structure) cause challenges in developing lignin applications [3].
Lignin in nanoscale can reduce some of the problems related to lignin processing. Nanolignin (NL) offer different or improved properties compared to parent material [4] due to the larger surface to volume ratio. NL polymer composites have high mechanical performance [5], enhanced thermal...
stability [6] and higher anti-oxidant activity [7]. Water-dispersed NL can be used to stabilise Pickering emulsions, carry silver ions in antimicrobial applications and drug delivery applications [8].

Many approaches have been reported to synthesize NL which include chemical methods (solvent shifting, pH shifting, carbon dioxide antisolvent and cross-linking/polymerisation), mechanical methods (homogenization and ultrasonication) or other methods such as ice-segregation, template base synthesis, aerosol processing and electrospinning [9]. Among the above methods, the most investigated methods are solvent and pH shifting. But both approaches require a massive amount of solvents and involve downstream processing which may not be cost effective in the industrial scale. In nanoparticle synthesis processes, many mechanical or physical methods are less energy intensive as compared to chemical pathway [10]. Hence, for this study mechanical homogenization was selected to produce NL. Currently, the NL is in lab production and a techno-economic analysis has only been done for aerosol lignin [11] and colloidal lignin manufacturing process [12].

Process simulation is an essential tool for the chemical industry to forecast the economic feasibility of new process model at the initial stage of process design. This study presents the preliminary economic analysis for NL production via mechanical homogenization. The process is simulated in SuperPro Designer v9.5 based on the laboratory data. The simulation data consists of estimated capital and operational costs and minimum selling price, which suggests the potential implementation of industrial scale NL plant.

2. Laboratory scale NL synthesis

The Alkali lignin, obtained from palm oil empty fruit bunch black liquor was dissolved in water using magnetic stirring. The solution was sent to high-pressure homogenizer to obtain NL. Later the NL solution was frozen at -40°C for 24 h and dried using a spray dryer to get solid NL particles. The particle size distribution of NL was examined by Malvern Nano-ZS Zetasizer (Malvern Instruments Ltd, UK) using dynamic light scattering (DLS) method. The Z-average was 283 nm, and polydispersity index (Pdi) was 0.390.

3. Process simulation

The production of NL in laboratory scale was conducted in batch mode. To improve the capacity and cost efficiency, the NL production was simulated in a continuous manner assuming that the plant would have operated 330 days in a year. The NL production rate was set at 625 kg/h (4950 t/y). The value was based on 10% lignin production from a general pulp mill [13]. Also, the lignin loss during the process was assumed to be negligible. Figure 1 shows the base case process flowsheet simulated in SuperPro Designer. First, lignin (625kg/h) was diluted in a blending tank with water. (1420 kg/h fresh water and recycled water 29194 kg/h). The concentration of lignin after the dilution was 2 wt. % (625kg/h lignin in 30614kg/h water). Then the dissolved lignin was pumped to high-pressure homogenizer. During the homogenization process, lignin size would be reduced to nanoscale. The NL solution was sent to spray dryer. The moisture content of the dried NL was less than 5wt. %. The solid particles in the vapour were removed by air filters. Then the vapour stream was subsequently cooled and air was emitted through a vent. The recovered water from the vapour stream (S-5) was reused for lignin dissolution.

Major costs considered for NL process were given as; Lignin 300USD/t [11], water 0.57USD/m³ and electricity 0.07USD/kWh (based on Malaysian water and electricity tariff),chilled water 0.4 USD/t and steam 12 USD/t (based on SuperPro 2019 values).

The details of the equipment sizing, number of units and purchase cost of 2019 were obtained from SuperPro designer and summarised in table 1. Figure 2 shows the percentage of contribution of each equipment to the total equipment purchase cost. The homogenizer unit is the most expensive equipment, and for the base case it contributes to 51% of the total equipment purchasing cost. Also, 13 units of homogenizers are required to maintain the process. This cost can be reduced by varying the homogenization condition such as lignin concentration and production rate, which will be studied in detail in the subsequent sensitivity analysis.
Figure 1. Simulation flowsheet for industrial scale NL production process from homogenization.

Table 1. Capacity and Purchase cost of equipment.

| Equipment       | Blending Tank (V-1) | Pump (PM-1) | Homogenizer (HG-1) | Spray Dryer (SDR-1) | Air Filter (AF-1) | Heat Exchanger (HX-1) | Storage Tank |
|-----------------|----------------------|-------------|--------------------|---------------------|-------------------|------------------------|--------------|
| Units           | 1                    | 1           | 13                 | 1                   | 7                 | 1                      | 1            |
| Capacity        | 80,000 L             | 1.23 W      | 20,000 L/h         | 305,751 L           | 14,163,872 L/h    | 100 m²                 | 80,000       |
| Unit Price ($ x 1000) | 311               | 22          | 121                | 378                 | 60                | 104                    | 371          |

4. Process economics

The economic evaluation was performed using the inbuilt function of SuperPro Designer v9.5. The minimum selling price (MSP) of NL was based on the desired payback period (5 years). Production cost for the base case was 5.1 USD/kg, and MSP was 6.1 USD/kg. Internal rate of return (IRR) needed to be more than 10% after the taxation to the project to be profitable. NL production plant with 4950t/y capacity claimed a capital investment of $ 27.6 Million and operating cost of $ 26.5 Million. Calculated annual revenue of the project was $ 31.7 Million. The IRR and the ROI values for the project calculated as 12.7% and 19.6%, respectively. The project could be considered profitable since the IRR was more than 10%, and ROI showed considerable value.

5. Sensitivity Analysis

Lignin concentration affects the capital cost (equipment sizing) and energy requirement significantly. Unit production cost for different lignin concentrations was calculated (figure 3). When the lignin concentration was low (less than 2 wt. %), larger capacity equipment needs to produce the same amount of NL. Hence the unit production cost increased significantly due to increment in capital investment and operational cost. On the other hand, when the lignin concentration was high, the unit cost of NL decreased as the capacity of equipment needed are lowered. For 6 wt. % lignin concentration, unit production cost and MSP are 2.46 USD/kg and 2.96 USD/kg. For this scenario, the production cost decreased by 48% compared to the base case (2 wt. %). Therefore, the lignin
concentration at the homogenizer seems to be a very sensitive parameter for project economics. Thus, optimization on lignin concentration should be considered to ensure the process remains cost effective.

**Figure 2.** Percentage contribution of equipment to total equipment cost.

**Figure 3.** Influence of lignin concentration on production cost and MSP of NL.

The production rate can influence the unit production cost of the product. For the base case simulation, the NL plant is assumed to integrate with pulp mill and consume approximately 10% of generated lignin to produce NL. Since NL falls under speciality material, it can be delivered as an independent product/precursor for another product in less volume. Also, the production capacity can be higher than the base scale, depending on the market demand. Hence different production rates vs unit production cost and MSP was simulated and presented in figure 4. When the production rate was lowered to 1 t/day, unit production cost increased by 3-fold. When the production rate heightened to 30 t/day, unit production cost decreased by 8% as compared to the base scale (15 t/day).

**Figure 4.** Influence of NL production rate on production cost and minimum selling price (MSP) of NL.

**Figure 5.** Impact of lignin price on production cost and minimum selling price (MSP) of NL.

Lignin was the primary input material of the process. Lignin market prices can vary depending on seasonality and purity. For the base scale, kraft lignin was selected (due to the abundance in the market). In figure 5, the lignin price is varied from 250 USD/t to 500 USD/t. Unit production cost
reduces 1% from the base case (300 USD/t) when the lignin price is 250 USD/t. If the lignin price rise to 500 USD/t, there would be a 4% unit production cost improvement.

6. Conclusion
A commercial feasibility study was conducted for industrial scale NL process using SuperPro Designer. For a NL plant with production capacity 15 t/day, the selling price of NL with 5 years payback period is $6.1/kg. The IRR and ROI values for the project is found to be 12.7% and 19.6% respectively, which indicate the feasibility of the process. The lignin concentration in the homogenizer has been recognised as the most sensitive parameters for project economics. The selling price is at $2.96/kg when the lignin concentration is increased to 6 wt. %. Even though the production rate and lignin market price may influence the manufacturing cost and selling price, they are not as prominent as the lignin concentration. According to the production and selling prices in this study, NL has the potential to use in high-value low volume applications such as a substitute for silver nanoparticles and stabilising agents for Pickering emulsions. However, to substitute lignin using NL for the high volume applications, i.e. Formaldehyde resins, the NL manufacturing cost requires to be lowered. To reduce the cost research on using low-grade lignin as feedstock for high volume low-value applications, optimising homogeniser conditions (pressure and number of passes) according to NL applications and investigating the effect of high lignin concentration at the homogeniser on the process and the final NL properties are suggested.

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