

## Electronic Supplementary Information

### **A modeling framework to identify environmentally greener and lower-cost pathways of nanomaterials**

Kai Lan,<sup>a,b</sup> Hannah Szu-Han Wang,<sup>a</sup> Tessa Lee,<sup>a</sup> Camilla Abbati de Assis,<sup>c</sup> Richard A. Venditti,<sup>b</sup> Yong Zhu,<sup>d</sup> Yuan Yao,<sup>\* a c</sup>

<sup>a</sup> Center for Industrial Ecology, Yale School of the Environment, Yale University,  
380 Edwards Street, New Haven, Connecticut, 06511, USA

<sup>b</sup> Department of Forest Biomaterials, North Carolina State University, 2820 Faucette  
Drive, Raleigh, North Carolina, 27695, USA

<sup>c</sup> Fisher International, Inc., 15720 Brixham Hill Ave. Suite 550, Charlotte, North Carolina, 28277,  
USA

<sup>d</sup> Department of Mechanical and Aerospace Engineering, North Carolina State University, 911  
Oval Drive, Raleigh, North Carolina, 27695, USA

<sup>e</sup> Chemical and Environmental Engineering, Yale School of Engineering and Applied Science,  
Yale University, 17 Hillhouse Avenue, New Haven, Connecticut, 06520, USA

\*Corresponding author: y.yao@yale.edu

Pages: 70

## Table of Contents

S1. Literature review for the case of cellulose nanomaterials .....	4
S2. CNC production.....	6
S3. CNF production .....	11
S4. Technical performance of CNC and CNF scenarios .....	14
S5. Sulfuric acid hydrolysis for CNC production.....	17
S6. CNC and CNF Landfilling .....	18
S7. Life cycle assessment methodology .....	19
S8. Capital expenditures for cellulose nanomaterial production .....	20
S9. Operating expenditures for cellulose nanomaterial production.....	21
S10. Sensitivity analysis for cellulose nanomaterials .....	22
Fig. S1. Process flowchart of the baseline. ....	25
Fig. S2. Process flowchart of Scenario CNC-1. ....	26
Fig. S3. Process flowchart of Scenario CNC-2. ....	27
Fig. S4. Process flowchart of Scenario CNC-3. ....	28
Fig. S5. Process flowchart of Scenario CNC-4. ....	29
Fig. S6. Process flowchart of CNF baseline process. ....	30
Fig. S7. Process flowchart of Scenario CNF-1.....	31
Fig. S8. The normalized life-cycle environmental impacts of CNC in the performance-based functional unit. ....	32
Fig. S9. Sensitivity analysis results of Scenario CNC-2 at 50 dry t day <sup>-1</sup> . a, global warming potential; b, minimum selling price. ....	33
Fig. S10. The normalized life-cycle environmental impacts of CNF in the performance-based functional unit. ....	34
Fig. S11. Sensitivity analysis results of Scenario CNF-1 at 50 dry t day <sup>-1</sup> . a, global warming potential; b, minimum selling price. ....	35
Fig. S12. Minimum selling price, operating cost, global warming potentials (in the performance-based functional unit, per MPa per m <sup>3</sup> ), and eco-efficiency analysis results of scenarios at 50 dry t day <sup>-1</sup> . ....	36
Fig. S13. Reaction pathways for sulfuric acid hydrolysis of dissolving pulp. ....	37
Table S1. Summarized input and output results for CNC scenarios. ....	38
Table S2. Summarized input and output results for CNF scenarios.....	39
Table S3. Parameter values for landfill and landfill gas recovery.....	40
Table S4. Ecoinvent processes used in this study.....	41

Table S5. Inputs and outputs of producing 1 air dried (10% moisture content) metric ton of NBSK pulp used in this study.....	42
Table S6. Life-cycle environmental impacts of producing 1 air dried (10% moisture content) metric ton of dissolving pulp used in this study. ....	43
Table S7. Financial assumptions for the discounted cash flow rate of return analysis. ....	44
Table S8. Project cost assumptions. ....	45
Table S9. Capital investment of CNC scenarios at varied plant capacities.....	46
Table S10. Capital investment of CNF scenarios at varied plant capacities. ....	48
Table S11. Purchased cost and installed cost of equipment in CNC scenarios.....	49
Table S12. Purchased cost and installed cost of equipment in CNF scenarios. ....	52
Table S13. Operating cost per dry t CNC of CNC scenarios at varied plant capacities.....	54
Table S14. Operating cost per dry t CNF of CNF scenarios at varied plant capacities.....	56
Table S15. Cost information (2020 US\$) for feedstocks, materials, and energy. ....	57
Table S16. Number of labor positions of the plant at 50 dry t nanocellulose produced per day (2020 US\$).....	58
Table S17. Summary of scenario settings for the case study of cellulose nanomaterials. ....	59
Table S18. Life-cycle environment impact results of producing 1 dry kg CNC.....	60
Table S19. Parameter range for sensitivity analysis for the case study of cellulose nanomaterials. ....	63
Table S20. Life-cycle environment impact results of producing 1 dry kg CNF. ....	64
Table S21. MSP of CNC and CNF scenarios at varied plant capacities. ....	66
Reference .....	67

## **S1. Literature review for the case of cellulose nanomaterials**

Several previous studies have employed LCA to investigate the environmental impacts of CNC or CNF production with varied methods.<sup>1–13</sup> For example, Arvidsson et al. conducted a cradle-to-gate LCA for CNF in three production routes. They showed that the no pretreatment and enzymatic routes had similar lower environmental impacts (i.e., cumulative energy demand, GWP, terrestrial acidification, and water depletion) than the carboxymethylation route.<sup>1</sup> Nadeem et al. performed a cradle-to-gate LCA to assess the life-cycle embodied energy and GWP of producing CNF film via four small-scale production routes.<sup>2</sup> They showed that refined and spray-deposited films have smaller life-cycle impacts.<sup>2</sup> Gu et al. developed a cradle-to-gate LCA for CNC production from wood pulp through sulfuric acid hydrolysis based on pilot scale data.<sup>8</sup> This study identified that the sodium hydroxide used to neutralize the acid solution (no acid recovery) contributed the most to the LCA results.<sup>8</sup> Zhang et al. investigated the cradle-to-gate life-cycle impacts of CNC production and showed considerable environmental benefits of recovering the sulfuric acid after acid hydrolysis compared to no recovery.<sup>9</sup> Zargar et al. evaluated the cradle-to-gate life-cycle environmental impacts of producing lignin-containing CNC using deep eutectic solvent.<sup>5</sup> Their results exhibited that the largest reduction potential was by reducing the eutectic solvent solution input, they also highlighted the usage of LCA in defining future research direction.<sup>5</sup>

Several previous studies used TEA to analyze the economics of producing CNC or CNF.<sup>10,14–17</sup> For instance, Bondancia et al. conduct a cradle-to-gate LCA and TEA for CNC production from sugar cane bagasse via three alternative acid hydrolysis routes — sulfuric acid, citric acid, and combination.<sup>10</sup> The sulfuric acid route showed both lower minimum product selling price (MPSP) (US\$6,897 per dry t) and life-cycle environmental impacts than the citric acid or citric/sulfuric acid route (US\$10,452–\$10,974 per dry t).<sup>10</sup> De Assis et al. analyzed the economics and risks of

cellulose micro- and nano-fibrils (CMNF) based on the pilot plant data.<sup>14</sup> The study showed that MPSP was US\$1,893–\$2,440 per dry t CMNF and pulp cost and energy consumption were the main drivers.<sup>14</sup> De Assis et al. studied the commercialization of CNC production via sulfuric acid hydrolysis and neutralization with CaO.<sup>15</sup> The results showed that the lowest MSP was achieved by co-location with a pulp mill (sharing infrastructures, utilities, effluent treatment system) and without acid recovery; the main economic driver was capital investment.<sup>15</sup>

## **S2. CNC production**

### **S2.1. Feedstock.**

In this study, the feedstock for CNC production is dissolving pulp.<sup>8,15,18,19</sup> Dissolving pulp can be produced from varied biomass sources (typically hardwood, softwood, and cotton fibers) via sulfite pulping or pre-hydrolysis kraft pulping.<sup>20</sup>

### **S2.2. CNC baseline process.**

The baseline process is based on the CNC batch-process pilot plant by the U.S. Department of Agriculture Forest Products Laboratory (USDA FPL).<sup>8</sup> ESI Fig. S1 shows the flowchart of the baseline process. The dissolving pulp is first fed into a shredder to generate small particles that allow for acid hydrolysis. The material loss during shredding is assumed to be 0.5%.<sup>15</sup> Then the shredded pulp is sent to acid hydrolysis using 64% *wt* sulfuric acid (pulp consistency 10% in acid hydrolysis).<sup>15</sup> The acid hydrolysis is operated at 45 °C for 60 minutes.<sup>8,15,21</sup> To maintain the reactor's temperature, steam at 454 °C and 62 atm from the natural gas boiler is used.<sup>22</sup> The boiler efficiency is assumed to be 80%.<sup>22</sup> In this study, the acid hydrolysis yield adopts the experimental data of Wang et al. on kinetic modeling of sulfuric acid hydrolysis of kraft pulp.<sup>21</sup> To determine the CNC yield of acid hydrolysis, the acid hydrolysis reactions are modeled into three pathways. The first and dominant one is that cellulose is hydrolyzed to CNC; the second one is that CNC is further hydrolyzed to glucose, and a portion of glucose is further degraded to 5-hydroxymethylfurfural (HMF); the third one is that xylan is hydrolyzed to xylose and a portion of xylose is degraded to furfural.<sup>21</sup> The detailed information and kinetic constants are available in ESI Section S5. Based on the kinetic model, the conversion rate of cellulose to CNC in acid hydrolysis is 53.1%.<sup>21</sup> Then, the hydrolysate is transferred to the tank for dilution with Reverse

Osmosis (RO) water to reach 2% *wt* CNC concentration.<sup>15</sup> Then sodium chlorite is added for keeping the brightness at the load of 0.07% *wt* of CNC and mixed with the solution for 30 minutes.<sup>8</sup> The exiting gas is scrubbed by a 10% NaOH solution.<sup>8</sup> After this step, the acid solution is neutralized by adding 10% NaOH solution for around 40 minutes. The suspension goes through filtration to remove the remaining large particles. Then the stream is fed to the diafiltration process for 36 hours to remove sugars and salts.<sup>8</sup> The CNC concentration is maintained at 2% *wt*.<sup>15</sup> Then, the ultrafiltration system further purifies and concentrates the CNC to 8% *wt*.<sup>15</sup>

### **S2.3. Scenario CNC-1: waste prevention by using CaO for sulfuric acid neutralization.**

The unrecovered weak sulfuric acid solution (around 13% *wt* H<sub>2</sub>SO<sub>4</sub>) from the acid recovery step needs to be neutralized with NaOH to generate an effluent consisting of only Na<sub>2</sub>SO<sub>4</sub> and water. One possible improvement to prevent waste generation can be using CaO to produce gypsum as a byproduct, as shown in ESI Fig. S2. Additionally, based on the ecoinvent database, the environmental burdens of producing and distributing CaO are lower than NaOH when neutralizing the same amount of sulfuric acid.<sup>23</sup> After the neutralization, the solids and liquid are separated in the decanter, and then gypsum is assumed to be sold.<sup>15</sup>

### **S2.4. Scenario CNC-2: waste prevention by recovering acid.**

In the CNC baseline process and Scenario CNC-1, the hydrolysate with high acid concentration (around 58%) is finally neutralized without recovering the acid, which leads to a high neutralizing agent load and wastewater stream. Based on the Green Chemistry principle of waste prevention, the acid is recovered in this scenario.<sup>24</sup> ESI Fig. S3 shows the process flowchart of the scenario with recovering acid. This process is modified from the work by de Assis et al.<sup>15</sup>

In this scenario, the sulfuric acid hydrolysis conditions are the same as the CNC baseline. After the acid hydrolysis, the hydrolysate passes through three-stage centrifuges with RO water dilution (loading with the same amount as the stream fed in) in each stage to separate impurities (e.g.,  $\text{H}_2\text{SO}_4$ , glucose, unreacted cellulose).<sup>15</sup> The outflow contains 10% *wt* CNC suspension, while the other outlet stream mainly containing  $\text{H}_2\text{SO}_4$  and glucose is sent for acid recovery.<sup>15</sup> To recover the sulfuric acid and use it for acid hydrolysis, the acid recovery includes two steps, namely separating  $\text{H}_2\text{SO}_4$  from the hydrolysate and then concentrating the acid solution to 64% *wt*. The separation step uses electrodialysis with 90% recovery efficiency.<sup>25,26</sup> Electrodialysis has been examined as a method to recover sulfuric acid from the hydrolysate of lignocellulosic feedstocks.<sup>25,26</sup> Then, the separated sulfuric acid solution is evaporated in a three-effect evaporator to achieve 64% *wt* and sent back to the acid hydrolysis reactor.<sup>27</sup> The heat demand is met by the steam from the boiler. The unrecovered acid solution (mainly  $\text{H}_2\text{SO}_4$  and glucose) is neutralized with CaO before exiting as a waste stream.<sup>15</sup>

For the 10% *wt* CNC suspension after centrifuges, it passes through the same brightness-preserving and neutralizing process as the CNC baseline. After neutralizing, one more centrifuge is deployed to further reduce the  $\text{Na}_2\text{SO}_4$  concentration in the suspension.<sup>15</sup> Then, the stream goes through filtration and is diluted with RO water to 2% *wt*. The remaining unit operations, namely diafiltration and ultrafiltration, are the same as the CNC baseline.

### **S2.5. Scenario CNC-3: solvent change by using organic acid hydrolysis.**

To improve the environmental performance of CNC production based on Green Chemistry Principle 5 of solvent change, two possible alternative solvents have been identified in the previous literature: citric acid and subcritical water.<sup>10,28–31</sup>



Citric acid, a commodity chemical, has been widely used in many industries (e.g., food, cosmetics, chemical, and packaging) for a long time.<sup>32,33</sup> In this study, as shown in ESI Fig. S4, the major changes of Scenario CNC-3 in unit operations compared to Scenario CNC-2 occur in acid hydrolysis and acid recovery. In addition, this scenario yields both CNC and CNF, which is different from other scenarios studied for CNC. Citric acid hydrolysis is operated at 120 °C for 4.5 h with 60% *wt* citric acid fed in and 7% pulp consistency.<sup>10</sup> The conversion rates of cellulose in citric acid hydrolysis adopt the experimental data by Bodancia et al. and are 14.2% to CNC and 55.5% to CNF. After being separated in the centrifuges, the citric acid solution is sent for recovery. Several methods are identified in the literature for citric acid recovery, including the calcium precipitation method, solvent extraction method, and ion exchange recovery method.<sup>34</sup> This study chose the ion exchange recovery method that has the lowest environmental impact among the three methods based on the study by Wang et al.<sup>34</sup> Before ion exchange, the solution is diluted to reach around pH 2.<sup>35</sup> Anion resin column first removes most of the anions; then HCl is used to elute anion resins and desorb the citric acid. The recovery rate of citric acid is assumed to be 90%.<sup>34</sup> Weak citric acid solution is further evaporated to achieve 60% *wt* and sent back to acid hydrolysis. The unrecovered citric acid is further neutralized with CaO.

#### **S2.6. Scenario CNC-4: solvent change by using subcritical water hydrolysis.**

Other than using citric acid, subcritical water is proposed to be used by Novo et al.<sup>29,30</sup> ESI Fig. S5 shows the batch process flowchart. Subcritical water hydrolysis uses water as the hydrolyzing agent in a high-pressurized reactor.<sup>29</sup> The shredded pulp is hydrolyzed in subcritical water at 120 °C and 20.3 MPa for 60 minutes with 9% pulp consistency.<sup>30</sup> In this scenario, the yield data of CNC and glucose follow the experimental results of Novo et al.<sup>30</sup> 30% of cellulose is

hydrolyzed to CNC and 70% to glucose, while the degradation of the glucose is neglected.<sup>30</sup> The following purification steps are the same as Scenario CNC-1.

#### **S2.7. Scenario CNC-5: minimizing the impacts of energy requirements by using wood pellets.**

In previous scenarios (i.e., baseline and Scenarios CNC-1 to CNC-4), the energy source for the boiler is natural gas to generate steam for acid hydrolysis and acid recovery. To reduce the usage of fossil fuels, this scenario explores the situation of using the biomass solid fuel boiler by combusting wood pellets to provide the heat source.<sup>36,37</sup> The Lower Heating Value (LHV) of pellets (forest residue-based) is 20.1 MJ kg<sup>-1</sup> based on GREET 2021.<sup>38</sup> Other than the feeding fuel, the other unit operations and assumptions are the same as Scenario CNC-2.

#### **S2.8. Scenario CNC-6: minimizing the impacts of energy requirements by using renewable electricity.**

Upon the basis of Scenario CNC-5, this study further explores the impacts of using renewable electricity for the CNC plant. In Scenario CNC-6, onshore wind power is investigated. Note that this study assumes several wind farms are interconnected to be able to supply baseload power and increase the stability of the power supply.<sup>39,40</sup>

### **S3. CNF production**

#### **S3.1. Feedstock.**

In this study, the feedstock for CNF production is northern bleached softwood kraft (NBSK) pulp, a common type of pulp in the market.<sup>14</sup>

#### **S3.2. CNF baseline process.**

The baseline process of CNF production is designed based on the CNF pilot plant at the University of Maine,<sup>41,42</sup> the TEA study by de Assis et al.,<sup>14</sup> and the LCA study by Arvidsson et al.<sup>1</sup> The CNF baseline process uses mechanical treatment as shown in ESI Fig. S6. The NBSK pulp and water are mixed in the hydropulper to achieve 3% *wt* consistency.<sup>14</sup> Note that if the CNF plant is co-located with a pulp mill, the pulp can be supplied as 3% *wt* without drying the pulp.<sup>14</sup> Then, the suspension is transferred to a buffer tank and re-circulated to a dual-disk disk refiner. The disk refiner reduces the particle size to achieve 90% fines (length below 0.2 mm).<sup>14</sup> The heat exchanger is employed to cool down the re-circulating stream.<sup>14</sup> After disk refining, the gel-like suspension is diluted to 1% *wt*.<sup>43</sup> Then, the stream passes through the homogenization at 1,000 bar with one pass.<sup>43</sup> The energy consumption of homogenization is 10.7 kWh per dry kg fiber based on the experimental literature data.<sup>43</sup> Finally, the CNF is concentrated by ultrafiltration to derive the final product.

#### **S3.3. Scenario CNF-1: minimizing the impacts of energy requirements by enzymatic pretreatment.**

To reduce the energy consumption of CNF production, pretreatment of the pulp can be one solution. Two types of pretreatment methods have been identified in the literature, namely

enzymatic and chemical pretreatment.<sup>14,24</sup> For enzymatic pretreatment, endoglucanase (a type of cellulase) is commonly used to reduce the molecular weight of cellulose polymer, then assist in nanofibrillating the pulp.<sup>44</sup> For chemical pretreatment, 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO)-oxidated and carboxymethylation are currently the most studied routes.<sup>1,7,43,45</sup> However, using the carboxymethylation method may result in higher environmental impacts than enzymatic pretreatment or no pretreatment. For example, Arvidsson et al. conducted an LCA to compare three routes of producing CNF, i.e., no pretreatment, enzymatic pretreatment, and carboxymethylation pretreatment.<sup>1</sup> The life-cycle environmental impact results show that no pretreatment and enzymatic pretreatment routes had similar magnitude, and both were much lower (>60%) than the carboxymethylation pretreatment route.<sup>1</sup> For TEMPO-oxidated methods, a recent study shows much higher GWP of TEMPO-oxidated methods for CNF production than enzymatic hydrolysis method.<sup>13</sup> However, this study does not model TEMPO production given the lack of life cycle inventory data and impact assessment method for TEMPO. Additionally, some literature has expressed potential concerns about the high cost and low environmental feasibility of TEMPO-oxidated methods.<sup>43,46–48</sup> Hence, this study does not include TEMPO-oxidated method, instead, enzymatic pretreatment is chosen to compare with the CNF baseline process.

As shown in ESI Fig. S7, after the pulp shredder, the pulp is mixed with enzyme and buffer solution for enzymatic hydrolysis.<sup>1,13,44</sup> The enzyme used in this study is endoglucanase (0.17g per kg dry pulp); the acetate buffer solution (1 mM sodium acetate (derived from sodium carbonate and acetic acid) and acetic acid ensures the hydrolysis efficiency at pH 5.<sup>1,49,50</sup> The pulp consistency is controlled at 2% *wt.*<sup>44</sup> The enzymatic hydrolysis is operated at 50 °C for 2-hour incubation and 80°C for 30-minute denaturation<sup>1</sup>. Then, the pulp is washed twice to remove the impurities.<sup>1,44</sup> The fiber loss, due to the degradation and loss of fines in washing, is assumed 6%

based on the literature data.<sup>49</sup> After the enzymatic hydrolysis, the pulp is diluted to 1% *wt* for disk refining and microfluidization. The electricity consumption of microfluidization is 2.2 kWh per dry kg fiber inflow.<sup>1</sup>

#### **S3.4. Scenario CNF-2: minimizing the impacts of energy requirements by using wood pellets.**

Similar to the improvement in Scenario CNC-5, this scenario explores the usage of renewable solid fuel instead of using natural gas. The fuel source is wood pellets to provide heat for enzymatic hydrolysis.<sup>36,37</sup> All the other unit operations and processes are the same as Scenario CNF-1.

#### **S3.5. Scenario CNF-3: minimizing the impacts of energy requirements by using renewable electricity.**

As mentioned above, the high energy consumption of CNF production is unfavorable.<sup>1</sup> Based on Scenario CNF-2 using enzymatic hydrolysis and renewable fuel, Scenario CNF-3 uses renewable electricity. Similar to Scenario CNC-6, onshore wind power is assumed to provide power in this study.

#### S4. Technical performance of CNC and CNF scenarios

The input and output results of the CNC plant at 50 dry t of nanocellulose per day are summarized in ESI Table S1. Due to the different final yields of nanocellulose materials, feedstock inputs vary by scenario. Scenario CNC-4 requires the highest quantity of feedstock, 176 dry t day<sup>-1</sup>, because of the lowest subcritical water hydrolysis yields 30% of CNC from cellulose, compared to 53.1% yield for the sulfuric acid and 69.7% (CNC and CNF) for the citric acid scenarios.<sup>30</sup> The scenario with the lowest feedstock demand is CNC-3. The other scenarios have minor differences in feedstock demand because they share the same acid hydrolysis settings and conversion rate. CNC baseline consumes a high amount of sulfuric acid (536 t day<sup>-1</sup>) and NaOH (438 t day<sup>-1</sup>) used to neutralize the sulfuric acid. At the same time, due to Na<sub>2</sub>SO<sub>4</sub> that generated by neutralization and finally passes through the RO system, the water demand and power consumption are 23.5%–424.1% and 36.4%–100.0% higher than other scenarios, respectively. Changing the neutralizing agent to CaO in Scenario CNC-1 largely reduces the water demand (from 10,083 to 1,924 t day<sup>-1</sup>) and power consumption (from 341,935 to 232,884 kWh day<sup>-1</sup>). This is because of CaSO<sub>4</sub> that can be easily filtered out to be sold as a byproduct, making the salt concentration of the flow entering the RO system much lower than the CNC baseline. However, the sulfuric acid load in Scenario CNC-1 is still high since no acid is recovered. To overcome this disadvantage, Scenario CNC-2 recovers sulfuric acid and evaporates the acid back to 64% for acid hydrolysis. Hence, compared to Scenario CNC-1, Scenario CNC-2 reduces 84.3% of the sulfuric acid consumption to 84 t day<sup>-1</sup>. It should be noted that due to the evaporation in acid recovery, natural gas consumption significantly increases from 1 t day<sup>-1</sup> (Scenario CNC-1) to 29 t day<sup>-1</sup> (Scenario CNC-2). At the same time, since more steps in separation and purification are deployed, water consumption increases by 19.7%.

Scenario CNC-3 changes sulfuric acid to citric acid and shows higher usage in water and electricity, when compared to CNC-2. This is majorly due to the acid recovery process where the citric acid solution needs to be diluted and then desorbed by using HCl solution. At the same time, the increased water usage enlarges the electricity consumption in the RO system. Other than using citric acid, this study also explores the subcritical water hydrolysis in Scenario CNC-4, where only water is used for hydrolysis. As mentioned above, due to the relatively lower CNC yield in the hydrolysis, the feedstock pulp demand in Scenario CNC-4 is the highest among all scenarios. However, Scenario CNC-4 employs a simpler process with fewer unit operations, lowering the power consumption (18.6%–50.0% lower than the other scenarios).

Scenario CNC-5 alternates the fuel source from natural gas in Scenario CNC-2 to wood pellets (68 dry t pellets day<sup>-1</sup>), while the other inputs and outputs stay the same as in Scenario CNC-2. To further reduce the potential GHG emissions, Scenario CNC-6 switches to wind power instead of typical grid power based on fossil energy. Hence, the input and output values in Scenarios CNC-5 and CNC-6 are the same.

For CNF, the inputs and output results for CNF scenarios are shown in ESI Table S2. CNF baseline adopts the pure mechanical treatment method and has the highest power consumption 729,883 kWh day<sup>-1</sup> (14.6 kWh dry kg<sup>-1</sup> CNF). The largest contributor to power consumption is homogenization (accounting for 73%) which is the last step of producing homogenized CNF suspension. As mentioned above, Scenario CNF-1 deploys enzymatic hydrolysis pretreatment to reduce energy consumption in the following mechanical treatment steps. As shown in ESI Table S2, Scenario CNF-1 reduces the power consumption by 55.7% to 322,925 kWh day<sup>-1</sup>. However, it is worth noticing that the water demand increases from 570 t day<sup>-1</sup> to 3,663 t day<sup>-1</sup>, caused by the added unit operations included in the enzymatic hydrolysis, washing, and dilution steps.

Natural gas is needed in Scenario CNF-1 to provide heat for the whole enzymatic hydrolysis process. In Scenario CNF-1, the material input of the enzyme and the chemicals for the buffer solution is relatively small.

To decarbonize the process, Scenario CNF-2 switches the fossil fuel to wood pellets; Scenario CNF-3 adopts wind power. Hence, Scenarios CNF-1, -2, and -3 share the same inputs and outputs (other than natural gas and wood pellets).



## S5. Sulfuric acid hydrolysis for CNC production

As shown in ESI Fig. S13, there are six rate constants of the modeled kinetics in sulfuric acid hydrolysis of pulp based on the work by Wang et al.<sup>21</sup> Then by applying first-order kinetics, cellulose reactions can be modeled as:

$$-\frac{dC_{Cellulose}}{dt} = (k_1 + k_3)(C_{Cellulose} - C_{Cellulose0}(1 - \gamma)) \quad (1)$$

$$\frac{dC_{CNC}}{dt} = k_1 C_{Cellulose} - k_2 C_{CNC} \quad (2)$$

$$\frac{dC_{Glucose}}{dt} = 1.111k_2 C_{CNC} + 1.111k_3 C_{Cellulose} - k_4 C_{Glucose} \quad (3)$$

$$\frac{dC_{HMF}}{dt} = 1.428k_4 C_{Glucose} \quad (4)$$

In eqn 1–4,  $C_{Cellulose}$ ,  $C_{CNC}$ ,  $C_{Glucose}$ ,  $C_{HMF}$  is the concentration (g L<sup>-1</sup>) of cellulose, CNC, glucose, and HMF, respectively;  $C_{Cellulose0}$  the initial value of  $C_{Cellulose}$ ;  $\gamma$  the fraction of cellulose that is depolymerized and equals 1 in this condition based on Wang et al.<sup>21</sup>  $k_1$ – $k_4$  (min<sup>-1</sup>) are the rate constants of the reactions shown in Fig. S13. The values for the sulfuric acid hydrolysis in this study (45 °C and 64% wt H<sub>2</sub>SO<sub>4</sub>) are  $k_1$ : 0.0334,  $k_2$ : 0.0068,  $k_3$ : 0.0107,  $k_4$ : 0.0034.

The kinetics related to hemicellulose reactions can be modeled as:

$$-\frac{dX_{h\_Xylan}}{dt} = k_5 X_{h\_Xylan} \quad (5)$$

$$X_{h\_Xylan} = X_{Xylan} - X_{Xylan0}(1 - \delta_X) \quad (6)$$

$$\frac{dX_{Xylose}}{dt} = 1.136k_5 X_{h\_Xylan} - k_6 X_{Xylose} \quad (7)$$

$$\frac{dX_{Furfural}}{dt} = k_6 X_{Xylose} \quad (8)$$

In eqn 5–8,  $X_{h\_Xylan}$ ,  $X_{Xylan}$ ,  $X_{Xylan0}$ ,  $X_{Xylose}$ ,  $X_{Furfural}$  is the concentration (g L<sup>-1</sup>) of hydrolysable xylan, xylan, initial xylan, xylose, and furfural, respectively;  $\delta_X$  is the fraction of hydrolysable xylan - 0.6836 according to Wang et al.;<sup>21</sup>  $k_5$  and  $k_6$  are rate constants of reactions shown in ESI Fig. S13 and their values are:  $k_5$ : 0.2200,  $k_6$ : 0.0009.<sup>21</sup>

## S6. CNC and CNF Landfilling

Based on the Intergovernmental Panel on Climate Change (IPCC) First Order Decay method,<sup>51,52</sup> eqn 9 and 10 show the method of quantifying methane emission from landfilling<sup>51</sup>.

$$C_{decomposed} = W \cdot DOC \cdot DOC_f \cdot (1 - e^{-kt}) \quad (9)$$

$$CH_4_{generated} = [(C_{decomposed} \cdot MCF \cdot F \cdot 16/12) \cdot (1 - R_p)] \cdot (1 - OX) \quad (10)$$

In eqn 9,  $C_{decomposed}$  is the accumulative decomposed carbon mass from year 0 to year  $t$ .  $W$  is the mass of deposited nanocellulose waste;  $DOC$  is degradable organic carbon of nanocellulose waste;  $DOC_f$  is the fraction of  $DOC$  that can decompose;  $k$  is the landfill decay rate.<sup>53</sup> In eqn 10,  $MCF$  is the  $CH_4$  correction factor which is determined by the site management;<sup>51</sup>  $F$  is the volume fraction of  $CH_4$  in landfill gas;  $R_p$  is the total recovered  $CH_4$  portion by energy recover device,<sup>53</sup> which is 0.75 (meaning 75% of methane is recovered) based on the review work by Anshassi et al.<sup>54</sup>  $OX$  is the average oxidation factor describing the fraction of oxidized methane.<sup>53</sup> After the  $CH_4$  emission is determined,  $CO_2$  emission is quantified using the experimental data on the volume rate of  $CH_4$  (before being recovered) to  $CO_2$ .<sup>55</sup> Then the recovered landfill gas is combusted to generate power. The generated power is calculated based on the total LHV of recovered landfill gas and electricity generation efficiency.<sup>54</sup> The values of the parameters are recorded in ESI Table S3.

## S7. Life cycle assessment methodology

In this study, the mass-based functional unit is 1 dry kg of cellulose nanomaterials produced. This study includes another functional unit to consider material performance that is important to decision-making in material synthesis and manufacturing. The study specifically chose specific tensile strength for CNC- and CNF-derived film,<sup>56,57</sup> but the framework is broadly applicable to other material performance indicators (e.g., elastic modulus, yield strength, stiffness). Examples can be found in the Ashby material selection framework and other adapted frameworks.<sup>58–60</sup>

Eqn 11 describes the conversion between the mass-based functional unit and the performance-based functional unit.  $EL_i^j$  (per dry kg) is the environmental impacts of 1 dry kg cellulose nanomaterials in impact category  $j$  for material  $i$ ;  $EL_i^j$  (per MPa per m<sup>3</sup>) is the environmental impact in the performance-based functional unit;  $\rho_i$  is the density of material  $i$ ;  $\sigma_i$  is the tensile strength of material  $i$ .

$$EL_i^j = EL_i^j \times \frac{\rho_i}{\sigma_i} \quad (11)$$

The density of the CNC film is 1,600 kg m<sup>-3</sup> (1.6 g cm<sup>-3</sup>).<sup>61</sup> The tensile strength for CNC film derived from sulfuric acid hydrolysis (i.e., baseline, CNC-1, CNC-2, CNC-5, CNC-6) was measured as 70 MPa;<sup>62</sup> the tensile strength for citric acid hydrolysis scenario (CNC-3) was measured as 107 MPa.<sup>28</sup> The tensile strength of CNC film for CNC-4 is not available in the literature. Hence, the results of the performance-based functional unit for CNC-4 are not included in this study and can be included in future research when the data is available. The density of the CNF film is 1,500 kg m<sup>-3</sup> (1.5 g cm<sup>-3</sup>).<sup>48</sup> The tensile strength for CNF film derived from mechanical refining (i.e., baseline) was measured as 153 MPa;<sup>48</sup> the tensile strength for citric acid hydrolysis scenario (i.e., CNF-1, CNF-2, CNF-3) was measured as 107 MPa.<sup>48</sup>



## S8. Capital expenditures for cellulose nanomaterial production

The total capital investment in each scenario includes total installed equipment cost, other direct costs, indirect cost, land, and working capital. Total installed equipment cost sums up the installed equipment costs that are calculated by multiplying purchased costs with installation factors, as shown in eqn 12.

$$\text{Installed cost} = \text{Purchased cost} \times \text{Installation factor} \quad (12)$$

As shown in eqn 13, scaling factors were used to scale the purchased costs found in the literature to the equipment capacities explored in this study. To adjust the year of equipment purchased costs to 2020, plant cost indices by Chemical Engineering Magazine are used.<sup>63</sup>

$$\begin{aligned} \text{Purchased cost} \\ = \text{Original purchased cost} \times \frac{\text{Plant cost index in 2020}}{\text{Plant cost index in the year of collected literature}} \times \left( \frac{\text{Equipment capacity in this study}}{\text{Original equipment capacity}} \right) \end{aligned} \quad (13)$$

The installed costs (2020 US\$) of each scenario 50 dry t nanocellulose produced per day are shown in ESI Tables S11 and S12. Other direct costs, including warehouse, site development, and additional piping, are shown in ESI Table S8). Indirect costs contain prorated expenses, field expenses, office and construction fees, project contingency, and other costs. ESI Table S8 shows the assumptions for project costs.

## S9. Operating expenditures for cellulose nanomaterial production

The operating expenditures in this study contain variable operating costs (e.g., feedstocks, materials, waste stream charges, byproduct credits) and fixed operating costs (e.g., labor cost, maintenance, insurance). For variable operating costs, the prices of feedstocks, materials, waste stream charges, and fuels were collected from the literature and shown in ESI Table S15. The Producer Price Index for chemical manufacturing is used to adjust the original prices to 2020 in this study.<sup>64</sup> For fixed operating costs, ESI Table S16 shows the labor cost at 50 dry t nanocellulose produced per day for each case. The positions and salaries are based on the report by the U.S. National Renewable Energy Laboratory.<sup>65</sup> The CNC and CNF plants are operated based on 3 shifts per day. The benefits and overhead are assumed to be 90% of the total salaries.<sup>65</sup> To adjust the salaries to 2020, the labor index from the Bureau of Labor Statistics is used.<sup>66</sup> As shown in eqn 14, the labor cost scaling factor (0.23) from the literature is used to adjust the number of shift operators in varied plant capacities.<sup>67</sup> Note that the number of shift operators per shift is rounded up to be an integer. The other positions (e.g., plant manager, shift supervisor) are assumed to be fixed for varied plant capacities. Other fixed operating costs cover plant maintenance and property insurance, assuming 3.7% of fixed capital investment.<sup>68</sup>

*Shift operators*

$$= 3 \times [(shift\ operators\ in\ reference\ plant\ capacity)/3] \times \left( \frac{New\ plant\ capacity}{Reference\ plant\ capacity} \right)^{Labor\ cost\ scaling\ factor}$$

(14)

## S10. Sensitivity analysis for cellulose nanomaterials

To identify the key drivers of the economic and environmental performance of CNC and CNF, this study includes a sensitivity analysis. The indicators chosen in sensitivity analysis are GWP and MSP, which are commonly reported in the literature for bio-based materials.<sup>69,70</sup> The processes for the sensitivity analysis are selected as the middle-road scenarios: Scenario CNC-2 (CaO with H<sub>2</sub>SO<sub>4</sub> recovery) and Scenario CNF-1 (enzymatic hydrolysis). There are two steps in the sensitivity analysis: 1) varying the parameters by  $\pm 50\%$  and omitting the parameters with less than 2% impact on results; 2) varying the parameters by the ranges that are collected from the literature or assumed if no data available (see ESI Table S19 for details of the ranges) and omitting the parameter with less than 2% impact on results.

ESI Fig. S9 shows the sensitivity analysis results for Scenario CNC-2 at 50 dry t day<sup>-1</sup>. In ESI Fig. S9, pulp consistency in acid hydrolysis shows the largest impacts on GWP and MSP. The key reason is that lower pulp consistency in acid hydrolysis directly leads to higher acid and neutralizing agent usage. At the same time, lower pulp consistency in acid hydrolysis reduces the stream volumes in acid recovery (lower capital investment) and natural gas usage in evaporating acid solution. CNC conversion rate is the second largest influencer on GWP and the third largest influencer on MSP. Hence, increasing the pulp consistency in acid hydrolysis and the CNC conversion rate can be the priority in future research in reducing GWP and MSP of CNC. CNC consistency in dilution also shows large impacts on GWP since the dilution water load decides the water demand and the electricity consumption of the reverse osmosis system. Increasing the landfill gas recovery rate from 75% to 90% decreases the GWP by 7.3% to 6.0 kgCO<sub>2</sub>e per kg dry CNC due to the high GWP factor of CH<sub>4</sub> (27.0 for biogenic methane).<sup>71</sup> Varying electricity consumption and electricity GHG emissions show impacts of  $\pm 7.2\%$  and  $\pm 5.5\%$  on GWP,



respectively. This is also highlighted by comparing Scenario CNC-6 (wind power) with Scenario CNC-5. Besides these parameters, since feedstock is a major contribution to MSP and GWP, varying the pulp cost exhibits a  $\pm 7.0\%$  effect on MSP; varying the cradle-to-gate GHG of pulp displays a  $\pm 5.6\%$  impact on total GWP results.

In ESI Fig. S9b, the internal rate of return (IRR) and the plant capacity show large impacts on MSP. Larger plant capacity decreases MSP (see ESI Table S21) due to the economy of scale, which has been commonly shown in previous TEA literature.<sup>72</sup> The cost of electricity, pulp, and natural gas also shows a large increasing effect on MSP. Since the capital investment in the equipment of acid hydrolysis and boiler system is the highest across all areas (see ESI Table S11), the installed costs of these two areas show  $\pm 5.1\%$  and  $\pm 2.3\%$  effects on MSP, respectively.

ESI Fig. S11 shows the sensitivity analysis results of Scenario CNF-2 at 50 dry t day<sup>-1</sup>. Similar to the sensitivity analysis results of Scenario CNC-2, pulp consistency in enzymatic hydrolysis shows the largest impact on GWP and the fourth largest impact on MSP as it determines the water consumption, energy consumption (heat for hydrolysis and electricity in hydrolysis and purification), and capital investment (by affecting equipment size). The landfill gas recovery rate is another important driver for GWP. Landfill gas recovery rate is the second largest impactor that varies the GWP from 4.9 to 5.2 kgCO<sub>2</sub>e per dry kg CNF. Electricity consumption and electricity GHG emissions are another two major influencers. Unlike CNC production that is affected largely by CNC conversion rate, the CNF yield of Scenario CNF-1 only shows  $\pm 4\%$  impact on GWP due to low cellulose degradation and loss (6%). For MSP, plant capacity, IRR, pulp consistency in enzymatic hydrolysis all show large impacts, similar to CNC. As the upper limit of electricity cost is high (see ESI Table S19) and energy cost is a major contributor, electricity cost is the third largest driver for MSP variation. The installed cost of the boiler system and pretreatment,

electricity consumption, and CNF yield show less than 5% impacts on MSP.

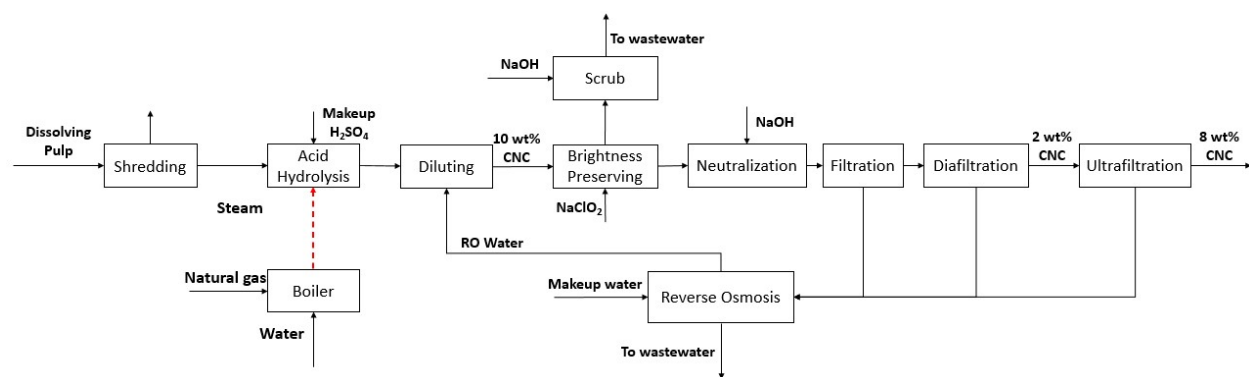


Fig. S1. Process flowchart of the baseline.

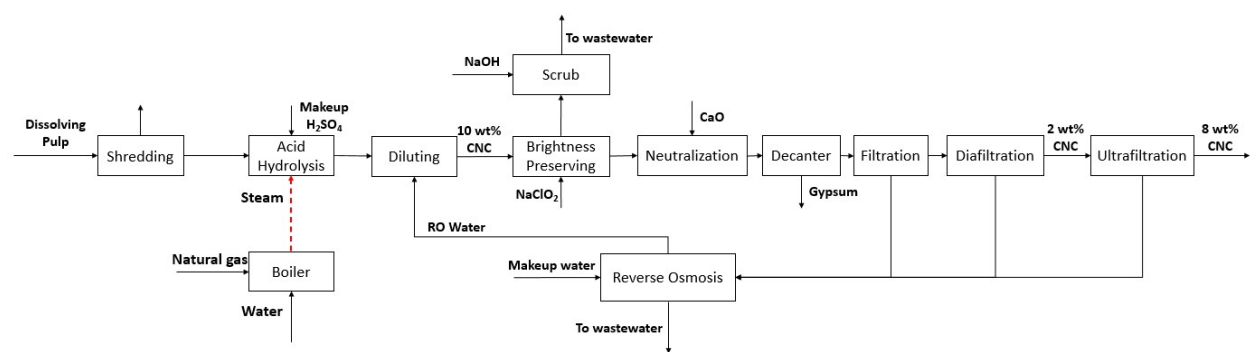


Fig. S2. Process flowchart of Scenario CNC-1.

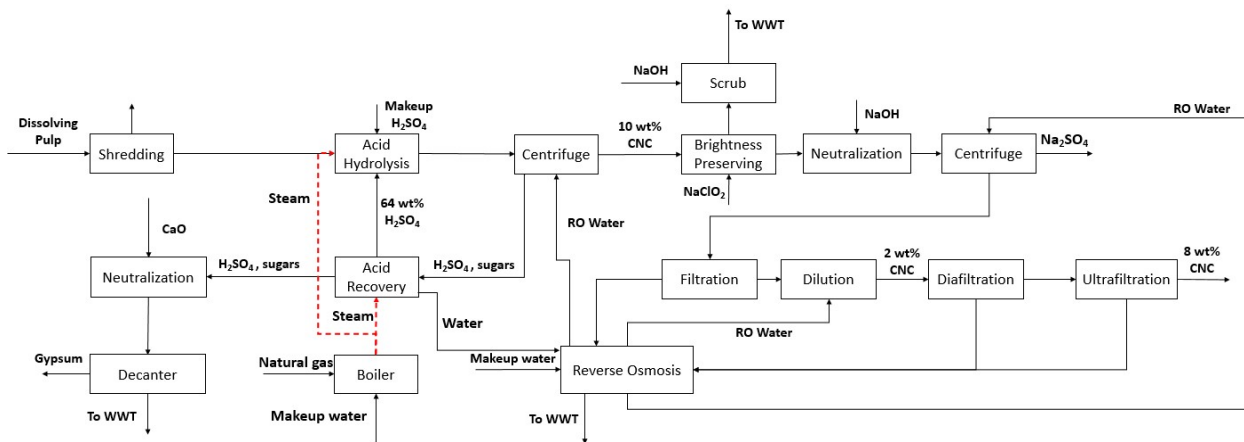


Fig. S3. Process flowchart of Scenario CNC-2.

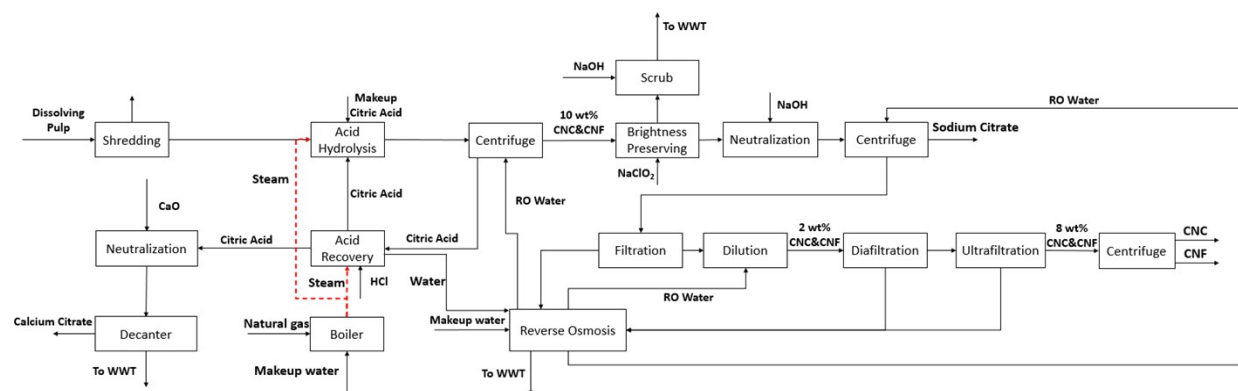


Fig. S4. Process flowchart of Scenario CNC-3.

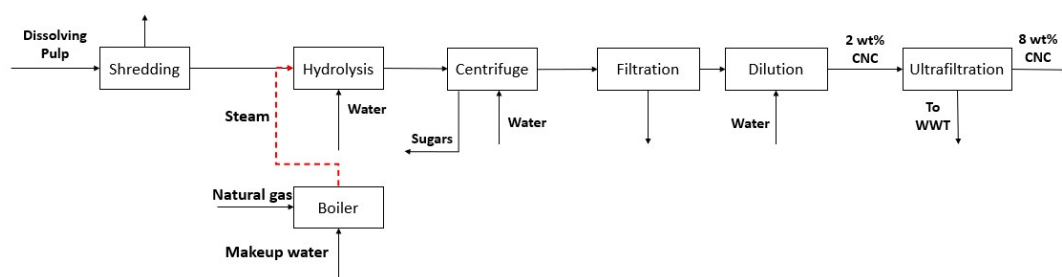


Fig. S5. Process flowchart of Scenario CNC-4.

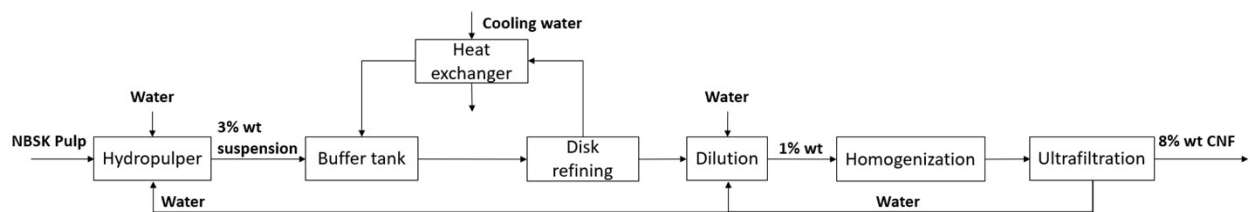


Fig. S6. Process flowchart of CNF baseline process.



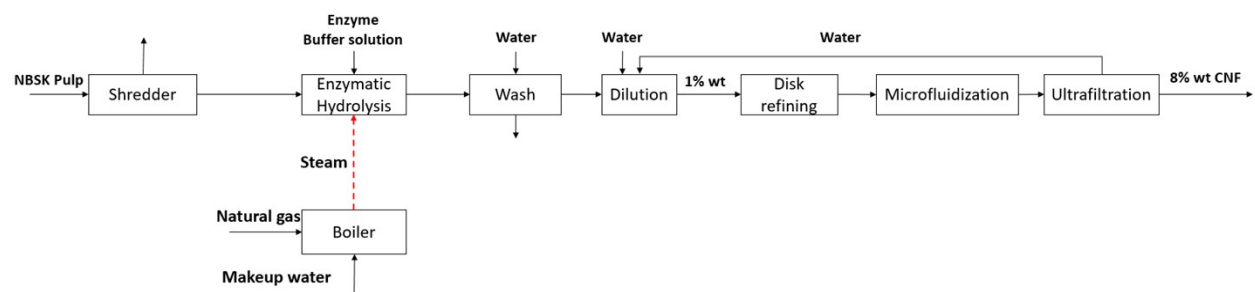


Fig. S7. Process flowchart of Scenario CNF-1.

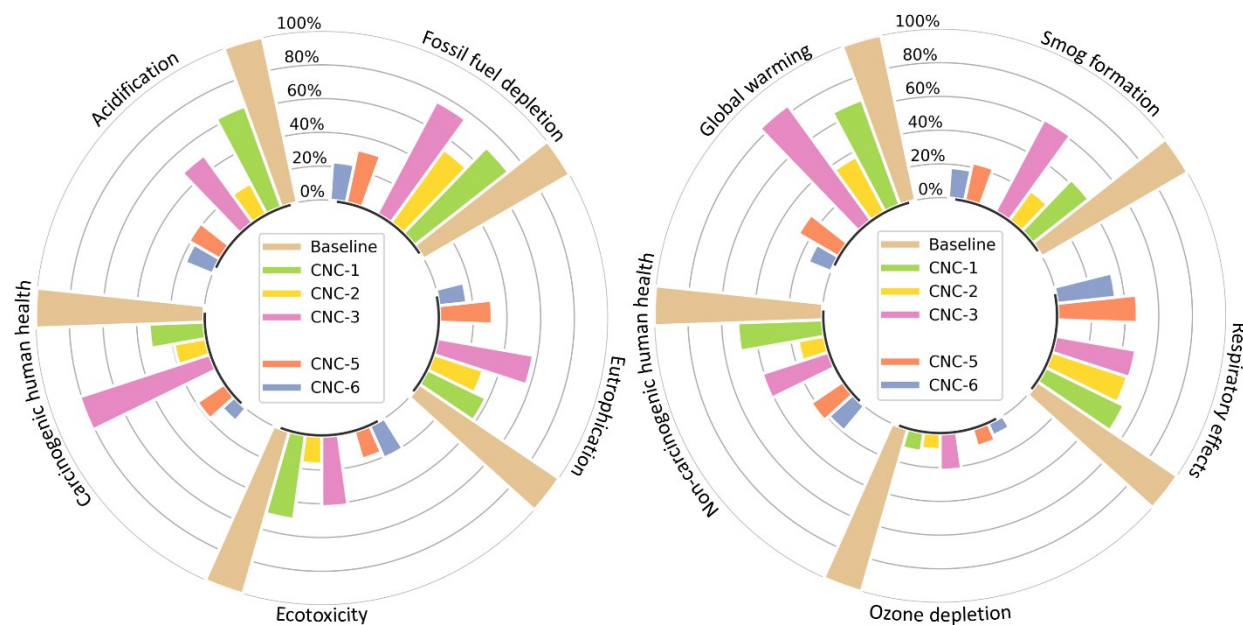


Fig. S8. The normalized life-cycle environmental impacts of CNC in the performance-based functional unit (per MPa per m<sup>3</sup>). CNC baseline: sulfuric acid for hydrolysis and NaOH for neutralization without acid recovery; Scenario CNC-1: sulfuric acid for hydrolysis and CaO for neutralization without acid recovery; Scenario CNC-2: sulfuric acid for hydrolysis and CaO for neutralization with acid recovery; Scenario CNC-3: citric acid for hydrolysis and CaO for neutralization with acid recovery; Scenario CNC-5: combusting wood pellets, all other conditions same as Scenario CNC-2; Scenario CNC-6: wind power, all other conditions same as Scenario CNC-5. Note that Scenario CNC-4 is shown due to the lack of material performance data.

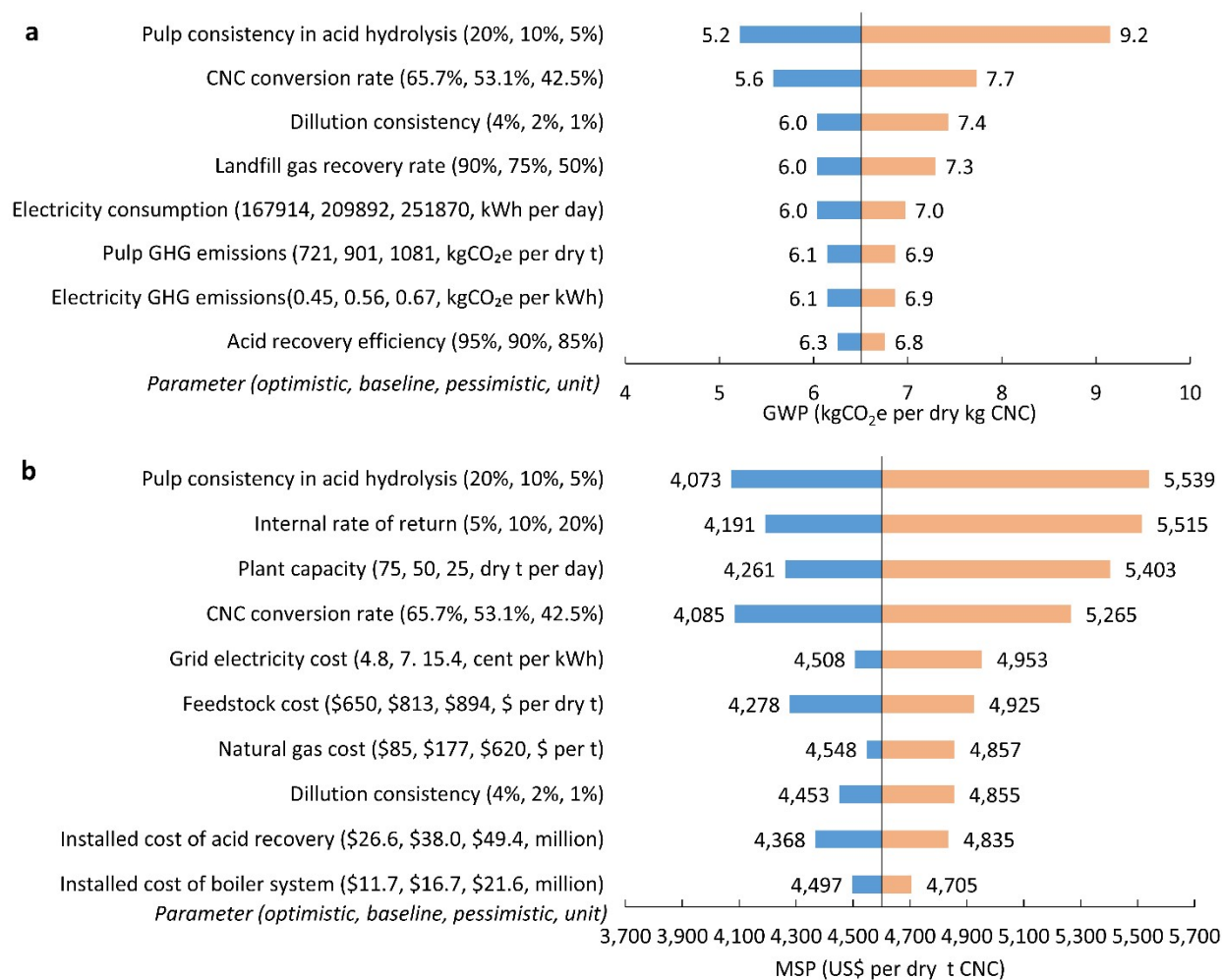


Fig. S9. Sensitivity analysis results of Scenario CNC-2 at 50 dry t day<sup>-1</sup>. a, global warming potential; b, minimum selling price.

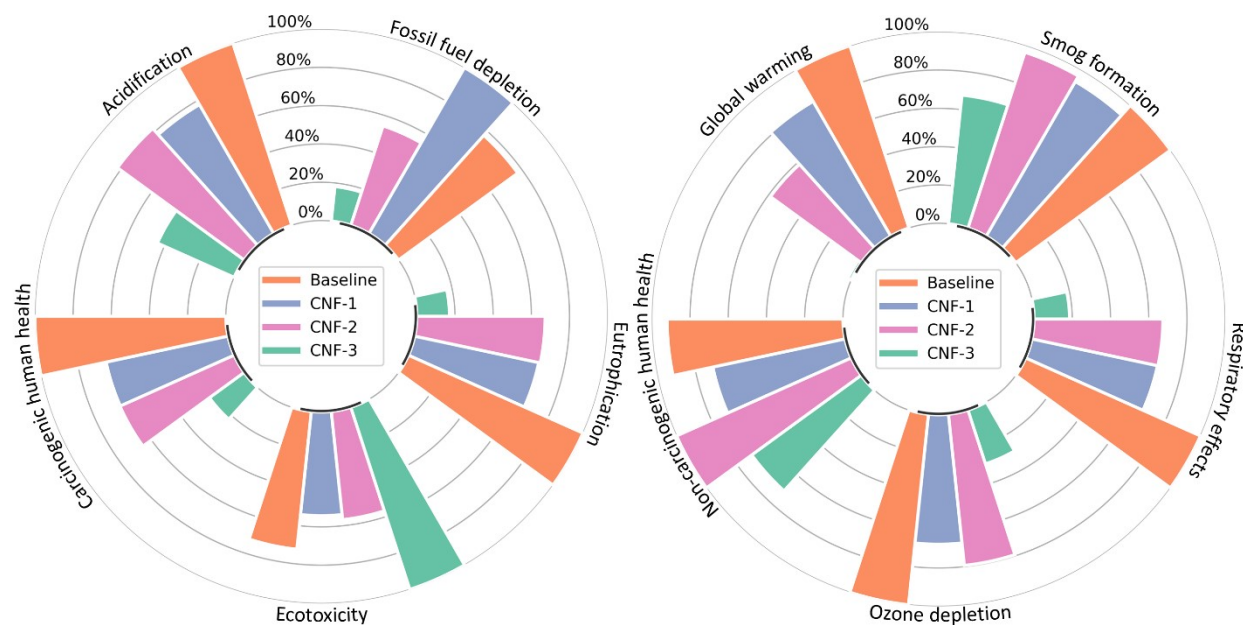


Fig. S10. The normalized life-cycle environmental impacts of CNF in the performance-based functional unit (per MPa per m<sup>3</sup>). CNF baseline: mechanical treatment; Scenario CNF-1: enzymatic hydrolysis as the pretreatment; Scenario CNF-2: combusting wood pellets, other settings are the same as Scenario CNF-1; Scenario CNF-3: wind power, other settings are the same with Scenario CNF-2.

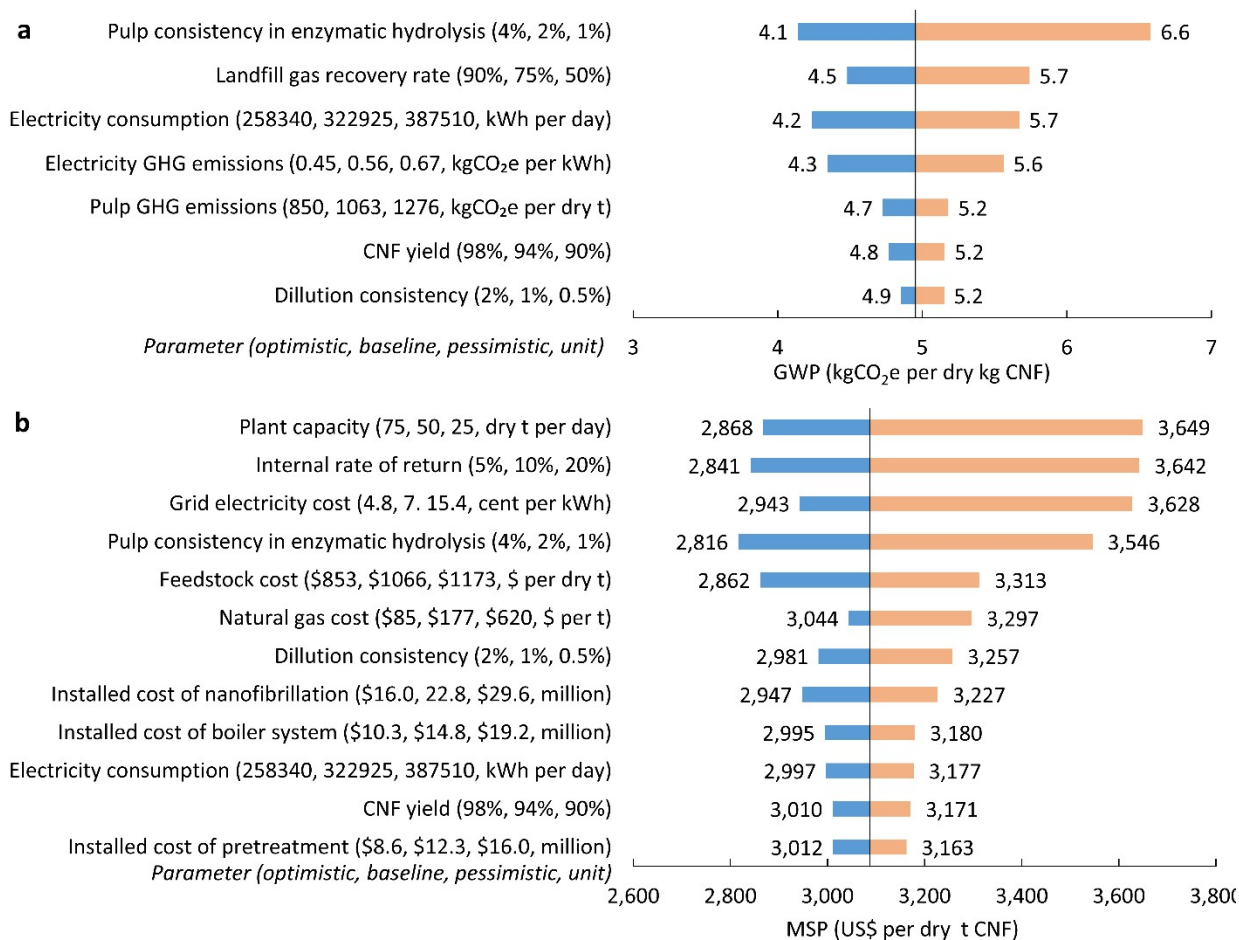


Fig. S11. Sensitivity analysis results of Scenario CNF-1 at 50 dry t day<sup>-1</sup>. a, global warming potential; b, minimum selling price.

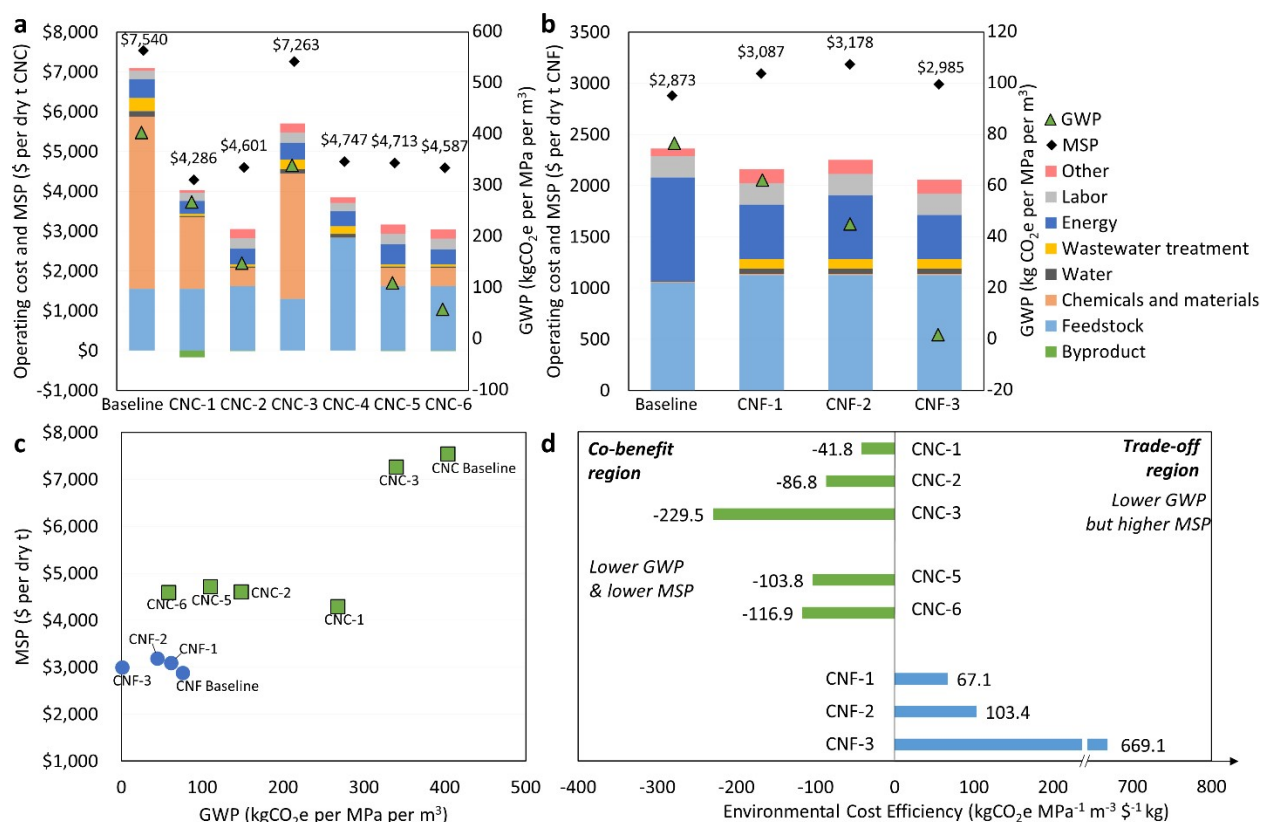


Fig. S12. Minimum selling price, operating cost, global warming potentials (in the performance-based functional unit, per MPa per m<sup>3</sup>), and eco-efficiency analysis results of scenarios at 50 dry t day<sup>-1</sup>. a, cellulose nanocrystal scenarios. b, cellulose nanofibril scenarios. c, minimum selling price and GWP in all scenarios. d, environmental cost efficiency results of scenarios compared to the baseline.

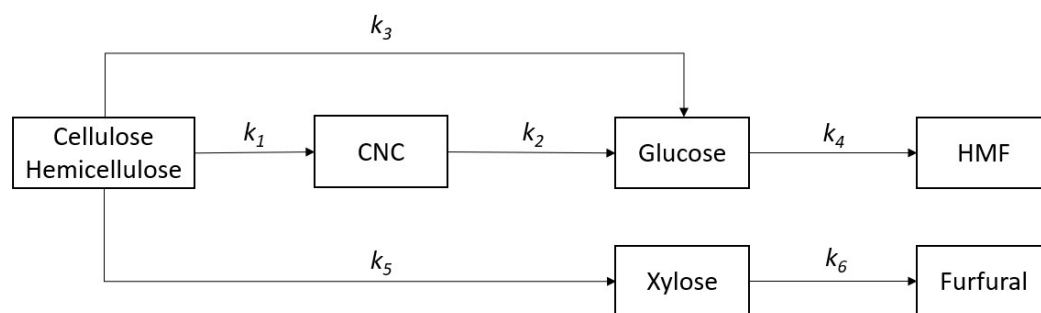


Fig. S13. Reaction pathways for sulfuric acid hydrolysis of dissolving pulp.

**Table S1.** Summarized input and output results for CNC scenarios.

Item	Unit	CNC Baseline	CNC-1 CaO	CNC-2 Acid recovery	CNC-3 Citric acid	CNC-4 Subcritical water	CNC-5 Wood pellets	CNC-6 Wind power
<b><i>Input</i></b>								
Dissolving pulp	dry t day <sup>-1</sup>	96	97	101	81	176	101	101
Sulfuric acid	t day <sup>-1</sup>	536	537	84	N/A	N/A	84	84
Citric acid	t day <sup>-1</sup>	N/A	N/A	N/A	96	N/A	N/A	N/A
NaOH	t day <sup>-1</sup>	438	0	26	20	N/A	26	26
NaClO <sub>2</sub>	kg day <sup>-1</sup>	125	125	130	104	N/A	130	130
CaO	t day <sup>-1</sup>	N/A	307	30	112	N/A	30	30
Natural gas	t day <sup>-1</sup>	1	1	29	22	40	N/A	N/A
HCl	t day <sup>-1</sup>	N/A	N/A	N/A	110	N/A	N/A	N/A
Makeup water	t day <sup>-1</sup>	10,083	1,924	2,302	8,167	6,914	2,302	2,302
Electricity	kWh day <sup>-1</sup>	341,935	232,884	209,893	250,691	170,932	209,893	209,893
Wood pellets	dry t day <sup>-1</sup>	N/A	N/A	N/A	N/A	N/A	68	68
<b><i>Output</i></b>								
CNC	dry t day <sup>-1</sup>	50	50	50	13	50	50	50
CNF	t day <sup>-1</sup>	N/A	N/A	N/A	37	N/A	N/A	N/A
Gypsum	t day <sup>-1</sup>	N/A	745	73	N/A	N/A	73	73
WWT	t day <sup>-1</sup>	10,537	1,501	1,852	9,044	6,474	1,852	1,852



**Table S2.** Summarized input and output results for CNF scenarios.

Item	Unit	CNF Baseline	CNF-1 Enzymatic hydrolysis	CNF-2 Wood pellets	CNF-3 Wind power
<b><i>Input</i></b>					
NBSK pulp	dry t day <sup>-1</sup>	50	53	53	53
Enzyme	kg day <sup>-1</sup>	N/A	9	9	9
Sodium carbonate	kg day <sup>-1</sup>	N/A	138	138	138
Acetate acid	kg day <sup>-1</sup>	N/A	158	158	158
Natural gas	t day <sup>-1</sup>	N/A	24	N/A	N/A
Makeup water	t day <sup>-1</sup>	570	3,663	3,663	3,663
Electricity	kWh day <sup>-1</sup>	729,883	322,925	322,925	322,925
Wood pellets	dry t day <sup>-1</sup>	N/A	N/A	56	56
<b><i>Output</i></b>					
CNF	dry t day <sup>-1</sup>	50	50	50	50
WWT	t day <sup>-1</sup>		3,092	3,092	3,092

**Table S3.** Parameter values for landfill and landfill gas recovery.

Parameter	Unit	Value
Fraction of degradable organic carbon that can decompose, $DOC_f$ <sup>51,53,73,74</sup>		0.7
Methane correction factor, $MCF$ <sup>51,53,73,74</sup>		0.75
Volume fraction of methane in landfill gas, $F$ <sup>51,53,73,74</sup>		0.50
Average oxidation factor, $OX$ <sup>51,53,73,74</sup>		0.1
Landfill decay rate, $k$ <sup>51–53,73,74</sup>		0.02
Volume rate of CH <sub>4</sub> to CO <sub>2</sub> in landfill gas emissions <sup>55</sup>		1.60
Landfill gas recovery efficiency <sup>54</sup>	%	75
Power generation efficiency by landfill gas incineration <sup>54</sup>	%	30

**Table S4.** Ecoinvent processes used in this study.

<b>Product</b>	<b>Process name<sup>23</sup></b>
Hydrogen peroxide	hydrogen peroxide production, product in 50% solution state   hydrogen peroxide, without water, in 50% solution state   Cutoff, U_RoW
Electricity	market group for electricity, high voltage   electricity, high voltage   Cutoff, U_US
Sulfuric acid	market for sulfuric acid   sulfuric acid   Cutoff, U_RoW
Transportation	market for transport, freight train   transport, freight train   Cutoff, U_US
Electricity	electricity production, wind, >3MW turbine, onshore   electricity, high voltage   Cutoff, U_US
Citric acid	market for citric acid   citric acid   Cutoff, U_GLO
Gypsum	market for gypsum, mineral   gypsum, mineral   Cutoff, U_RoW
Wastewater treatment	treatment of wastewater, average, capacity 1E9l/year   wastewater, average   Cutoff, U_RoW
Calcium oxide	quicklime production, in pieces, loose   quicklime, in pieces, loose   Cutoff, U_RoW
Wood pellet	wood pellet production   wood pellet, measured as dry mass   Cutoff, U_RoW
Sodium hydroxide	market for sodium hydroxide, without water, in 50% solution state   sodium hydroxide, without water, in 50% solution state   Cutoff, U_GLO
Sodium chlorate	sodium chlorate production, powder   sodium chlorate, powder   Cutoff, U_RoW
Tap water	market for tap water   tap water   Cutoff, U_RoW
Natural gas	natural gas production   natural gas, high pressure   Cutoff, U_US
Magnesium sulfate	market for magnesium sulfate   magnesium sulfate   Cutoff, U_GLO
Methanol	market for methanol   methanol   Cutoff, U_GLO
Oxygen	market for oxygen, liquid   oxygen, liquid   Cutoff, U_RoW
Diesel	market for diesel, low-sulfur   diesel, low-sulfur   Cutoff, U_RoW
Sodium perchlorate	sodium perchlorate production   sodium perchlorate   Cutoff, U_GLO
Pulp wood	softwood forestry, spruce, sustainable forest management   pulpwood, softwood, measured as solid wood under bark   Cutoff, U_RoW
Enzyme	enzymes production   enzymes   Cutoff, U_RoW
Deionized water	market for water, deionised   water, deionised   Cutoff, U_RoW
Acetic acid	market for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U
Sodium Carbonate	market for soda ash, light, crystalline, heptahydrate   soda ash, light, crystalline, heptahydrate   Cutoff, U_GLO
Sodium sulfate	market for sodium sulfate, anhydrite   sodium sulfate, anhydrite   Cutoff, U_RoW
Quicklime	quicklime production, in pieces, loose   quicklime, in pieces, loose   Cutoff, U_CA_QC
Limestone	market for limestone, crushed, washed   limestone, crushed, washed   Cutoff, U_RoW
Ammonia	market for ammonia, liquid   ammonia, liquid   Cutoff, U_RoW
Sodium Chloride	salt production from seawater, evaporation pond   Cutoff, U_GLO

**Table S5.** Inputs and outputs of producing 1 air dried (10% moisture content) metric ton of NBSK pulp used in this study.

<b>Item</b>	<b>Unit</b>	<b>Value<sup>75</sup></b>
<b><i>Input</i></b>		
Wood chips	dry kg	2340
Transportation	km	150
NaOH	kg	49.2
H <sub>2</sub> O <sub>2</sub>	kg	4.4
O <sub>2</sub>	kg	5.7
Na <sub>2</sub> ClO <sub>4</sub>	kg	59.7
H <sub>2</sub> SO <sub>4</sub>	kg	44
CH <sub>3</sub> OH	kg	5.4
Electricity	kWh	39
Diesel	MJ	3070
<b><i>Output (emissions to water)</i></b>		
Biological oxygen demand	kg	1.9
Chemical oxygen demand	kg	57.9
Suspended solids	kg	1.8
Adsorbable organic halides	kg	0.25
Nitrogen	kg	0.65
Phosphorus	kg	0.13
Polycyclic aromatic hydrocarbons	kg	0.002
<b><i>Output (emissions to air)</i></b>		
CO	kg	18
CH <sub>4</sub>	kg	0.1
N <sub>2</sub> O	kg	0.07
NO <sub>x</sub>	kg	2.4
SO <sub>x</sub>	kg	0.09
VOC	kg	1.9
Total suspended particulates	kg	2.5
PM10	kg	2.1
PM2.5	kg	1.6
Polychlorinated dibenzo-dioxins	kg	6.8E-06
Polycyclic aromatic hydrocarbons	kg	0.01

**Table S6.** Life-cycle environmental impacts of producing 1 air dried (10% moisture content) metric ton of dissolving pulp used in this study.

<b>Impact category<sup>20</sup></b>	<b>Unit</b>	<b>Value</b>
Acidification	kg SO <sub>2</sub> eq	3
Carcinogenicity	CTUh	0
Ecotoxicity	CTUe	10669
Eutrophication	kg N eq	6
Fossil fuel depletion	MJ surplus	1008
Global warming	kg CO <sub>2</sub> eq	786
Non carcinogenicity	CTUh	0
Ozone depletion	kg CFC-11 eq	0
Respiratory effects	kg PM2.5 eq	1
Smog	kg O <sub>3</sub> eq	33

**Table S7.** Financial assumptions for the discounted cash flow rate of return analysis.

<b>Assumptions</b>	<b>Value<sup>76</sup></b>
Year of analysis	2020
Internal rate of return	10%
Income tax rate	21%
Loan interest	8%
Loan years	10 years
Financing	40% by equity
Plant life	20 years
Plant construction time	36 months
Percentage of spending in year 1, 2, and 3	8% in year 1; 60% in year 2; 32% in year 3
Working capital	5% of fixed capital investment
Salvage value of plant	0
Start-up time	6 months
Revenues during start-up time	50%
Variable cost during start-up time	75%
Fixed cost during start-up time	100%

**Table S8.** Project cost assumptions.

<b>Assumptions</b>	<b>Value<sup>22</sup></b>
<b>Direct costs</b>	
Warehouse	4.0% of total installed equipment costs
Site development	9.0% of total installed equipment costs
Additional piping	4.5% of total installed equipment costs
<b>Indirect costs</b>	
Prorated expenses	10% of total direct costs
Field expenses	10% of total direct costs
Home office & construction fees	20% of total direct costs
Project contingency	10% of total direct costs
Other costs	10% of total direct costs
Working Capital	5% of fixed capital investment

**Table S9.** Capital investment of CNC scenarios at varied plant capacities.

<b>Plant Capacity (dry t day<sup>-1</sup>)</b>	<b>25</b>	<b>50</b>	<b>75</b>	<b>100</b>
CNC Baseline				
Feedstock handling and shredding	\$2,212,171	\$3,375,444	\$4,322,794	\$5,152,639
Hydrolysis and neutralization	\$4,531,851	\$7,314,969	\$9,883,448	\$12,331,234
Acid recovery	\$0	\$0	\$0	\$0
Purification	\$2,753,794	\$4,173,972	\$5,323,586	\$6,326,558
Boiler	\$1,852,894	\$2,808,606	\$3,582,278	\$4,257,284
Utilities	\$3,752,974	\$5,738,468	\$7,359,036	\$8,780,817
Other direct cost	\$2,643,145	\$4,097,005	\$5,332,450	\$6,448,493
Indirect cost	\$13,310,122	\$20,631,348	\$26,852,694	\$32,472,768
Land and working capital	\$3,400,848	\$4,254,991	\$4,980,814	\$5,636,490
CNC-1 CaO				
Feedstock handling and shredding	\$2,214,268	\$3,378,647	\$4,326,897	\$5,157,532
Hydrolysis and neutralization	\$5,722,744	\$9,251,866	\$12,457,803	\$15,481,432
Acid recovery	\$0	\$0	\$0	\$0
Purification	\$2,756,364	\$4,177,867	\$5,328,554	\$6,332,462
Boiler	\$1,854,624	\$2,811,227	\$3,585,621	\$4,261,257
Utilities	\$1,629,826	\$2,491,144	\$3,193,965	\$3,810,471
Other direct cost	\$2,481,120	\$3,869,381	\$5,056,247	\$6,132,552
Indirect cost	\$12,494,209	\$19,485,099	\$25,461,815	\$30,881,780
Land and working capital	\$3,305,658	\$4,121,262	\$4,818,545	\$5,450,874
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery				
Feedstock handling and shredding	\$2,271,155	\$3,465,535	\$4,438,240	\$5,290,308
Hydrolysis and neutralization	\$6,868,489	\$10,741,776	\$14,166,647	\$17,347,155
Acid recovery	\$25,064,838	\$38,018,426	\$48,511,425	\$57,670,249
Purification	\$9,004,318	\$13,866,102	\$17,865,533	\$21,394,230
Boiler	\$10,985,930	\$16,652,700	\$21,240,163	\$25,242,632
Utilities	\$2,295,282	\$3,509,265	\$4,500,098	\$5,369,387
Other direct cost	\$9,885,752	\$15,094,416	\$19,376,368	\$23,154,943
Indirect cost	\$49,781,824	\$76,011,165	\$97,573,856	\$116,601,677
Land and working capital	\$7,655,879	\$10,715,969	\$13,231,616	\$15,451,529
CNC-3 Citric Acid				
Feedstock handling and shredding	\$1,983,182	\$3,025,717	\$3,874,658	\$4,618,254
Hydrolysis and neutralization	\$7,550,685	\$11,898,149	\$15,753,832	\$19,341,469
Acid recovery	\$23,327,137	\$39,433,445	\$53,877,751	\$67,380,691
Purification	\$7,422,408	\$11,466,668	\$14,803,888	\$17,754,588
Boiler	\$9,343,446	\$14,162,963	\$18,064,536	\$21,468,576
Utilities	\$2,369,910	\$3,622,079	\$4,643,697	\$5,539,761
Other direct cost	\$9,099,435	\$14,631,579	\$19,428,213	\$23,818,084
Indirect cost	\$45,822,153	\$73,680,450	\$97,834,932	\$119,941,066



Land and working capital	\$7,193,918	\$10,444,052	\$13,262,075	\$15,841,124
CNC-4 Subcritical Water				
Feedstock handling and shredding	\$3,195,737	\$4,878,037	\$6,248,524	\$7,449,287
Hydrolysis and neutralization	\$10,137,620	\$16,783,826	\$22,753,766	\$28,355,073
Acid recovery	\$0	\$0	\$0	\$0
Purification	\$2,966,443	\$4,557,047	\$5,868,451	\$7,028,521
Boiler	\$13,369,461	\$20,265,752	\$25,848,571	\$30,719,473
Utilities	\$2,206,931	\$3,371,976	\$4,322,224	\$5,155,515
Other direct cost	\$5,578,334	\$8,724,912	\$11,382,269	\$13,773,877
Indirect cost	\$28,090,895	\$43,936,162	\$57,317,853	\$69,361,310
Land and working capital	\$5,125,271	\$6,973,886	\$8,535,083	\$9,940,153
CNC-5 Wood Pellets				
Feedstock handling and shredding	\$2,271,155	\$3,465,535	\$4,438,240	\$5,290,308
Hydrolysis and neutralization	\$6,868,489	\$10,741,776	\$14,166,647	\$17,347,155
Acid recovery	\$25,064,838	\$38,018,426	\$48,511,425	\$57,670,249
Purification	\$9,004,318	\$13,866,102	\$17,865,533	\$21,394,230
Boiler	\$10,985,930	\$16,652,700	\$21,240,163	\$25,242,632
Utilities	\$2,295,282	\$3,509,265	\$4,500,098	\$5,369,387
Other direct cost	\$9,885,752	\$15,094,416	\$19,376,368	\$23,154,943
Indirect cost	\$49,781,824	\$76,011,165	\$97,573,856	\$116,601,677
Land and working capital	\$7,655,879	\$10,715,969	\$13,231,616	\$15,451,529
CNC-6 Wind Power				
Feedstock handling and shredding	\$2,271,155	\$3,465,535	\$4,438,240	\$5,290,308
Hydrolysis and neutralization	\$6,868,489	\$10,741,776	\$14,166,647	\$17,347,155
Acid recovery	\$25,064,838	\$38,018,426	\$48,511,425	\$57,670,249
Purification	\$9,004,318	\$13,866,102	\$17,865,533	\$21,394,230
Boiler	\$10,985,930	\$16,652,700	\$21,240,163	\$25,242,632
Utilities	\$2,295,282	\$3,509,265	\$4,500,098	\$5,369,387
Other direct cost	\$9,885,752	\$15,094,416	\$19,376,368	\$23,154,943
Indirect cost	\$49,781,824	\$76,011,165	\$97,573,856	\$116,601,677
Land and working capital	\$7,655,879	\$10,715,969	\$13,231,616	\$15,451,529

**Table S10.** Capital investment of CNF scenarios at varied plant capacities.

<b>Plant Capacity (dry t day<sup>-1</sup>)</b>	<b>25</b>	<b>50</b>	<b>75</b>	<b>100</b>
<b>CNF Baseline</b>				
Feedstock handling and shredding	\$483,276	\$747,115	\$964,401	\$1,156,143
Pretreatment	\$3,059,058	\$4,969,454	\$6,600,435	\$8,072,902
Nanofibrillation	\$14,103,315	\$21,376,629	\$27,264,276	\$32,400,910
Boiler	\$0	\$0	\$0	\$0
Utilities	\$38,990	\$63,340	\$84,128	\$102,896
Other direct cost	\$3,094,812	\$4,752,394	\$6,109,817	\$7,303,249
Indirect cost	\$15,584,588	\$23,931,699	\$30,767,292	\$36,777,075
Land and working capital	\$3,666,202	\$4,640,032	\$5,437,517	\$6,138,659
<b>CNF-1 Enzymatic Hydrolysis</b>				
Feedstock handling and shredding	\$504,003	\$779,233	\$1,005,916	\$1,205,962
Pretreatment	\$8,043,718	\$12,321,788	\$15,847,648	\$18,960,637
Nanofibrillation	\$15,045,844	\$22,806,003	\$29,087,973	\$34,568,772
Boiler	\$9,739,142	\$14,762,772	\$18,829,585	\$22,377,793
Utilities	\$142,528	\$231,538	\$307,529	\$376,134
Other direct cost	\$5,858,166	\$8,907,733	\$11,388,764	\$13,560,627
Indirect cost	\$29,500,051	\$44,856,800	\$57,350,562	\$68,287,445
Land and working capital	\$5,289,673	\$7,081,293	\$8,538,899	\$9,814,869
<b>CNF-2 Wood Pellets</b>				
Feedstock handling and shredding	\$504,003	\$779,233	\$1,005,916	\$1,205,962
Pretreatment	\$8,043,718	\$12,321,788	\$15,847,648	\$18,960,637
Nanofibrillation	\$15,045,844	\$22,806,003	\$29,087,973	\$34,568,772
Boiler	\$9,739,142	\$14,762,772	\$18,829,585	\$22,377,793
Utilities	\$142,528	\$231,538	\$307,529	\$376,134
Other direct cost	\$5,858,166	\$8,907,733	\$11,388,764	\$13,560,627
Indirect cost	\$29,500,051	\$44,856,800	\$57,350,562	\$68,287,445
Land and working capital	\$5,289,673	\$7,081,293	\$8,538,899	\$9,814,869
<b>CNF-3 Wind Power</b>				
Feedstock handling and shredding	\$504,003	\$779,233	\$1,005,916	\$1,205,962
Pretreatment	\$8,043,718	\$12,321,788	\$15,847,648	\$18,960,637
Nanofibrillation	\$15,045,844	\$22,806,003	\$29,087,973	\$34,568,772
Boiler	\$9,739,142	\$14,762,772	\$18,829,585	\$22,377,793
Utilities	\$142,528	\$231,538	\$307,529	\$376,134
Other direct cost	\$5,858,166	\$8,907,733	\$11,388,764	\$13,560,627
Indirect cost	\$29,500,051	\$44,856,800	\$57,350,562	\$68,287,445
Land and working capital	\$5,289,673	\$7,081,293	\$8,538,899	\$9,814,869

**Table S11.** Purchased cost and installed cost of equipment in CNC scenarios.

		CNC Baseline	CNC Baseline	CNC-1	CNC-1	CNC-2	CNC-2
	Items	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost
<b>Feedstock handling and shredding</b>	Telehandler <sup>77</sup>	\$33,251	\$33,251	\$33,287	\$33,287	\$34,272	\$34,272
	Pulp shredder <sup>78</sup>	\$43,219	\$62,667	\$43,266	\$62,735	\$44,545	\$64,591
	Dust collection <sup>79</sup>	\$102,612	\$184,702	\$102,724	\$184,903	\$105,761	\$190,370
	Miscellaneous equipment <sup>79</sup>	\$30,096	\$54,173	\$30,129	\$54,232	\$31,020	\$55,835
	Feedstock storage <sup>80</sup>	\$1,788,619	\$3,040,652	\$1,790,288	\$3,043,490	\$1,835,569	\$3,120,467
<b>Reaction</b>	Acid solution pump <sup>80</sup>	\$3,706	\$8,524	\$3,711	\$8,534	\$3,836	\$8,823
	Hydrolysis Mixer <sup>80</sup>	\$40,703	\$69,195	\$40,734	\$69,248	\$41,591	\$70,705
	Hydrolysis storage <sup>80</sup>	\$508,992	\$916,185	\$509,546	\$917,182	\$524,613	\$944,303
	Acid hydrolysis reactor <sup>81</sup>	\$1,823,187	\$2,734,781	\$1,826,024	\$2,739,036	\$1,903,646	\$2,855,468
	Outlet pump <sup>80</sup>	\$4,059	\$9,336	\$4,064	\$9,347	\$4,202	\$9,664
	Acid Tank <sup>80</sup>	\$51,062	\$153,187	\$51,118	\$153,354	\$52,630	\$157,889
	Hydrolysate cooler <sup>80</sup>	\$101,186	\$222,608	\$101,186	\$222,608	\$101,186	\$222,608
	Dilution tank <sup>22</sup>	\$1,546,813	\$2,320,219	\$1,548,497	\$2,322,745	\$0	\$0
	Centrifuge system <sup>80</sup>	\$0	\$0	\$0	\$0	\$5,759,520	\$5,759,520
	Bleaching mixer <sup>80</sup>	\$66,336	\$112,771	\$66,387	\$112,858	\$29,860	\$50,762
	Scrubber <sup>22</sup>	\$250,263	\$600,632	\$250,263	\$600,632	\$250,263	\$600,632
	Pump for bleaching effluent <sup>80</sup>	\$8,867	\$20,393	\$8,878	\$20,419	\$2,473	\$5,688
	Neutralizing mixer <sup>80</sup>	\$86,552	\$147,138	\$80,604	\$137,026	\$32,772	\$55,712
	Gypsum filter <sup>81</sup>	\$0	\$0	\$1,065,316	\$1,938,874	\$0	\$0
<b>Acid recovery</b>	Acid recovery electrodialysis <sup>82</sup>	\$0	\$0	\$0	\$0	\$5,599,513	\$13,998,782
	Neutralizing mixer <sup>80</sup>	\$0	\$0	\$0	\$0	\$2,061	\$4,740
	Transfer pump <sup>80</sup>	\$0	\$0	\$0	\$0	\$27,632	\$46,974
	Transfer pump <sup>80</sup>	\$0	\$0	\$0	\$0	\$1,885	\$4,335
	Three-effect evaporator <sup>83</sup>	\$0	\$0	\$0	\$0	\$9,409,636	\$23,524,091
	Ion Exchanger <sup>80</sup>	\$0	\$0	\$0	\$0	\$0	\$0
	Decanter <sup>68</sup>	\$0	\$0	\$0	\$0	\$32,650	\$59,424
	Gypsum filter <sup>81</sup>	\$0	\$0	\$0	\$0	\$208,835	\$380,080
<b>Neutralization and purification</b>	Centrifuge <sup>80</sup>	\$0	\$0	\$0	\$0	\$2,787,845	\$2,787,845
	Transfer pump <sup>80</sup>	\$0	\$0	\$0	\$0	\$5,348	\$12,300
	Filtration pump <sup>80</sup>	\$0	\$0	\$0	\$0	\$2,453	\$5,641
	Filtration <sup>80</sup>	\$0	\$0	\$0	\$0	\$145,958	\$248,129
	Diafiltration <sup>84</sup>	\$0	\$0	\$0	\$0	\$1,722,267	\$4,305,667
	Ultrafiltration <sup>84</sup>	\$1,669,589	\$4,173,972	\$1,671,147	\$4,177,867	\$1,672,580	\$4,181,450
	Dilution tank <sup>80</sup>	\$0	\$0	\$0	\$0	\$1,550,046	\$2,325,070
<b>Boiler</b>	Deaerator and boiler feed water heater <sup>80,84</sup>	\$12,940	\$38,042	\$12,953	\$38,078	\$78,698	\$229,883
	Boiler <sup>84</sup>	\$1,120,167	\$2,016,300	\$1,121,212	\$2,018,182	\$6,639,911	\$11,951,839
	Combustion gas baghouse <sup>84</sup>	\$419,035	\$754,263	\$419,426	\$754,967	\$2,483,876	\$4,470,977
<b>Utilities</b>	Transfer pumps <sup>80</sup>	\$47,893	\$110,153	\$23,955	\$55,096	\$33,624	\$77,336
	RO system <sup>84</sup>	\$2,830,146	\$5,094,262	\$1,240,063	\$2,232,113	\$1,738,581	\$3,129,445
	Process water tank <sup>80</sup>	\$314,149	\$534,053	\$119,962	\$203,935	\$177,931	\$302,484

**Continued Table S11**

		CNC-3	CNC-3	CNC-4	CNC-4	CNC-5	CNC-5
	Items	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost
<b>Feedstock handling and shredding</b>	Telehandler <sup>77</sup>	\$29,328	\$29,328	\$50,729	\$50,729	\$34,272	\$34,272
	Pulp shredder <sup>78</sup>	\$38,119	\$55,273	\$65,936	\$95,607	\$44,545	\$64,591
	Dust collection <sup>79</sup>	\$90,505	\$162,909	\$156,548	\$281,787	\$105,761	\$190,370
	Miscellaneous equipment <sup>79</sup>	\$26,545	\$47,781	\$45,915	\$82,648	\$31,020	\$55,835
	Feedstock storage <sup>80</sup>	\$1,606,133	\$2,730,426	\$2,568,980	\$4,367,266	\$1,835,569	\$3,120,467
<b>Reaction</b>	Acid solution pump <sup>80</sup>	\$4,463	\$10,265	\$6,972	\$16,035	\$3,836	\$8,823
	Hydrolysis Mixer <sup>80</sup>	\$44,881	\$76,298	\$0	\$0	\$41,591	\$70,705
	Hydrolysis storage <sup>80</sup>	\$583,619	\$1,050,514	\$873,434	\$1,572,181	\$524,613	\$944,303
	Acid hydrolysis reactor <sup>81</sup>	\$2,216,742	\$3,325,113	\$3,943,294	\$5,914,941	\$1,903,646	\$2,855,468
	Outlet pump <sup>80</sup>	\$4,746	\$10,916	\$7,524	\$17,305	\$4,202	\$9,664
	Acid Tank <sup>80</sup>	\$60,084	\$180,252	\$0	\$0	\$52,630	\$157,889
	Hydrolysate cooler <sup>80</sup>	\$101,186	\$222,608	\$101,186	\$222,608	\$101,186	\$222,608
	Dilution tank <sup>22</sup>	\$0	\$0	\$0	\$0	\$0	\$0
	Centrifuge system <sup>80</sup>	\$6,310,499	\$6,310,499	\$8,915,591	\$8,915,591	\$5,759,520	\$5,759,520
	Bleaching mixer <sup>80</sup>	\$29,859	\$50,760	\$73,627	\$125,166	\$29,860	\$50,762
	Scrubber <sup>22</sup>	\$250,263	\$600,632	\$0	\$0	\$250,263	\$600,632
	Pump for bleaching effluent <sup>80</sup>	\$2,473	\$5,687	\$0	\$0	\$2,473	\$5,688
	Neutralizing mixer <sup>80</sup>	\$32,119	\$54,603	\$0	\$0	\$32,772	\$55,712
	Gypsum filter <sup>81</sup>	\$0	\$0	\$0	\$0	\$0	\$0
<b>Acid recovery</b>	Acid recovery electrodialysis <sup>82</sup>	\$0	\$0	\$0	\$0	\$5,599,513	\$13,998,782
	Neutralizing mixer <sup>80</sup>	\$18,404	\$42,329	\$0	\$0	\$2,061	\$4,740
	Transfer pump <sup>80</sup>	\$105,650	\$179,604	\$0	\$0	\$27,632	\$46,974
	Transfer pump <sup>80</sup>	\$18,274	\$42,031	\$0	\$0	\$1,885	\$4,335
	Three-effect evaporator <sup>83</sup>	\$6,979,345	\$17,448,363	\$0	\$0	\$9,409,636	\$23,524,091
	Ion Exchanger <sup>80</sup>	\$12,067,288	\$21,721,118	\$0	\$0	\$0	\$0
	Decanter <sup>68</sup>	\$0	\$0	\$0	\$0	\$32,650	\$59,424
	Gypsum filter <sup>81</sup>	\$0	\$0	\$0	\$0	\$208,835	\$380,080
<b>Neutralization and purification</b>	Centrifuge <sup>80</sup>	\$2,721,391	\$2,721,391	\$0	\$0	\$2,787,845	\$2,787,845
	Transfer pump <sup>80</sup>	\$5,114	\$11,763	\$0	\$0	\$5,348	\$12,300
	Filtration pump <sup>80</sup>	\$2,453	\$5,641	\$2,451	\$5,637	\$2,453	\$5,641
	Filtration <sup>80</sup>	\$145,959	\$248,130	\$145,831	\$247,913	\$145,958	\$248,129
	Diafiltration <sup>84</sup>	\$1,706,735	\$4,266,838	\$0	\$0	\$1,722,267	\$4,305,667
	Ultrafiltration <sup>84</sup>	\$764,912	\$1,912,280	\$1,721,399	\$4,303,497	\$1,672,580	\$4,181,450
	Dilution tank <sup>80</sup>	\$1,533,750	\$2,300,625	\$0	\$0	\$1,550,046	\$2,325,070
<b>Boiler</b>	Deaerator and boiler feed water heater <sup>80,84</sup>	\$66,758	\$195,132	\$96,084	\$280,442	\$78,698	\$229,883
	Boiler <sup>84</sup>	\$5,647,335	\$10,165,203	\$8,080,263	\$14,544,473	\$6,639,911	\$11,951,839
	Combustion gas baghouse <sup>84</sup>	\$2,112,571	\$3,802,628	\$3,022,687	\$5,440,837	\$2,483,876	\$4,470,977
<b>Utilities</b>	Transfer pumps <sup>80</sup>	\$29,835	\$68,621	\$24,961	\$57,410	\$33,624	\$77,336
	RO system <sup>84</sup>	\$1,799,237	\$3,238,627	\$1,679,970	\$3,023,945	\$1,738,581	\$3,129,445
	Process water tank <sup>80</sup>	\$185,195	\$314,831	\$170,953	\$290,620	\$177,931	\$302,484

**Continued Table S11**

		CNC-6	CNC-6
	Items	Purchased Cost	Installed Cost
<b>Feedstock handling and shredding</b>	Telehandler <sup>77</sup>	\$34,272	\$34,272
	Pulp shredder <sup>78</sup>	\$44,545	\$64,591
	Dust collection <sup>79</sup>	\$105,761	\$190,370
	Miscellaneous equipment <sup>79</sup>	\$31,020	\$55,835
	Feedstock storage <sup>80</sup>	\$1,835,569	\$3,120,467
<b>Reaction</b>	Acid solution pump <sup>80</sup>	\$3,836	\$8,823
	Hydrolysis Mixer <sup>80</sup>	\$41,591	\$70,705
	Hydrolysis storage <sup>80</sup>	\$524,613	\$944,303
	Acid hydrolysis reactor <sup>81</sup>	\$1,903,646	\$2,855,468
	Outlet pump <sup>80</sup>	\$4,202	\$9,664
	Acid Tank <sup>80</sup>	\$52,630	\$157,889
	Hydrolysate cooler <sup>80</sup>	\$101,186	\$222,608
	Dilution tank <sup>22</sup>	\$0	\$0
	Centrifuge system <sup>80</sup>	\$5,759,520	\$5,759,520
	Bleaching mixer <sup>80</sup>	\$29,860	\$50,762
	Scrubber <sup>22</sup>	\$250,263	\$600,632
	Pump for bleaching effluent <sup>80</sup>	\$2,473	\$5,688
	Neutralizing mixer <sup>80</sup>	\$32,772	\$55,712
	Gypsum filter <sup>81</sup>	\$0	\$0
<b>Acid recovery</b>	Acid recovery electrodialysis <sup>82</sup>	\$5,599,513	\$13,998,782
	Neutralizing mixer <sup>80</sup>	\$2,061	\$4,740
	Transfer pump <sup>80</sup>	\$27,632	\$46,974
	Transfer pump <sup>80</sup>	\$1,885	\$4,335
	Three-effect evaporator <sup>83</sup>	\$9,409,636	\$23,524,091
	Ion Exchanger <sup>80</sup>	\$0	\$0
	Decanter <sup>68</sup>	\$32,650	\$59,424
	Gypsum filter <sup>81</sup>	\$208,835	\$380,080
<b>Neutralization and purification</b>	Centrifuge <sup>80</sup>	\$2,787,845	\$2,787,845
	Transfer pump <sup>80</sup>	\$5,348	\$12,300
	Filtration pump <sup>80</sup>	\$2,453	\$5,641
	Filtration <sup>80</sup>	\$145,958	\$248,129
	Diafiltration <sup>84</sup>	\$1,722,267	\$4,305,667
	Ultrafiltration <sup>84</sup>	\$1,672,580	\$4,181,450
	Dilution tank <sup>80</sup>	\$1,550,046	\$2,325,070
<b>Boiler</b>	Deaerator and boiler feed water heater <sup>80,84</sup>	\$78,698	\$229,883
	Boiler <sup>84</sup>	\$6,639,911	\$11,951,839
	Combustion gas baghouse <sup>84</sup>	\$2,483,876	\$4,470,977
<b>Utilities</b>	Transfer pumps <sup>80</sup>	\$33,624	\$77,336
	RO system <sup>84</sup>	\$1,738,581	\$3,129,445
	Process water tank <sup>80</sup>	\$177,931	\$302,484

**Table S12.** Purchased cost and installed cost of equipment in CNF scenarios.

		CNF Baseline	CNF Baseline	CNF-1	CNF-1	CNF-2	CNF-2
	Items	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost
<b>Feedstock handling and shredding</b>	Telehandler <sup>77</sup>	\$21,663	\$21,663	\$22,701	\$22,701	\$22,701	\$22,701
	Pulp shredder <sup>78</sup>	\$28,156	\$40,827	\$29,506	\$42,784	\$29,506	\$42,784
	Dust collection <sup>79</sup>	\$66,850	\$120,331	\$70,055	\$126,099	\$70,055	\$126,099
	Miscellaneous equipment <sup>79</sup>	\$19,607	\$35,293	\$20,547	\$36,985	\$20,547	\$36,985
	Feedstock storage <sup>80</sup>	\$311,178	\$529,002	\$323,920	\$550,664	\$323,920	\$550,664
<b>Reaction</b>	Enzymatic hydrolysis reactor <sup>80</sup>	\$0	\$0	\$5,470,262	\$8,205,394	\$5,470,262	\$8,205,394
	Hydrolysis Mixer <sup>80</sup>	\$0	\$0	\$68,519	\$116,483	\$68,519	\$116,483
	Hydrolysate cooler <sup>80</sup>	\$0	\$0	\$101,186	\$222,608	\$101,186	\$222,608
	Dilution tank <sup>22</sup>	\$0	\$0	\$2,518,202	\$3,777,303	\$2,518,202	\$3,777,303
	Hydropulper <sup>14</sup>	\$3,600,000	\$3,600,000	\$0	\$0	\$0	\$0
<b>Neutralization and purification</b>	Washer <sup>69</sup>	\$0	\$0	\$889,654	\$1,423,447	\$889,654	\$1,423,447
	Washer water pump <sup>80</sup>	\$0	\$0	\$2,577	\$5,927	\$2,577	\$5,927
	Disk refiner <sup>14</sup>	\$9,011,908	\$12,616,671	\$9,011,908	\$12,616,671	\$9,011,908	\$12,616,671
	Homogenizer <sup>85</sup>	\$4,454,079	\$4,454,079	\$0	\$0	\$0	\$0
	Microfluidizer <sup>85</sup>	\$0	\$0	\$4,454,079	\$4,454,079	\$4,454,079	\$4,454,079
	Ultrafiltration <sup>84</sup>	\$1,722,351	\$4,305,879	\$1,722,351	\$4,305,879	\$1,722,351	\$4,305,879
<b>Boiler</b>	Deaerator and boiler feed water heater <sup>80,84</sup>	\$0	\$0	\$69,631	\$203,497	\$69,631	\$203,497
	Boiler <sup>84</sup>	\$0	\$0	\$5,886,462	\$10,595,632	\$5,886,462	\$10,595,632
	Combustion gas baghouse <sup>84</sup>	\$0	\$0	\$2,202,024	\$3,963,643	\$2,202,024	\$3,963,643
<b>Utilities</b>	Process water tank <sup>80</sup>	\$37,259	\$63,340	\$136,199	\$231,538	\$136,199	\$231,538

**Continued Table S12**

		CNF-3	CNF-3
	Items	Purchased Cost	Installed Cost
<b>Feedstock handling and shredding</b>			
	Telehandler <sup>77</sup>	\$22,701	\$22,701
	Pulp shredder <sup>78</sup>	\$29,506	\$42,784
	Dust collection <sup>79</sup>	\$70,055	\$126,099
	Miscellaneous equipment <sup>79</sup>	\$20,547	\$36,985
	Feedstock storage <sup>80</sup>	\$323,920	\$550,664
		\$0	\$0
<b>Reaction</b>	Enzymatic hydrolysis reactor <sup>80</sup>	\$5,470,262	\$8,205,394
	Hydrolysis Mixer <sup>80</sup>	\$68,519	\$116,483
	Hydrolysate cooler <sup>80</sup>	\$101,186	\$222,608
	Dilution tank <sup>22</sup>	\$2,518,202	\$3,777,303
	Hydropulper <sup>14</sup>	\$0	\$0
		\$0	\$0
<b>Neutralization and purification</b>	Washer <sup>69</sup>	\$889,654	\$1,423,447
	Washer water pump <sup>80</sup>	\$2,577	\$5,927
	Disk refiner <sup>14</sup>	\$9,011,908	\$12,616,671
	Homogenizer <sup>85</sup>	\$0	\$0
	Microfluidizer <sup>85</sup>	\$4,454,079	\$4,454,079
	Ultrafiltration <sup>84</sup>	\$1,722,351	\$4,305,879
		\$0	\$0
<b>Boiler</b>	Deaerator and boiler feed water heater <sup>80,84</sup>	\$69,631	\$203,497
	Boiler <sup>84</sup>	\$5,886,462	\$10,595,632
	Combustion gas baghouse <sup>84</sup>	\$2,202,024	\$3,963,643
		\$0	\$0
<b>Utilities</b>	Process water tank <sup>80</sup>	\$136,199	\$231,538

**Table S13.** Operating cost per dry t CNC of CNC scenarios at varied plant capacities.

<b>Plant Capacity (dry t day<sup>-1</sup>)</b>	<b>25</b>	<b>50</b>	<b>75</b>	<b>100</b>
<b>CNC Baseline</b>				
Feedstock	\$1,550	\$1,550	\$1,550	\$1,550
Chemicals and materials	\$4,331	\$4,330	\$4,330	\$4,329
Water	\$136	\$136	\$136	\$136
Wastewater treatment	\$327	\$327	\$327	\$327
Energy	\$479	\$479	\$479	\$479
Byproduct credit	\$0	\$0	\$0	\$0
Labor	\$416	\$208	\$151	\$123
Other	\$82	\$63	\$55	\$50
<b>CNC-1 CaO</b>				
Feedstock	\$1,552	\$1,552	\$1,552	\$1,552
Chemicals and materials	\$1,805	\$1,804	\$1,803	\$1,803
Water	\$29	\$29	\$29	\$29
Wastewater treatment	\$47	\$47	\$47	\$47
Energy	\$328	\$328	\$328	\$328
Byproduct credit	-\$168	-\$168	-\$168	-\$168
Labor	\$416	\$208	\$151	\$123
Other	\$77	\$60	\$52	\$47
<b>CNC-2 H<sub>2</sub>SO<sub>4</sub> Recovery</b>				
Feedstock	\$1,618	\$1,618	\$1,618	\$1,618
Chemicals and materials	\$467	\$461	\$458	\$457
Water	\$30	\$30	\$30	\$30
Wastewater treatment	\$57	\$57	\$57	\$57
Energy	\$392	\$392	\$392	\$392
Byproduct credit	-\$16	-\$16	-\$16	-\$16
Labor	\$490	\$264	\$188	\$150
Other	\$305	\$233	\$200	\$179
<b>CNC-3 Citric Acid</b>				
Feedstock	\$1,296	\$1,296	\$1,296	\$1,296
Chemicals and materials	\$3,155	\$3,153	\$3,153	\$3,152
Water	\$112	\$112	\$112	\$112
Wastewater treatment	\$234	\$234	\$234	\$234
Energy	\$425	\$425	\$425	\$425
Byproduct credit	\$0	\$0	\$0	\$0
Labor	\$490	\$264	\$188	\$150
Other	\$281	\$226	\$200	\$184
<b>CNC-4 Subcritical Water</b>				
Feedstock	\$2,834	\$2,834	\$2,834	\$2,834



Chemicals and materials	\$5	\$4	\$3	\$3
Water	\$90	\$90	\$90	\$90
Wastewater treatment	\$196	\$196	\$196	\$196
Energy	\$378	\$378	\$378	\$378
Byproduct credit	\$0	\$0	\$0	\$0
Labor	\$416	\$208	\$151	\$123
Other	\$172	\$135	\$117	\$106
<b>CNC-5 Wood Pellets</b>				
Feedstock	\$1,618	\$1,618	\$1,618	\$1,618
Chemicals and materials	\$467	\$461	\$458	\$457
Water	\$30	\$30	\$30	\$30
Wastewater treatment	\$57	\$57	\$57	\$57
Energy	\$503	\$503	\$503	\$503
Byproduct credit	-\$16	-\$16	-\$16	-\$16
Labor	\$490	\$264	\$188	\$150
Other	\$305	\$233	\$200	\$179
<b>CNC-6 Wind Power</b>				
Feedstock	\$1,618	\$1,618	\$1,618	\$1,618
Chemicals and materials	\$467	\$461	\$458	\$457
Water	\$30	\$30	\$30	\$30
Wastewater treatment	\$57	\$57	\$57	\$57
Energy	\$378	\$378	\$378	\$378
Byproduct credit	-\$16	-\$16	-\$16	-\$16
Labor	\$490	\$264	\$188	\$150
Other	\$305	\$233	\$200	\$179

**Table S14.** Operating cost per dry t CNF of CNF scenarios at varied plant capacities.

<b>Plant Capacity (dry t day<sup>-1</sup>)</b>	<b>25</b>	<b>50</b>	<b>75</b>	<b>100</b>
<b>CNF Baseline</b>				
Feedstock	\$1,055	\$1,055	\$1,055	\$1,055
Chemicals and materials	\$11	\$8	\$7	\$6
Water	\$8	\$8	\$8	\$8
Wastewater treatment	\$0	\$0	\$0	\$0
Energy	\$1,011	\$1,011	\$1,011	\$1,011
Labor	\$416	\$208	\$151	\$123
Other	\$96	\$73	\$63	\$56
<b>CNF-1 Enzymatic Hydrolysis</b>				
Feedstock	\$1,128	\$1,128	\$1,128	\$1,128
Chemicals and materials	\$16	\$13	\$12	\$11
Water	\$48	\$48	\$48	\$48
Wastewater treatment	\$96	\$96	\$96	\$96
Energy	\$530	\$530	\$530	\$530
Labor	\$416	\$208	\$151	\$123
Other	\$181	\$138	\$117	\$105
<b>CNF-2 Wood Pellets</b>				
Feedstock	\$1,128	\$1,128	\$1,128	\$1,128
Chemicals and materials	\$16	\$13	\$12	\$11
Water	\$48	\$48	\$48	\$48
Wastewater treatment	\$96	\$96	\$96	\$96
Energy	\$621	\$621	\$621	\$621
Labor	\$416	\$208	\$151	\$123
Other	\$181	\$138	\$117	\$105
<b>CNF-3 Wind Power</b>				
Feedstock	\$1,128	\$1,128	\$1,128	\$1,128
Chemicals and materials	\$16	\$13	\$12	\$11
Water	\$48	\$48	\$48	\$48
Wastewater treatment	\$96	\$96	\$96	\$96
Energy	\$429	\$429	\$429	\$429
Labor	\$416	\$208	\$151	\$123
Other	\$181	\$138	\$117	\$105

**Table S15.** Cost information (2020 US\$) for feedstocks, materials, and energy.

<b>Item</b>	<b>Value</b>	<b>Unit</b>
Dissolving pulp <sup>15</sup>	804.3	US\$ dry t <sup>-1</sup>
NBSK pulp <sup>14</sup>	1,054.7	US\$ dry t <sup>-1</sup>
Sulfuric acid <sup>15</sup>	89.0	US\$ t <sup>-1</sup>
NaOH <sup>15</sup>	383.9	US\$ t <sup>-1</sup>
NaClO <sub>2</sub> (ref. <sup>15</sup> )	4,950.9	US\$ t <sup>-1</sup>
CaO <sup>15</sup>	135.5	US\$ t <sup>-1</sup>
Water <sup>15</sup>	0.6	US\$ t <sup>-1</sup>
Enzyme <sup>10</sup>	5,000.0	US\$ t <sup>-1</sup>
Na <sub>2</sub> CO <sub>3</sub> (ref. <sup>86</sup> )	260.3	US\$ t <sup>-1</sup>
Acetic acid <sup>69</sup>	890.4	US\$ t <sup>-1</sup>
Grid electricity <sup>87</sup>	6.9	cent kWh <sup>-1</sup>
Wind farm electricity <sup>88</sup>	3.9	US\$ t <sup>-1</sup>
Wood pellets <sup>89</sup>	156.1	US\$ t <sup>-1</sup>
Citric acid <sup>10</sup>	1,400.0	US\$ t <sup>-1</sup>
Natural gas <sup>90</sup>	173.4	US\$ t <sup>-1</sup>
Gypsum <sup>10</sup>	11.3	US\$ t <sup>-1</sup>
Wastewater treatment <sup>91</sup>	1.5	US\$ t <sup>-1</sup>
Solid disposal <sup>22</sup>	45.2	US\$ t <sup>-1</sup>
Limestone <sup>92</sup>	12.0	US\$ t <sup>-1</sup>
NaCl <sup>92</sup>	133.3	US\$ t <sup>-1</sup>

**Table S16.** Number of labor positions of the plant at 50 dry t nanocellulose produced per day (2020 US\$).

<b>Position</b>	<b>Annual salary<sup>65</sup></b>	<b>CNC baseline</b>	<b>CNC-1</b>	<b>CNC-2</b>	<b>CNC-3</b>	<b>CNC-4</b>	<b>CNC-5</b>	<b>CNC-6</b>	<b>CNF baseline</b>	<b>CNF-1</b>	<b>CNF-2</b>	<b>CNF-3</b>
Plant manager	\$195,724	1	1	1	1	1	1	1	1	1	1	1
Plant engineer	\$186,404	2	2	2	2	2	2	2	2	2	2	2
Maintenance supervisor	\$75,893	1	1	1	1	1	1	1	1	1	1	1
Maintenance technician	\$106,517	2	2	2	2	2	2	2	2	2	2	2
Lab manager	\$74,562	1	1	1	1	1	1	1	1	1	1	1
Lab technician	\$53,258	1	1	1	1	1	1	1	1	1	1	1
Shift supervisor	\$63,910	1	1	1	1	1	1	1	1	1	1	1
Shift operators	\$958,650	18	18	27	27	27	27	27	18	18	18	18
Yard employees	\$37,281	1	1	1	1	1	1	1	1	1	1	1
Clerks & secretaries	\$47,932	1	1	1	1	1	1	1	1	1	1	1
Overhead and benefits	90% of labor annual salary											

**Table S17.** Summary of scenario settings for the case study of cellulose nanomaterials.

<b>CNC Scenarios</b>	<b>Neutralizing agent</b>	<b>Hydrolysis solution</b>	<b>Acid recovery</b>	<b>Boiler fuel</b>	<b>Electricity</b>	<b>Products</b>
CNC Baseline	NaOH	H <sub>2</sub> SO <sub>4</sub>	No	Natural gas	Grid	CNC
CNC-1	CaO	H <sub>2</sub> SO <sub>4</sub>	No	Natural gas	Grid	CNC
CNC-2	CaO	H <sub>2</sub> SO <sub>4</sub>	Yes	Natural gas	Grid	CNC
CNC-3	CaO	Citric acid	Yes	Natural gas	Grid	CNC and CNF
CNC-4	CaO	Subcritical water	Yes	Natural gas	Grid	CNC
CNC-5	CaO	H <sub>2</sub> SO <sub>4</sub>	Yes	Wood pellets	Grid	CNC
CNC-6	CaO	H <sub>2</sub> SO <sub>4</sub>	Yes	Wood pellets	Wind power	CNC
<b>CNF Scenarios</b>	<b>Pretreatment</b>			<b>Boiler fuel</b>	<b>Electricity</b>	<b>Products</b>
CNF Baseline	No			Natural gas	Grid	CNF
CNF-1	Yes			Natural gas	Grid	CNF
CNF-2	Yes			Wood pellets	Grid	CNF
CNF-3	Yes			Wood pellets	Wind power	CNF

**Table S18.** Life-cycle environment impact results of producing 1 dry kg CNC.

<b>Acidification</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	Wastewater treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	9.30E-03	7.63E-02	5.73E-02	9.56E-04	1.03E-03	1.08E-02	0.00E+00	-1.54E-03		1.54E-01
CNC-1 CaO	9.31E-03	7.64E-02	7.51E-03	1.82E-04	1.47E-04	7.37E-03	-1.42E-03	-1.54E-03		9.80E-02
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	9.71E-03	1.20E-02	4.18E-03	2.18E-04	1.82E-04	6.88E-03	-1.39E-04	-1.54E-03		3.15E-02
CNC-3 Citric Acid	7.77E-03	9.47E-02	5.37E-03	7.75E-04	7.59E-04	8.11E-03	0.00E+00	-1.54E-03		1.16E-01
CNC-4 Subcritical Water	1.70E-02	0.00E+00	0.00E+00	6.56E-04	6.36E-04	5.75E-03	0.00E+00	-1.54E-03		2.25E-02
CNC-5 Wood Pellets	9.71E-03	1.20E-02	4.18E-03	2.18E-04	1.82E-04	8.10E-03	-1.39E-04	-1.54E-03		3.27E-02
CNC-6 Wind Power	9.71E-03	1.20E-02	4.18E-03	2.18E-04	1.82E-04	2.36E-03	-1.39E-04	-1.54E-03		2.70E-02
<b>Carcinogenicity</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	1.49E-08	2.60E-07	7.97E-07	7.03E-08	3.63E-08	2.73E-07	0.00E+00	-3.90E-08		1.41E-06
CNC-1 CaO	1.50E-08	2.60E-07	2.70E-08	1.34E-08	5.17E-09	1.86E-07	-7.16E-09	-3.90E-08		4.61E-07
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	1.56E-08	4.09E-08	5.17E-08	1.61E-08	6.37E-09	1.79E-07	-6.98E-10	-3.90E-08		2.70E-07
CNC-3 Citric Acid	1.25E-08	1.44E-06	4.69E-08	5.70E-08	2.66E-08	2.09E-07	0.00E+00	-3.90E-08		1.75E-06
CNC-4 Subcritical Water	2.73E-08	0.00E+00	0.00E+00	4.82E-08	2.23E-08	1.53E-07	0.00E+00	-3.90E-08		2.12E-07
CNC-5 Wood Pellets	1.56E-08	4.09E-08	5.17E-08	1.61E-08	6.37E-09	1.81E-07	-6.98E-10	-3.90E-08		2.72E-07
CNC-6 Wind Power	1.56E-08	4.09E-08	5.17E-08	1.61E-08	6.37E-09	4.65E-08	-6.98E-10	-3.90E-08		1.37E-07
<b>Ecotoxicity</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	1.92E+01	2.34E+02	2.57E+02	3.50E+00	4.11E+00	2.85E+01	0.00E+00	-4.07E+00		5.43E+02
CNC-1 CaO	1.92E+01	2.34E+02	4.94E+00	6.68E-01	5.85E-01	1.95E+01	-1.87E+00	-4.07E+00		2.73E+02
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	2.00E+01	3.69E+01	1.59E+01	7.99E-01	7.22E-01	1.91E+01	-1.82E-01	-4.07E+00		8.92E+01
CNC-3 Citric Acid	1.60E+01	2.92E+02	1.36E+01	2.84E+00	3.02E+00	2.21E+01	0.00E+00	-4.07E+00		3.46E+02
CNC-4 Subcritical Water	3.51E+01	0.00E+00	0.00E+00	2.40E+00	2.52E+00	1.65E+01	0.00E+00	-4.07E+00		5.24E+01
CNC-5 Wood Pellets	2.00E+01	3.69E+01	1.59E+01	7.99E-01	7.22E-01	2.16E+01	-1.82E-01	-4.07E+00		9.17E+01
CNC-6 Wind Power	2.00E+01	3.69E+01	1.59E+01	7.99E-01	7.22E-01	4.33E+01	-1.82E-01	-4.07E+00		1.13E+02
<b>Eutrophication</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	1.19E-02	9.86E-03	4.81E-02	1.03E-03	6.77E-03	2.51E-02	0.00E+00	-3.59E-03		9.92E-02
CNC-1 CaO	1.19E-02	9.88E-03	1.94E-03	1.96E-04	9.64E-04	1.71E-02	-2.77E-04	-3.59E-03		3.81E-02
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	1.24E-02	1.55E-03	3.08E-03	2.35E-04	1.19E-03	1.57E-02	-2.71E-05	-3.59E-03		3.05E-02
CNC-3 Citric Acid	9.92E-03	5.37E-02	2.91E-03	8.34E-04	4.97E-03	1.86E-02	0.00E+00	-3.59E-03		8.74E-02
CNC-4 Subcritical Water	2.17E-02	0.00E+00	0.00E+00	7.06E-04	4.16E-03	1.29E-02	0.00E+00	-3.59E-03		3.59E-02
CNC-5 Wood Pellets	1.24E-02	1.55E-03	3.08E-03	2.35E-04	1.19E-03	1.61E-02	-2.71E-05	-3.59E-03		3.10E-02

CNC-6 Wind Power	1.24E-02	1.55E-03	3.08E-03	2.35E-04	1.19E-03	1.65E-03	-2.71E-05	-3.59E-03		1.65E-02
<b>Fossil fuel depletion</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	2.89E+00	5.82E+00	8.70E+00	1.98E-01	1.03E-01	3.48E+00	0.00E+00	-4.63E-01		2.07E+01
CNC-1 CaO	2.89E+00	5.83E+00	4.17E+00	3.77E-02	1.46E-02	2.44E+00	-2.83E-01	-4.63E-01		1.46E+01
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	3.01E+00	9.16E-01	9.34E-01	4.51E-02	1.81E-02	6.65E+00	-2.76E-02	-4.63E-01		1.11E+01
CNC-3 Citric Acid	2.41E+00	1.38E+01	1.92E+00	1.60E-01	7.54E-02	5.94E+00	0.00E+00	-4.63E-01		2.39E+01
CNC-4 Subcritical Water	5.28E+00	0.00E+00	0.00E+00	1.35E-01	6.31E-02	8.09E+00	0.00E+00	-4.63E-01		1.31E+01
CNC-5 Wood Pellets	3.01E+00	9.16E-01	9.34E-01	4.51E-02	1.81E-02	2.18E+00	-2.76E-02	-4.63E-01		6.62E+00
CNC-6 Wind Power	3.01E+00	9.16E-01	9.34E-01	4.51E-02	1.81E-02	2.81E-01	-2.76E-02	-4.63E-01		4.72E+00
<b>Global warming</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life	Biogenic carbon uptake	Total
CNC Baseline	1.90E+00	1.51E+00	1.14E+01	2.17E-01	1.63E+00	3.91E+00	0.00E+00	2.12E-01	-3.14E+00	1.77E+01
CNC-1 CaO	1.90E+00	1.51E+00	7.13E+00	4.14E-02	1.53E+00	2.69E+00	-1.47E-01	2.12E-01	-3.15E+00	1.17E+01
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	1.98E+00	2.37E-01	1.39E+00	4.95E-02	1.67E+00	4.26E+00	-1.44E-02	2.12E-01	-3.28E+00	6.51E+00
CNC-3 Citric Acid	1.59E+00	1.49E+01	3.13E+00	1.76E-01	1.08E+00	4.26E+00	0.00E+00	2.12E-01	-2.63E+00	2.28E+01
CNC-4 Subcritical Water	3.47E+00	0.00E+00	0.00E+00	1.49E-01	4.19E+00	4.57E+00	0.00E+00	2.12E-01	-5.74E+00	6.85E+00
CNC-5 Wood Pellets	1.98E+00	2.37E-01	1.39E+00	4.95E-02	1.67E+00	2.58E+00	-1.44E-02	2.12E-01	-3.28E+00	4.83E+00
CNC-6 Wind Power	1.98E+00	2.37E-01	1.39E+00	4.95E-02	1.67E+00	3.29E-01	-1.44E-02	2.12E-01	-3.28E+00	2.57E+00
<b>Non carcinogenicity</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	2.61E-08	4.33E-06	4.21E-06	1.04E-07	6.36E-07	9.71E-07	0.00E+00	-1.39E-07		1.01E-05
CNC-1 CaO	2.61E-08	4.33E-06	1.53E-07	1.98E-08	9.05E-08	6.62E-07	-3.58E-08	-1.39E-07		5.11E-06
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	2.72E-08	6.81E-07	2.67E-07	2.37E-08	1.12E-07	6.32E-07	-3.49E-09	-1.39E-07		1.60E-06
CNC-3 Citric Acid	2.18E-08	4.97E-06	2.49E-07	8.40E-08	4.67E-07	7.38E-07	0.00E+00	-1.39E-07		6.39E-06
CNC-4 Subcritical Water	4.77E-08	0.00E+00	0.00E+00	7.11E-08	3.90E-07	5.36E-07	0.00E+00	-1.39E-07		9.06E-07
CNC-5 Wood Pellets	2.72E-08	6.81E-07	2.67E-07	2.37E-08	1.12E-07	1.32E-06	-3.49E-09	-1.39E-07		2.29E-06
CNC-6 Wind Power	2.72E-08	6.81E-07	2.67E-07	2.37E-08	1.12E-07	9.56E-07	-3.49E-09	-1.39E-07		1.93E-06
<b>Ozone depletion</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	3.05E-08	2.06E-07	7.25E-06	7.31E-08	9.55E-09	3.65E-07	0.00E+00	-5.21E-08		7.88E-06
CNC-1 CaO	3.06E-08	2.06E-07	4.65E-07	1.39E-08	1.36E-09	2.49E-07	-3.11E-08	-5.21E-08		8.83E-07
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	3.19E-08	3.24E-08	4.74E-07	1.67E-08	1.68E-09	2.32E-07	-3.03E-09	-5.21E-08		7.34E-07
CNC-3 Citric Acid	2.55E-08	1.78E-06	4.99E-07	5.92E-08	7.01E-09	2.74E-07	0.00E+00	-5.21E-08		2.60E-06
CNC-4 Subcritical Water	5.58E-08	0.00E+00	0.00E+00	5.01E-08	5.87E-09	1.94E-07	0.00E+00	-5.21E-08		2.54E-07

CNC-5 Wood Pellets	3.19E-08	3.24E-08	4.74E-07	1.67E-08	1.68E-09	3.28E-07	-3.03E-09	-5.21E-08		8.30E-07
CNC-6 Wind Power	3.19E-08	3.24E-08	4.74E-07	1.67E-08	1.68E-09	1.12E-07	-3.03E-09	-5.21E-08		6.13E-07
<b>Respiratory effects</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	1.36E-02	5.53E-03	1.62E-02	3.63E-04	2.01E-04	9.08E-03	0.00E+00	-1.30E-03		4.37E-02
CNC-1 CaO	1.36E-02	5.54E-03	1.09E-03	6.93E-05	2.86E-05	6.19E-03	-2.70E-03	-1.30E-03		2.26E-02
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	1.42E-02	8.71E-04	1.08E-03	8.29E-05	3.53E-05	5.82E-03	-2.63E-04	-1.30E-03		2.06E-02
CNC-3 Citric Acid	1.14E-02	1.36E-02	1.14E-03	2.94E-04	1.47E-04	6.84E-03	0.00E+00	-1.30E-03		3.21E-02
CNC-4 Subcritical Water	2.49E-02	0.00E+00	0.00E+00	2.49E-04	1.23E-04	4.88E-03	0.00E+00	-1.30E-03		2.89E-02
CNC-5 Wood Pellets	1.42E-02	8.71E-04	1.08E-03	8.29E-05	3.53E-05	5.88E-03	-2.63E-04	-1.30E-03		2.06E-02
CNC-6 Wind Power	1.42E-02	8.71E-04	1.08E-03	8.29E-05	3.53E-05	4.91E-04	-2.63E-04	-1.30E-03		1.52E-02
<b>Smog formation</b>	Feedstock	Hydrolysis chemicals	Other chemicals	Water consumption	WWT treatment	Energy	Byproduct	End-of-life		Total
CNC Baseline	1.12E-01	2.81E-01	7.45E-01	1.19E-02	1.07E-02	1.05E-01	0.00E+00	-1.51E-02		1.25E+00
CNC-1 CaO	1.12E-01	2.82E-01	1.08E-01	2.27E-03	1.53E-03	7.19E-02	-3.40E-02	-1.51E-02		5.28E-01
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	1.17E-01	4.43E-02	5.53E-02	2.72E-03	1.88E-03	6.87E-02	-3.31E-03	-1.51E-02		2.72E-01
CNC-3 Citric Acid	9.38E-02	9.31E-01	7.35E-02	9.66E-03	7.87E-03	8.03E-02	0.00E+00	-1.51E-02		1.18E+00
CNC-4 Subcritical Water	2.05E-01	0.00E+00	0.00E+00	8.17E-03	6.59E-03	5.82E-02	0.00E+00	-1.51E-02		2.63E-01
CNC-5 Wood Pellets	1.17E-01	4.43E-02	5.53E-02	2.72E-03	1.88E-03	8.08E-02	-3.31E-03	-1.51E-02		2.84E-01
CNC-6 Wind Power	1.17E-01	4.43E-02	5.53E-02	2.72E-03	1.88E-03	2.34E-02	-3.31E-03	-1.51E-02		2.26E-01



**Table S19.** Parameter range for sensitivity analysis for the case study of cellulose nanomaterials.

<b>Item</b>	<b>Minimum</b>	<b>Maximum</b>
IRR <sup>93,94</sup>	5%	20%
Installed cost of different areas <sup>67</sup>	-30%	+30%
Electricity <sup>95</sup>	4.80 US cent kWh <sup>-1</sup>	15.4 US cent kWh <sup>-1</sup>
Natural gas <sup>90</sup>	US\$0.085 kg <sup>-1</sup>	US\$0.62 kg <sup>-1</sup>
Project contingency	10%	35% (assumed)
Pulp consistency in acid hydrolysis <sup>8,15</sup>	5%	20%
CNC conversion rate <sup>21</sup>	-20%	+20%
CNC consistency in dilution	1% (assumed)	4% (assumed)
CNF consistency in dilution	0.5% (assumed)	2% (assumed)
Landfill gas recovery rate <sup>54</sup>	50%	90%
Electricity consumption	-20% (assumed)	20% (assumed)
Cradle-to-gate GHG emissions of pulp	-20% (assumed)	20% (assumed)
Electricity GHG emissions	-20% (assumed)	20% (assumed)
Acid recovery efficiency <sup>25,26</sup>	85%	95%
CNF yield <sup>49</sup>	90%	98%

**Table S20.** Life-cycle environment impact results of producing 1 dry kg CNF.

<b>Acidification</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	8.05E-03	0.00E+00	5.41E-05	0.00E+00	2.30E-02	-1.54E-03		2.96E-02
CNF-1 Enzymatic Hydrolysis	8.61E-03	2.04E-05	2.41E-04	3.03E-04	1.04E-02	-1.54E-03		1.80E-02
CNF-2 Wood Pellets	8.61E-03	2.04E-05	2.41E-04	3.03E-04	1.14E-02	-1.54E-03		1.90E-02
CNF-3 Wind Power	8.61E-03	2.04E-05	2.41E-04	3.03E-04	2.57E-03	-1.54E-03		1.02E-02
<b>Carcinogenicity</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	6.55E-08	0.00E+00	3.97E-09	0.00E+00	5.82E-07	-3.90E-08		6.12E-07
CNF-1 Enzymatic Hydrolysis	7.00E-08	1.52E-10	3.91E-09	1.06E-08	2.67E-07	-3.90E-08		3.13E-07
CNF-2 Wood Pellets	7.00E-08	1.52E-10	3.91E-09	1.06E-08	2.68E-07	-3.90E-08		3.14E-07
CNF-3 Wind Power	7.00E-08	1.52E-10	3.91E-09	1.06E-08	6.19E-08	-3.90E-08		1.08E-07
<b>Ecotoxicity</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	1.43E+01	0.00E+00	1.98E-01	0.00E+00	6.07E+01	-4.07E+00		7.12E+01
CNF-1 Enzymatic Hydrolysis	1.53E+01	5.85E-02	1.03E+00	1.21E+00	2.82E+01	-4.07E+00		4.18E+01
CNF-2 Wood Pellets	1.53E+01	5.85E-02	1.03E+00	1.21E+00	3.03E+01	-4.07E+00		4.39E+01
CNF-3 Wind Power	1.53E+01	5.85E-02	1.03E+00	1.21E+00	6.36E+01	-4.07E+00		7.72E+01
<b>Eutrophication</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	6.60E-03	0.00E+00	5.82E-05	0.00E+00	5.36E-02	-3.59E-03		5.67E-02
CNF-1 Enzymatic Hydrolysis	7.06E-03	2.03E-05	1.17E-04	1.99E-03	2.39E-02	-3.59E-03		2.95E-02
CNF-2 Wood Pellets	7.06E-03	2.03E-05	1.17E-04	1.99E-03	2.43E-02	-3.59E-03		2.99E-02
CNF-3 Wind Power	7.06E-03	2.03E-05	1.17E-04	1.99E-03	2.03E-03	-3.59E-03		7.62E-03
<b>Fossil fuel depletion</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	1.46E+00	0.00E+00	1.12E-02	0.00E+00	6.90E+00	-4.63E-01		7.91E+00
CNF-1 Enzymatic Hydrolysis	1.56E+00	2.32E-03	4.04E-02	3.01E-02	6.87E+00	-4.63E-01		8.04E+00
CNF-2 Wood Pellets	1.56E+00	2.32E-03	4.04E-02	3.01E-02	3.22E+00	-4.63E-01		4.39E+00
CNF-3 Wind Power	1.56E+00	2.32E-03	4.04E-02	3.01E-02	2.89E-01	-4.63E-01		1.46E+00
<b>Global warming</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life	Biogenic Uptake	Total
CNF Baseline	1.06E+00	0.00E+00	1.23E-02	-1.82E-16	8.13E+00	2.12E-01	-1.64E+00	7.78E+00
CNF-1 Enzymatic Hydrolysis	1.14E+00	2.23E-03	3.39E-02	1.47E-01	5.17E+00	2.12E-01	-1.75E+00	4.95E+00
CNF-2 Wood Pellets	1.14E+00	2.23E-03	3.39E-02	1.47E-01	3.80E+00	2.12E-01	-1.75E+00	3.58E+00
CNF-3 Wind Power	1.14E+00	2.23E-03	3.39E-02	1.47E-01	3.30E-01	2.12E-01	-1.75E+00	1.14E-01
<b>Non carcinogenicity</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	3.31E-07	0.00E+00	5.86E-09	0.00E+00	2.07E-06	-1.39E-07		2.27E-06
CNF-1 Enzymatic Hydrolysis	3.53E-07	2.96E-09	1.66E-08	1.86E-07	9.45E-07	-1.39E-07		1.37E-06
CNF-2 Wood Pellets	3.53E-07	2.96E-09	1.66E-08	1.86E-07	1.51E-06	-1.39E-07		1.93E-06
CNF-3 Wind Power	3.53E-07	2.96E-09	1.66E-08	1.86E-07	9.46E-07	-1.39E-07		1.37E-06
<b>Ozone depletion</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	1.22E-07	0.00E+00	4.13E-09	0.00E+00	7.78E-07	-5.21E-08		8.52E-07

CNF-1 Enzymatic Hydrolysis	1.31E-07	2.40E-10	1.87E-08	2.80E-09	3.51E-07	-5.21E-08		4.52E-07
CNF-2 Wood Pellets	1.31E-07	2.40E-10	1.87E-08	2.80E-09	4.30E-07	-5.21E-08		5.30E-07
CNF-3 Wind Power	1.31E-07	2.40E-10	1.87E-08	2.80E-09	9.67E-08	-5.21E-08		1.97E-07
<b>Respiratory effects</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	3.57E-03	0.00E+00	2.05E-05	0.00E+00	1.93E-02	-1.30E-03		2.16E-02
CNF-1 Enzymatic Hydrolysis	3.82E-03	2.71E-06	4.26E-05	5.89E-05	8.77E-03	-1.30E-03		1.14E-02
CNF-2 Wood Pellets	3.82E-03	2.71E-06	4.26E-05	5.89E-05	8.82E-03	-1.30E-03		1.14E-02
CNF-3 Wind Power	3.82E-03	2.71E-06	4.26E-05	5.89E-05	5.30E-04	-1.30E-03		3.15E-03
<b>Smog formation</b>	Feedstock	Pretreatment	Water consumption	Wastewater treatment	Energy	End-of-life		Total
CNF Baseline	1.79E-01	0.00E+00	6.74E-04	0.00E+00	2.25E-01	-1.51E-02		3.90E-01
CNF-1 Enzymatic Hydrolysis	1.92E-01	1.80E-04	2.10E-03	3.15E-03	1.03E-01	-1.51E-02		2.85E-01
CNF-2 Wood Pellets	1.92E-01	1.80E-04	2.10E-03	3.15E-03	1.13E-01	-1.51E-02		2.95E-01
CNF-3 Wind Power	1.92E-01	1.80E-04	2.10E-03	3.15E-03	2.44E-02	-1.51E-02		2.06E-01

**Table S21.** MSP of CNC and CNF scenarios at varied plant capacities.

<b>Plant Capacity (dry t nanocellulose day<sup>-1</sup>)</b>	<b>25</b>	<b>50</b>	<b>75</b>	<b>100</b>
CNC Baseline	\$7,909	\$7,540	\$7,412	\$7,341
CNC-1 CaO	\$4,644	\$4,286	\$4,164	\$4,096
CNC-2 H <sub>2</sub> SO <sub>4</sub> Recovery	\$5,403	\$4,601	\$4,261	\$4,061
CNC-3 Citric Acid	\$7,930	\$7,263	\$6,982	\$6,818
CNC-4 Subcritical Water	\$5,264	\$4,747	\$4,549	\$4,434
CNC-5 Wood Pellets	\$5,515	\$4,713	\$4,372	\$4,172
CNC-6 Wind Power	\$5,389	\$4,587	\$4,247	\$4,046
CNF Baseline	\$3,273	\$2,873	\$2,729	\$2,647
CNF-1 Enzymatic Hydrolysis	\$3,649	\$3,087	\$2,868	\$2,740
CNF-2 Wood Pellets	\$3,740	\$3,178	\$2,959	\$2,831
CNF-3 Wind Power	\$3,547	\$2,985	\$2,766	\$2,638

## Reference

- 1 R. Arvidsson, D. Nguyen and M. Svanström, *Environ. Sci. Technol.*, 2015, **49**, 6881–6890.
- 2 H. Nadeem, M. Dehghani, G. Garnier and W. Batchelor, *J. Clean. Prod.*, 2022, **342**, 130890.
- 3 K. C. Teh, R. R. Tan, K. B. Aviso, M. A. B. Promentilla and J. Tan, *Food Bioprod. Process.*, 2019, **118**, 13–31.
- 4 M. C. B. De Figueirêdo, M. De Freitas Rosa, C. M. Lie Ugaya, M. D. S. M. De Souza Filho, A. C. C. Da Silva Braid and L. F. L. De Melo, *J. Clean. Prod.*, 2012, **35**, 130–139.
- 5 S. Zargar, J. Jiang, F. Jiang and Q. Tu, *Biofuels, Bioprod. Biorefining*, 2022, **16**, 68–80.
- 6 X. Z. Sun, D. Moon, T. Yagishita and T. Minowa, *Trans. ASABE*, 2013, **56**, 1061–1067.
- 7 S. Haroni, H. Zaki Dizaji, H. Bahrami and M. González Alriols, *Ind. Crops Prod.*, , DOI:10.1016/j.indcrop.2021.114084.
- 8 H. Gu, R. Reiner, R. Bergman and A. Rudie, in *Proceedings from the LCA XV Conference*, 2015, pp. 33–42.
- 9 L. Zhang, X. Jia, Y. Ai, R. Huang, W. Qi, Z. He, J. J. Klemeš and R. Su, *J. Clean. Prod.*, , DOI:10.1016/j.jclepro.2022.131073.
- 10 T. J. Bondancia, G. Batista, J. de Aguiar, M. V. Lorevice, A. J. G. Cruz, J. M. Marconcini, L. H. C. Mattoso and C. S. Farinas, *ACS Sustain. Chem. Eng.*, 2022, **10**, 4660–4676.
- 11 D. M. do Nascimento, A. F. Dias, C. P. de Araújo Junior, M. de F. Rosa, J. P. S. Moraes and M. C. B. de Figueirêdo, *Ind. Crops Prod.*, 2016, **93**, 58–65.
- 12 R. M. Leão, P. C. Miléo, J. M. L. L. Maia and S. M. Luz, *Carbohydr. Polym.*, 2017, **175**, 518–529.
- 13 P. Gallo Stampino, L. Riva, C. Punta, G. Elegir, D. Bussini and G. Dotelli, *Molecules*, 2021, **26**, 1–20.
- 14 C. A. De Assis, M. C. Iglesias, M. Bilodeau, D. Johnson, R. Phillips, M. S. Peresin, E. M. Bilek, O. J. Rojas, R. Venditti and R. Gonzalez, *Biofuels, Bioprod. Biorefining*, 2017, **12**, 251–264.
- 15 C. A. de Assis, C. Houtman, R. Phillips, E. M. Bilek, O. J. Rojas, L. Pal, M. S. Peresin, H. Jameel and R. Gonzalez, *Biofuels, Bioprod. Biorefining*, 2017, **11**, 682–700.
- 16 M. Jonoobi, A. P. Mathew and K. Oksman, *Ind. Crops Prod.*, 2012, **40**, 232–238.
- 17 D. Moon, M. Sagisaka, K. Tahara and K. Tsukahara, *Sustain.*, DOI:10.3390/su9122368.
- 18 W. Wang, S. Fu, S. Y. Leu and C. Dong, *Cellulose*, 2018, **25**, 6465–6478.
- 19 Z. Zhu, W. Wang, X. Wang, X. Zhao, N. Xia, F. Kong and S. Wang, *Cellulose*, 2021, **28**, 9661–9676.
- 20 D. Echeverria, R. Venditti, H. Jameel and Y. Yao, *Environ. Sci. Technol.*, , DOI:10.1021/acs.est.1c06523.
- 21 Q. Wang, X. Zhao and J. Y. Zhu, *Ind. Eng. Chem. Res.*, 2014, **53**, 11007–11014.
- 22 D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton and D. Dudgeon, *Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover (No. NREL/TP-5100-47764)*, Golden, CO, 2011.
- 23 G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz and B. Weidema, *Int. J. Life Cycle Assess.*, 2016, **21**, 1218–1230.
- 24 P. Anastas and N. Eghbali, *Chem. Soc. Rev.*, 2010, **39**, 301–312.

- 25 J. Lemaire, C. L. Blanc, F. Duval, M. A. Théoleyre and D. Pareau, *Sep. Purif. Technol.*, 2016, **166**, 181–186.
- 26 F. J. Wolfaardt, L. G. Leite Fernandes, S. K. Cangussu Oliveira, X. Duret, J. F. Görgens and J. M. Lavoie, *Energy Convers. Manag.* *X*, DOI:10.1016/j.ecmx.2020.100074.
- 27 W. L. Luyben, *Chem. Eng. Process. - Process Intensif.*, 2018, **131**, 106–115.
- 28 Y. Cen, Z. Xiang, T. Han, Y. Long and T. Song, *Cellulose*, 2022, **29**, 7193–7209.
- 29 L. P. Novo, J. Bras, A. García, N. Belgacem and A. A. da S. Curvelo, *Ind. Crops Prod.*, 2016, **93**, 88–95.
- 30 L. P. Novo, J. Bras, A. García, N. Belgacem and A. A. S. Curvelo, *ACS Sustain. Chem. Eng.*, 2015, **3**, 2839–2846.
- 31 L. Chen, J. Y. Zhu, C. Baez, P. Kitin and T. Elder, *Green Chem.*, 2016, **18**, 3835–3843.
- 32 S. Mores, L. P. de S. Vandenberghe, A. I. Magalhães Júnior, J. C. de Carvalho, A. F. M. de Mello, A. Pandey and C. R. Soccol, *Bioresour. Technol.*, , DOI:10.1016/j.biortech.2020.124426.
- 33 M. Berovic and M. Legisa, *Biotechnol. Annu. Rev.*, 2007, **13**, 303–343.
- 34 J. Wang, Z. Cui, Y. Li, L. Cao and Z. Lu, *J. Clean. Prod.*, 2020, **249**, 119315.
- 35 M. Van den Bergh, B. Van de Voorde and D. De Vos, *ChemSusChem*, 2017, **10**, 4864–4871.
- 36 L. J. R. Nunes, J. C. O. Matias and J. P. S. Catalão, *Appl. Energy*, 2014, **127**, 135–140.
- 37 M. Jach-Nocoń, G. Pełka, W. Luboń, T. Mirowski, A. Nocoń and P. Pachytel, *Energies*, 2021, **14**, 4465.
- 38 Argonne National Laboratory, *The greenhouse gases, regulated emissions, and energy use in technologies (GREET) model*, 2022.
- 39 C. L. Archer and M. Z. Jacobson, *J. Appl. Meteorol. Climatol.*, 2007, **46**, 1701–1717.
- 40 F. Cassola, M. Burlando, M. Antonelli and C. F. Ratto, *J. Appl. Meteorol. Climatol.*, 2008, **47**, 3099–3116.
- 41 D. A. Johnson, in *TAPPI Nanotechnology Conference*, Vancouver, CA, 2014.
- 42 The University of Maine, UMaine Nanomaterial Pilot Plant, <https://umaine.edu/pdc/nanocellulose/umaine-nanomaterial-pilot-plant/>.
- 43 S. Ang, V. Haritos and W. Batchelor, *Cellulose*, 2019, **26**, 4767–4786.
- 44 X. Tian, P. Lu, X. Song, S. Nie, Y. Liu, M. Liu and Z. Wang, *Cellulose*, 2017, **24**, 3929–3942.
- 45 O. Nechyporchuk, M. N. Belgacem and J. Bras, *Ind. Crops Prod.*, 2016, **93**, 2–25.
- 46 S. H. Osong, S. Norgren and P. Engstrand, *Cellulose*, 2016, **23**, 93–123.
- 47 R. Ciriminna and M. Pagliaro, *Org. Process Res. Dev.*, 2010, **14**, 245–251.
- 48 Y. Qing, R. Sabo, J. Y. Zhu, U. Agarwal, Z. Cai and Y. Wu, *Carbohydr. Polym.*, 2013, **97**, 226–234.
- 49 W. Wang, M. D. Mozuch, R. C. Sabo and P. Kersten, *Cellulose*, 2015, **22**, 351–361.
- 50 W. Geng, R. A. Venditti, J. J. Pawlak, T. De Assis, R. W. Gonzalez, R. B. Phillips and H. min Chang, *Biofuels, Bioprod. Biorefining*, 2020, **14**, 225–241.
- 51 S. Towprayoon, T. Ishigaki, C. Chiemchaisri, A. O. Abdel-Aziz, M. E. Hunstone, C. Jarusutthirak, M. Ritzkowski and M. Thomsen, in *2019 Refinement to the 2006 IPCC Guidelines for National Greenhouse Gas Inventories*, 2019, vol. 5, pp. 6.1–6.49.
- 52 K. Lan, S. S. Kelley, P. Nepal and Y. Yao, *Environ. Res. Lett.*, 2020, **15**, 124036.
- 53 IPCC, in *Good practice guidance and uncertainty management in national greenhouse gas inventories*, 2000.

- 54 M. Anshassi, H. Sackles and T. G. Townsend, *Resour. Conserv. Recycl.*, 2021, **174**, 105810.
- 55 X. Chai, Z. Lou, T. Shimaoka, H. Nakayama, Y. Zhu, X. Cao, T. Komiya, T. Ishizaki and Y. Zhao, *Waste Manag.*, 2010, **30**, 446–451.
- 56 Q. Xia, C. Chen, Y. Yao, J. Li, S. He, Y. Zhou, T. Li, X. Pan, Y. Yao and L. Hu, *Nat. Sustain.*, 2021, **4**, 627–635.
- 57 S. Xiao, C. Chen, Q. Xia, Y. Liu, Y. Yao, Q. Chen, M. Hartsfield, A. Brozena, K. Tu, S. J. Eichhorn, Y. Yao, J. Li, W. Gan, S. Q. Shi, V. W. Yang, M. Lo Ricco, J. Y. Zhu, I. Burgert, A. Luo, T. Li and L. Hu, *Science (80-. )*, 2021, **374**, 465–471.
- 58 M. F. Ashby, *Materials and the environment: eco-informed material choice*, Elsevier, 2012.
- 59 M. M. Falinski, D. L. Plata, S. S. Chopra, T. L. Theis, L. M. Gilbertson and J. B. Zimmerman, *Nat. Nanotechnol.*, 2018, **13**, 708–714.
- 60 L. M. Gilbertson, L. Pourzahedi, S. Laughton, X. Gao, J. B. Zimmerman, T. L. Theis, P. Westerhoff and G. V. Lowry, *Nat. Nanotechnol.*, 2020, **15**, 801–810.
- 61 Y. Habibi, L. A. Lucia and O. J. Rojas, *Chem. Rev.*, 2010, **110**, 3479–3500.
- 62 A. B. Reising, R. J. Moon and J. P. Youngblood, *J-for*, 2012, **2**, 32–41.
- 63 Chemical Engineering Magazine, *Chem. Eng. Mag.*, 2015.
- 64 US BLS, Producer Price Indexes.
- 65 A. Dutta, M. Talmadge, J. Hensley, M. Worley, D. D. Harris, D. Barton, P. Groenendijk, D. Ferrari, B. S. D. Chemical, E. M. Searcy, C. T. Wright and J. R. Hess, *Process design and economics for conversion of lignocellulosic biomass to ethanol: thermochemical pathway by indirect gasification and mixed alcohol synthesis (No. NREL/TP-5100-51400)*, Golden, CO (United States), 2011.
- 66 US BLS, Labor Index by Bureau of Labor Statistics, <https://data.bls.gov/cgi-bin/srgate>.
- 67 M. S. Peters, K. D. Timmerhaus, R. E. West, K. Timmerhaus and R. West, *Plant design and economics for chemical engineers*, McGraw-Hill, New York, 2003.
- 68 A. Dutta, A. Sahir, E. Tan, D. Humbird, L. J. Snowden-swan, P. Meyer, J. Ross, D. Sexton, R. Yap and J. Lukas, *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels Thermochemical Research Pathways with In Situ and Ex Situ Upgrading of Fast Pyrolysis Vapors (NREL/TP-5100-62455;PNNL-23823)*, 2015.
- 69 K. Lan, Y. Xu, H. Kim, C. Ham, S. S. Kelley and S. Park, *Bioresour. Technol.*, 2021, **340**, 125726.
- 70 K. Lan, L. Ou, S. Park, S. S. Kelley and Y. Yao, *Energy Technol.*, 2019, 1900850.
- 71 IPCC, *Climate Change 2021: The Physical Science Basis AR 6 Work Group I*, 2022.
- 72 K. Lan, L. Ou, S. Park, S. S. Kelley, B. C. English, T. E. Yu, J. Larson and Y. Yao, *Renew. Sustain. Energy Rev.*, 2021, 110881.
- 73 J. E. F. Jensen and R. Pipatti, in *Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories*, 2006, pp. 339–348.
- 74 R. Pipatti, C. Sharma, M. Yamada, J. W. S. Alves, Q. Gao, G. H. S. Guendehou, M. Koch, C. L. Cabrera, K. Mareckova, H. Oonk, E. Scheehle, A. Smith, P. Svardal and S. M. M. Vieira, in *2006 IPCC Guidelines for National Greenhouse Gas Inventories*, 2006.
- 75 V. M. Thomas and W. Liu, *Assessment of Alternative Fibers for Pulp Production*, 2013.
- 76 R. Davis, L. Tao, E. C. D. Tan, M. J. Bidy, G. T. Beckham, C. Scarlata, J. Jacobson, K. Cafferty, J. Ross, J. Lukas, D. Knorr and P. Schoen, *Process Design and Economics for*

*the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons*, 2013.

- 77 K. Q. Fan, P. F. Zhang and Z. J. Pei, *Renew. Energy*, 2013, **50**, 786–794.
- 78 A. Pirraglia, R. Gonzalez, D. Saloni and J. Denig, *Energy Convers. Manag.*, 2013, **66**, 153–164.
- 79 P. Lamers, M. S. Roni, J. S. Tumuluru, J. J. Jacobson, K. G. Cafferty, J. K. Hansen, K. Kenney, F. Teymouri and B. Bals, *Bioresour. Technol.*, 2015, **194**, 205–213.
- 80 R. Davis, L. Tao, C. Scarlata, E. C. D. Tan, J. Ross, J. Lukas and D. Sexton, *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Catalytic Conversion of Sugars to Hydrocarbons*, Golden, CO (United States), 2015.
- 81 T. J. Bondancia, J. De Aguiar, G. Batista, A. J. G. Cruz, J. M. Marconcini, L. H. C. Mattoso and C. S. Farinas, *Ind. Eng. Chem. Res.*, 2020, **59**, 11505–11516.
- 82 F. Giacalone, M. Papapetrou, G. Kosmadakis, A. Tamburini, G. Micale and A. Cipollina, *Energy*, 2019, **181**, 532–547.
- 83 J. Hong, N. Van Duc Long, G. R. Harvianto, J. Haider and M. Lee, *Chem. Eng. Process. - Process Intensif.*, 2019, **136**, 107–115.
- 84 R. Davis, N. Grundl, L. Tao, M. J. Bidy, E. C. D. Tan, G. T. Beckham, D. Humbird, D. N. Thompson and M. S. Roni, *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update: Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Path*, Golden, CO (United States), 2018.
- 85 S. Kang, S. Heo and J. H. Lee, *Ind. Eng. Chem. Res.*, 2019, **58**, 944–955.
- 86 A. Yusuf, A. Giwa, E. O. Mohammed, O. Mohammed, A. Al Hajaj and M. R. M. Abu-Zahra, *J. Clean. Prod.*, DOI:10.1016/j.jclepro.2019.117760.
- 87 US EIA, Electricity-Sales (consumption), revenue, prices & customers, <https://www.eia.gov/electricity/data.php>.
- 88 T. Stehly, P. Beiter and P. Duffy, *2019 Cost of Wind Energy Review*, Golden, CO (United States), 2020.
- 89 D. Thrän, K. Schaubach, D. Peetz, M. Junginger, T. Mai-Moulin, F. Schipfer, O. Olsson and P. Lamers, *Biofuels, Bioprod. Biorefining*, 2019, **13**, 267–280.
- 90 US EIA, Natural Gas Prices, [https://www.eia.gov/dnav/ng/NG\\_PRI\\_SUM\\_A\\_EPG0\\_PIN\\_DMCF\\_M.htm](https://www.eia.gov/dnav/ng/NG_PRI_SUM_A_EPG0_PIN_DMCF_M.htm).
- 91 US DOE Office of EERE, *Water and Wastewater Annual Price Escalation Rates for Selected Cities across the United States*, 2017.
- 92 USGS, *Mineral commodity summaries 2022*, 2022.
- 93 J. R. Frank, T. R. Brown, T. A. Volk, J. P. Heavey and R. W. Malmsheimer, *Biofuels, Bioprod. Biorefining*, 2018, **12**, 846–856.
- 94 M. D. Lynch, *Metab. Eng.*, 2021, **65**, 42–51.
- 95 US EIA, Electric Power Monthly, [https://www.eia.gov/electricity/monthly/epm\\_table\\_grapher.php?t=epmt\\_5\\_6\\_a](https://www.eia.gov/electricity/monthly/epm_table_grapher.php?t=epmt_5_6_a).