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Conversion Economics of Forest Biomaterials: Risk and Financial Analysis of CNC Manufacturing

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Abstract: Commercialization of cellulose nanocrystals (CNC) presents opportunities for a wide range of new products. Techno-economic assessments can provide insightful information for the efficient design of conversion processes, drive cost-saving efforts, and reduce financial risks. In this study, we conducted techno-economic assessments for CNC production using information from the USDA Forest Products Laboratory Pilot Plant, literature, and discussions with experts. Scenarios considered included variations related to greenfield, co-location, and acid recovery. Operating costs, capital investment, minimum product selling price (MPSP), financial performance metrics, and the effect of drying and higher reaction yields on CNC manufacturing financials were estimated for each scenario. The lowest MPSP was found for the co-location without acid recovery scenario, mainly driven by capital investment. Risk analysis indicates 95% probability of manufacturing costs lower than USD 5900/t of CNC (dry equivalent) and a MPSP lower than USD 7200/t of CNC (dry equivalent). Finally, based on our analysis, we provide guidance on process optimizations that can improve the economic performance of CNC manufacturing process. In addition, a risk profile of the CNC manufacturing business is provided. © 2017 Society of Chemical Industry and John Wiley & Sons, Ltd

Keywords: cellulose nanocrystals; risk analysis; techno-economic analysis; CNC; conversion economics

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Introduction

Cellulose is the most abundant biopolymer available in nature,[1] obtained mainly from wood and plants, but also synthesized by algae, tunicates, and bacteria.[2] Its notable characteristics, such as biodegradability, optical and mechanical properties, have led to several studies of this material in its nanoscale form (nanocellulose). [3] Nanocellulose can be produced in different ways, resulting in different properties and dimensions: cellulose nanocrystals (CNC), cellulose nanofibrils (CNF), and bacterial cellulose (BC). CNC are obtained by acid hydrolysis, and consist of crystalline particles with 3–5 nm width and 50–500 nm length.[1,4] CNF are produced via mechanical treatments and present both amorphous and crystalline regions, with widths of 5–60 nm and lengths from 500 nm to several micrometers.[4,5] Wood is the preferred source of cellulose due to its availability and high cellulose content.[6] BC is produced by micro-organisms, with typical dimensions of 6–50 nm width by several micrometers in length.[4,7]

According to the Web of Science database, there are more than 5000 publications on nanocellulose (1994 to 2016),[8] with a significant increase in interest in the last decade. Patents granted during the same period, according to Google Patents database,[9] totaled more than 500 (Fig. 1). However, these publications are mainly related to technical assessments of production pathways,[2,3,10] evaluation of properties,[4,5] strategies for nanocellulose surface modifications, [11] and its applications.[12,13] To the best of our knowledge, no studies have been published considering the economic feasibility of the process (with detailed mass and energy balance as well as capital and operational costs). Currently, there is no industrial production of CNC, although pilot and demonstration facilities have been assembled with production capacities as high as 1000 kg/day (dry equivalent).[14] Additionally, information from companies is confidential and rarely shared. With the goal of addressing this need for information, the present work aims to collect and discuss technical, financial, and business intelligence information that may be suitable for future techno-economic analyses in CNC manufacturing. This work includes the development of a block diagram and a computational model to provide a comprehensive view of the CNC production process. Through a complete mass and energy balance and techno-economic analysis, major cost drivers, further opportunities for cost optimization, and supply chain for CNC manufacturing are assessed. In this work, we narrowed the analysis to the conversion process through sulfuric acid hydrolysis.

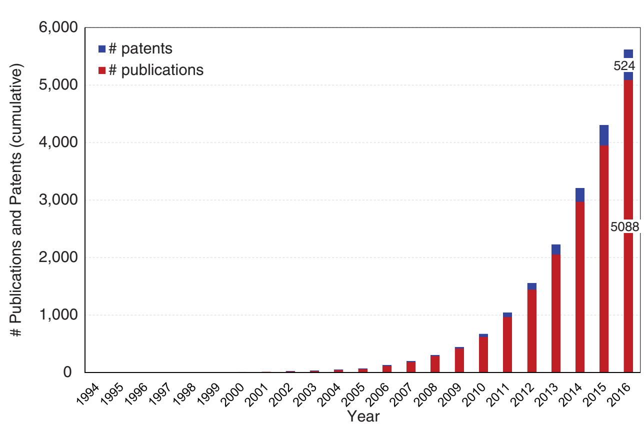

Figure 1. Cumulative number of patents and publications with the keywords *nanocellulose, cellulose nanocrystal(s), cellulose nanofibril(s), cellulose nanowhisker(s)* and *nanocrystalline cellulose*, from 1994 to 2016.

Motivation

As previously discussed, the remarkable characteristics of nanocellulose make it suitable for numerous applications. Moreover, growing research interest in nanotechnology, combined with the need for high value renewable materials, opens potential opportunities for nanocellulose production and commercialization.[15,16] For 2015, the global market for nanocellulose was estimated at USD 65 million and is expected to increase by a compounded annual growth rate (CAGR) of 30% between 2016 and 2021.[17] In terms of volume, the nanocellulose market size was 13 870 t (dry equivalent) in 2015 (t stands for metric tons) with main applications in composites and paper-processing segments.[17] Preliminary projections have estimated the nanocellulose market to range from 18 to 56 million t (dry equivalent), although there are uncertainties in market estimations, especially when novel applications are considered.[18] Main potential markets for nanocellulose include paints and coatings, cement manufacturing, automotive parts, and paper and paper packaging. [16,18,19] Some examples of specific applications of nanocellulose are: (i) viscosity modifier for paints,[19,20] (ii) reinforcing material for cement and polymers,[18,19,21] (iii) additive to improve barrier performance in coatings,[22] and (iv) wet-end additive to enhance strength and improve dewatering of paper.[23] Application of CNC at industrial scale has not been reported, although CNF is being industrially used in Japan as a thickening agent for pen ink, and to produce deodorant sheets for incontinence pads.[24,25]

Considering the potential of CNC in the near future, it seems appropriate to link the development of the production process and applications with financial/business intelligence. The results of conversion economics done at early stages of design may provide relevant information for potential players (producers and consumers), help identify opportunities for process improvement, guide future research and development efforts, and aid in the understanding of risks inherent to nanocellulose business.[26] This work aims to make the connection between technical and financial evaluations, providing information to guide future research work and inform investors or start-up companies considering to invest in the nanocellulose industry.

Literature review

Nanocellulose production processes

The processes to manufacture CNC and CNF are illustrated in Fig. 2. The starting material is biomass, mainly wood, non-woody plants, and crop residues. Biomass is processed in order to remove hemicellulose, lignin, extractives, and inorganic contaminants (an optional step for the CNF production).[2,27,28] These refinement processes have usually been executed in the pulp and paper industries (e.g. pulping and bleaching) and for the manufacturing of second-generation biofuels.[2,6] The resulting material after purification is pulp, containing at least 85% cellulose by mass.

CNF are produced when aqueous suspensions of pulp are subjected to an intensive mechanical process.[29] Common mechanical treatments are homogenization, microfluidization, and microgrinding.[11] Other treatments comprise cryocrushing, high-intensity ultrasonication, disk refining, and steam explosion.[30–32] Several pre-treatments have been proposed in order to reduce energy consumption and modify nanocellulose surface.[2] Examples of those are: TEMPO mediated oxidation (2,2,6,6-tetramethylpiperidine-1-oxyl radical),[33,34] enzymatic hydrolysis,[35] carboxymethylation, treatment with electrolyte solution, cryocrushing, acetylation,[36] and treatment using microemulsions.[37] Reported energy consumptions for CNF production from wood pulp can range from 500 kWh/t to 70 MWh/t, depending on pre-treatment and mechanical treatment applied.[5] We will cover the economics of CNF in a future publication.

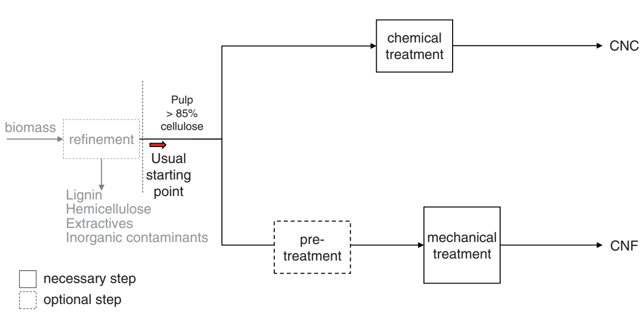

Figure 2. Production processes for CNC and CNF.

CNC are produced by the chemical treatment of pulp. Acid hydrolysis can be applied to dissolve the amorphous regions of the fibrils.[7,27] Sulfuric acid is one of the most common used acids for hydrolysis,[2,6] due to its low cost and better stability of the CNC suspensions.[7] CNC can be also obtained from microcrystalline, microfibrillated, or nanofibrillated cellulose.[2,7] There are also proprietary processes for CNC production, such as the AVAP® technology from American Process Inc. (API), and the R3™ technology from Blue Goose Biorefineries. The AVAP® process uses wood as a starting material, which is pre-treated with sulfur dioxide and ethanol to remove hemicelluloses, lignin, and amorphous cellulose. The material is then washed, bleached, and mechanically treated to disperse the nanocelluloses. Additional products include ethanol from sugars fermentation and energy from lignin combustion.[27] In R3™ technology, CNC is produced from agricultural and forestry biomass, through an oxidative process involving hydrogen peroxide and citric acid.[38,39] Other products obtained are specialty cellulose and microcrystalline cellulose (MCC).[39] Reported yields for CNC production from acid hydrolysis are usually low, between 30% and 50% based on pulp,[40] and between 15% and 30% based on wood (assuming 50% cellulose content in dry wood,[41] and 90% cellulose content in pulp).[42] However, there has been ongoing research aiming to minimize cellulose losses during the process. An example is the integrated production of CNC and CNF.[40,43]

CNC is usually obtained as a water-dispersed material, with concentrations varying from 3% to 11%.[27] Drying this material can be challenging due to the tendency of CNC to aggregate and cellulose's hydrophilic nature,[2,44] but these issues need to be overcome to reduce transportation costs and enhance additional applications.[6] Spray drying and freeze drying seem to be the most common technologies studied, probably because they are established at industrial scale for other manufacturing processes and may be able to maintain the nanoscale of the material to a certain extent.[27,30] Other processes studied include oven drying, supercritical drying, and drying at room temperature.[44,45]

Techno-economic assessments on CNC

From our literature research, we found only one techno-economic assessment involving CNC. This study evaluated the economic potential of CNC production in addition to a 2nd generation ethanol facility, using the residue of enzymatic hydrolysis as raw material. Only feedstock costs and an assumed price for CNC (USD 2210 / t) were taken into consideration in the analysis.[46] In addition, few information is available on the manufacturing costs of CNC. Cowie (2015) has estimated manufacturing costs to increase from USD 4000 / t to USD 16 000 / t when depreciation of equipment is considered.[47] However, no additional information on the manufacturing process and input values have been disclosed. Others have estimated production costs between USD 2000 / t and USD 15 000 / t.[48] Once more, there is no available information on how the cost estimation was performed, and no information on mass and energy balances.

Materials and methods

A description of materials and methods used to perform the techno-economic assessment for CNC manufacturing is presented next.

Feedstock

Dissolving pulp, viscose grade (> 90% cellulose content),[42] is used as feedstock.

Base-case scenario description

CNC manufacturing process is similar to the one available at USDA Forest Products Laboratory Pilot Plant. The main difference from the USDA facility to the simulated scenario in this study, in addition to plant capacity (pilot facility capacity is 10 kg / day),[14,49] is the existence of an acid recovery section in the simulated scenario. The base-case scenario (scenario 1) is a greenfield facility to produce CNC via acid hydrolysis, including an acid recovery section. By greenfield we mean that the project starts from bare ground. Plant capacity for all scenarios is 50 t / day of dry-equivalent CNC, and the process runs in continuous mode. Figure 3 shows the block diagram for scenario 1.

CNC manufacturing process starts at the feedstock handling and size reduction, where dissolving pulp (1) is shredded into small particles to allow acid penetration during hydrolysis. An exhaust system consisting of a cyclone and bag filters is connected to the shredder to prevent loss of material and emission of particulates to the atmosphere. The exhaust system vent is free of particulates (2). The shredded pulp (3) is then sent to the reaction step, where it is intensively mixed with sulfuric acid (H_2SO_4) at 64% (wt) concentration from the recovery section (4), in addition to acid makeup (5). Hydrolysis reaction occurs at 45°C with a residence time of one hour. After hydrolysis, the reactor output (6) is sent to a liquid–solid separation stage, where it is diluted with water (8), and passes through a series of centrifuges. The purpose of this step is to wash the CNC suspension from acid and sugars formed in the hydrolysis step, and to separate the suspended CNC particles from the liquid phase. The liquid outflow (9) consists of low concentration sulfuric acid (19% wt) and sugars (3% wt) that are sent to the acid recovery section; the centrifuge heavy phase is a CNC suspension at 10% (wt) solid content. Sodium chlorite ($NaOCl_2$) (7) is added to preserve the brightness in the final product and the excess of $NaOCl_2$ (10) is trapped in a scrubber using sodium sulfite (21) and caustic soda (NaOH) (23). The remaining acid in the CNC suspension is neutralized with caustic soda (NaOH) (11), generating sodium sulfate (Na_2SO_4). Before the CNC concentration step, the CNC suspension (12) passes through a filter to retain particles that may contaminate the final product. Then, the suspension is diluted with water (30) to reach a 2% (wt) CNC concentration. Next, the suspension passes through a diafiltration step, which separates the remaining salt and sugars from CNC. The retentate of diafiltration, a 2% (wt) CNC suspension with very small quantities of salt, is re-concentrated through ultrafiltration. The ultrafiltration retentate is the final CNC product (14), a suspension with 8% (wt) CNC. The permeates from diafiltration and ultrafiltration (13) are sent to the water reverse osmosis (RO) system to be purified. The purified water is reused in the plant as boiler feed water (28), to dilute the CNC suspension after reaction (8), and to dilute the CNC suspension before diafiltration (30). The retentate of the reverse osmosis, which has higher salt concentration, is then sent to the wastewater treatment (25).

The feed of the acid recovery section (9) is the weak acid solution from the liquid-solid separation phase. This stream is passed through a membrane system that removes CNC and sugars from the permeate. We have considered the permeate free of CNC and sugars for mass balance purposes, although it is known that there will be trace amounts of these materials in the real stream. The permeate is then concentrated from 19% (wt) to 64% (wt) of sulfuric acid in a sequence of evaporators. The recovered acid (4) is fed back to the reaction, and an acid makeup is necessary to replace system losses and sulfate that was bounded

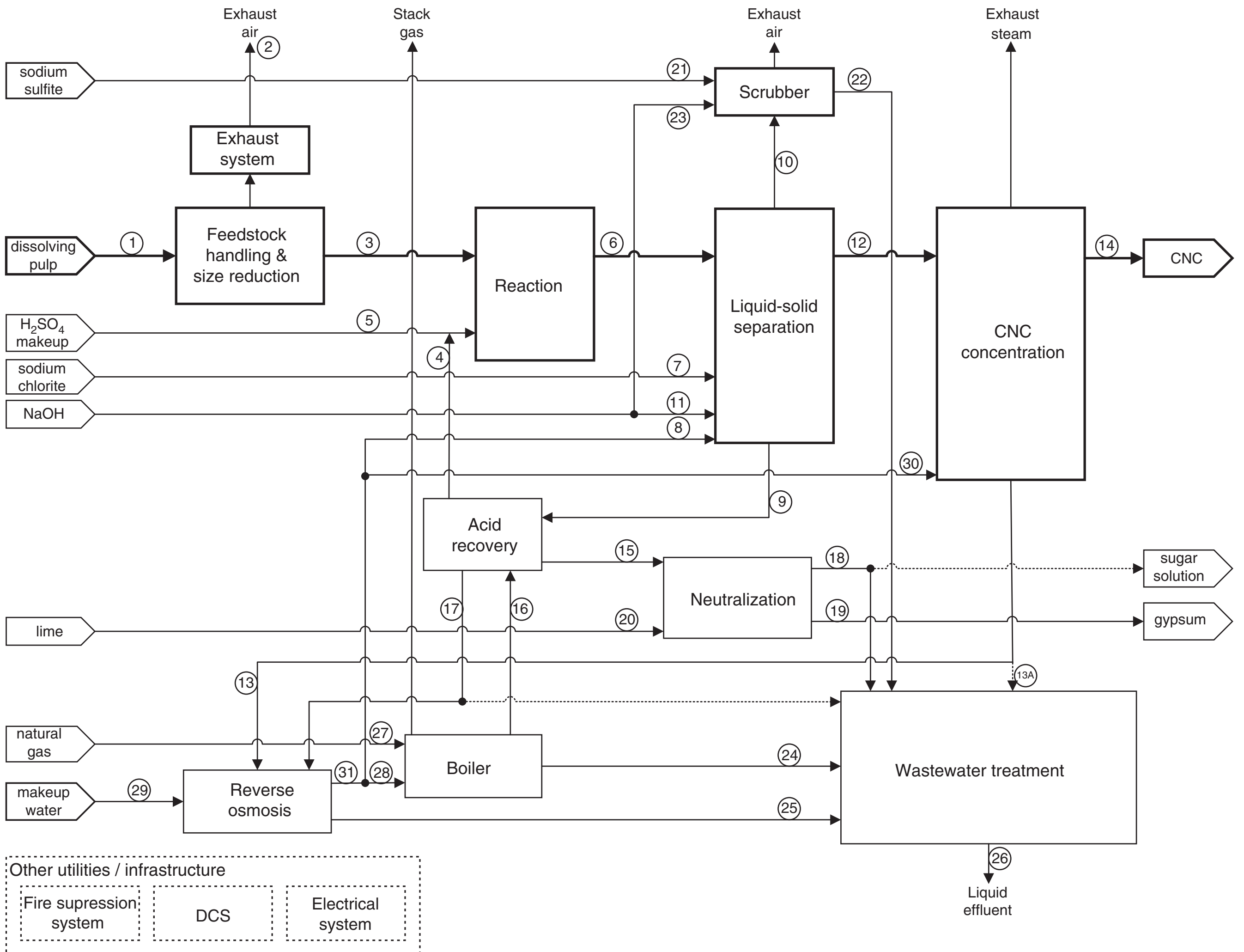

Figure 3. Block diagram for CNC manufacturing - scenario 1.

to CNC (5). As previously addressed, the pilot plant at Forest Products Laboratory does not include an acid recovery system; therefore we have assumed that the traces of CNC and sugars are not affecting the quality of the recovered acid, so it is being continuously recycled. The remaining CNC and sugar solution (15), which still contains about 15% (wt) of sulfuric acid, is then sent to the neutralization step. In this stage, lime (CaO) (20) is used to neutralize the acid, forming gypsum, which is further separated in a decanter and then sold (19). The liquid outlet is a 25% (wt) sugar solution (18) that is directed to the wastewater treatment, but can be sold if there is an available market. CNC concentrations in gypsum and in sugar solution are as low as 0.1% (wt).

In addition to the process equipment, investment in a greenfield facility includes additional areas, usually related to site infrastructure. Main utility equipment includes a steam boiler, a reverse osmosis system for water purification, and a wastewater treatment section. Additionally, a fire suppression system, distributed control system (DCS) and electrical system (motor control center, switchgear, and power distribution) have been considered in the capital investment.

Scenarios assessed

As previously described, the base-case scenario (scenario 1) contemplates a greenfield facility to produce CNC via acid hydrolysis, including an acid recovery section. Three additional scenarios were examined (Table 1). Scenario 2, greenfield context, considers the exclusion of the acid recovery section, which minimizes the capital investment. However, all the acid used in reaction must be neutralized with lime after the separation of CNC suspension

Table 1. CNC production scenarios assessed.

	Base-case (scenario 1)	Scenario 2	Scenario 3	Scenario 4
Context	Greenfield	Greenfield	Independent company co-location	Independent company co-location
Configuration	Acid recovery	No acid recovery	Acid recovery	No acid recovery

Table 2. Major process information used for mass balances.

Process information	Unit	Value adopted	Reference
CNC production	t/day (dry-equivalent)	50	Assumption
CNC hydrolysis yield (based on pulp)	% (wt)	50	Pilot plant[a]
Pulp consistency in reactor	% (wt)	20	Pilot plant[a]
Sulfuric acid concentration	% (wt)	64	Pilot plant[a]
Sulfuric acid makeup	t/t CNC dry	0.9[b] / 6.4[c]	Mass balance
Lime consumption	t/t CNC dry	0.5[b] / 3.6[c]	Mass balance
CNC concentration at centrifuges outlet	% (wt)	10	Laboratory result[d]
CNC concentration after ultrafiltration	% (wt)	8	Pilot plant[a]

[a]Pilot plant process data from trials at USDA Forest Product Lab (Madison, WI).[49]
[b]With acid recovery.
[c]Without acid recovery.
[d]Data from experiments ran at USDA Forest Product Laboratories (Madison, WI).

using centrifuges. Therefore, the production costs are expected to increase in relation to the base-case scenario. Significant quantities of gypsum ($CaSO_4$) are generated in the neutralization reaction, which is recovered by precipitation, and might be sold as a byproduct. Additionally, the boiler and reverse osmosis areas will suffer modifications due to lower steam demand and higher fresh water consumption.

Scenario 3 contemplates the co-location of the CNC plant (with acid recovery) within a pulp mill, done by an independent company. *Independent company* means a company that is not the same as that of the pulp mill. If the co-location is done by the same company, some additional savings are possible, such as labor and land cost (one example would be the Metsä Group Biorefinery in Finland).[50] In the co-location context, pulp for CNC production is readily available, and freight costs are not summed to the feedstock cost. However, the main savings would be on capital investment, due to shared infrastructure, utilities, and effluent treatment system when compared to the greenfield context. It is assumed that the adjacent mill can supply utilities and treat the CNC effluent in the co-location scenarios. The CNC manufacturer pays by quantity of steam consumed and effluent treated. Scenario 4 also considers co-location; however, it eliminates the acid recovery section. Additional revenues are possible if the sugar solution is sold, but this case is not in the scope of this publication.

Process information

Table 2 lists the main process information used for mass and energy balances, for all four scenarios assessed. Most of the information is based on data obtained from the USDA Forest Products Laboratory Pilot Plant facility in Madison, WI, USA.[49,51] Other sources of information are literature, experimental results from USDA laboratory trials,[51] and information kindly supplied by companies,[52] based on their commercial experience. The complete mass balance is not available in this paper, but the authors can be contacted to share the working files.

Cost information

Major cost information used to run the analysis are listed in Table 3. Unless otherwise noted, raw materials costs are considered as delivered to the manufacturing facility. Several cost data were retrieved from FisherSolve™ for the 1st quarter of 2016. When not available on FisherSolve™, other sources were consulted, such as ICIS for chemical costs and U.S. Energy Information Administration (EIA) for electricity cost.[53,54] All cost values were corrected to the start-up year (2019), using an inflation rate of 1.2% (average from

Table 3. Major cost information for CNC production.

Input	Value (2019)	Unit	Reference
Dissolving pulp (viscose grade)	763	USD/t (FOB in pulp mill)	RISI database[57]
Sodium sulfite	342	USD/t	FisherSolve™
Sulfuric acid (100%)	90	USD/t	ICIS website[53]
Sodium chlorite (crystals, 80%)	5,004	USD/t	ICIS website[53]
Caustic soda (100%)	388	USD/t	FisherSolve™
Lime	137	USD/t	FisherSolve™
Natural gas	4.5	USD/MBTU	FisherSolve™
Steam	11.5	USD/t	FisherSolve™
Tap water	0.66	USD/t	Environmental Protection Agency[58]
Electricity	69.5	USD/MWh	US Energy Information Administration[54]
Effluent treatment	0.6	USD/t treated	Ulrich and Vasudevan (2006)[56]
Gyspum	9.5	USD/t (FOB)	US Geological Survey (2015)[59]
Freight for pulp	50	USD/t	Expert info – 500-mile radius (additional to pulp cost)

2012 – 2015, according to U.S. Treasury data).[55] Costs were considered as average values for US, without taking into account any specific location. For the co-location context, steam is bought from the adjacent pulp mill and the cost to treat effluents externally is based on the quantity treated.[56] For all scenarios, tap water is used as water makeup.

Financial assumptions

Financial assumptions for this study are listed in Table 4. For all scenarios, it is assumed that the construction starts in 2016 (year -3) and the plant will be built in 3 years. We acknowledge that for co-location scenarios construction time can be shortened; however, this was not considered for this analysis. The facility starts-up in 2019 (defined as year 0), producing 80% of its capacity, and reaching 100% on year 1 (2020). It is assumed that the production rate will then increase by 0.5% per year, due to process improvements. Project financial horizon evaluation is 10 years after start-up; terminal value at year 10 was estimated as 5 times EBITDA (Earnings Before Interest, Taxes, Depreciation and Amortization), although the estimated terminal value is close to 8 times EBITDA (based on the discounted value at year 10 for additional 10 years of operation). Tax rates are based on NREL report for lignocellulosic ethanol production,[60] and have been compared to other sources.[61,62] The minimum product selling price (MPSP) is calculated at zero net present value (NPV) at an assumed hurdle rate of 16%. This hurdle rate was chosen considering the weighted average cost of capital (WACC) for the specialty chemicals industry, which is around 8%.[63]

Financial metrics

Main financial metrics used in this work are briefly explained.

Net Present Value (NPV) is the sum of the all discounted cash outflows and inflows of the project.[64] The values are discounted to the end of year -3 (2016) using a hurdle rate.

Hurdle rate is the minimum rate that a project should achieve to be accepted.[65]

Return on Investment (ROI) is calculated by dividing the after-tax profit by the capital employed (working capital + asset value) year by year.[64]

Minimum product selling price (MPSP) is the minimum price that the product should be sold to set NPV zero at the defined hurdle rate.

Payback period is the time required to pay off the initial investment.[66] It is calculated as the number of years needed for the cumulative free cash flow to become positive.

Capital investment

Capital investment was based on information provided by American Process Inc. (API).[52] This estimate includes ISBL and OSBL equipment, with an accuracy of + 35% / - 20%. ISBL stands for inside battery limits and includes equipment associated with the primary streams of the process; OSBL stands for outside battery limits and refers to equipment not included in ISBL (units that support the main process, such as utilities, fire-suppression systems and effluent treatment). Land development and infrastructure were assumed as a fixed value of USD 15 million for the

Table 4. Financial assumptions.

Input	Value	Units	Reference
Project start	2016	year	assumed
Financial evaluation horizon	10[a]	years	assumed
Production on year 0 (2019)	80%	% of plant capacity	assumed
Production on year 1 (2020)	100%	% of plant capacity	assumed
% of CAPEX spent in year –3 (2016)	50% 35%	% of direct costs % of indirect costs	assumed
% of CAPEX spent in year –2	50% 35%	% of direct costs % of indirect costs	assumed
% of CAPEX spent in year –1	30%	% of indirect costs	assumed
Hurdle rate	16%	%	Damodaran (2016)[63]
Depreciation schedule, straight line	10	years	assumed
Working capital,	10%	% of sales of next year	assumed
Tax rate on EBIT	35%	%	NREL[60]
Terminal value in year 10	5	multiple of EBITDA	assumed
Overall equipment efficiency	90%	%	assumed
Maintenance cost	2%	% of RAV[b]	assumed
Capital reinvestment	1%	% of RAV[b]	
Hourly and administrative staff	42 40	in greenfield context in co-location context	assumed
Overhead costs	3%	% of sales	assumed
Other fixed costs (insurance, property taxes and emissions)	1.5%	% of RAV[b]	assumed

[a] Years after production start.
[b] RAV = Replacement Asset Value.

greenfield context. For the co-location context, land and infrastructure costs were assumed as 75% of the greenfield value. Project management and engineering expenses sum up to 22% of installed equipment costs and a contingency of 25% of installed equipment cost was considered to cover unforeseen and unexpected issues. Scale factors were used, and varied from 0.6 (tailor designed equipment) to 1 (modular equipment).

Block diagrams

Microsoft Visio® was used to create block diagrams and process flowsheets for each scenario accessed.

Techno-economic assessment

Microsoft Excel® spreadsheets were used to perform the mass and energy balances and financial analysis. Detailed mass and energy balances were performed to estimate flowrates and the consumption of feedstock, chemicals, and energy. Financial assessment was performed through cash flow analysis and main financial metrics were calculated (NPV, ROI, payback).

Sensitivity and probability analyses

For the scenario with the lowest MPSP, sensitivity and probability analyses were executed to assess the impact of uncertainties on the distribution probability of manufacturing costs and MPSP. For sensitivity analysis, all input costs were varied by ± 25% independently, and the impact on the MPSP was recorded. Those inputs with major impacts were selected to perform probability analysis.

Probability analysis allows us to understand what the chances for an event to happen are. For example, it is possible to understand what is the probability for CNC manufacturing cost (output) to be within a range or below or above a value, based on the variation of the inputs. In short, the process is as follows: (i) Major cost driver variation is gathered (based on historical data, forecasted trends, or other source of information). If historical data is used, it is recommended to use the same period for all inputs (e.g. five years), and to adjust the data using a price index, so inflation is not considered as part of the variability assessed. Then (ii) a distribution probability model is adjusted to the data collected. Next, (iii) all inputs are linked to the output using a probability software simulator, and iv) a Monte Carlo simulation is executed using a specialized software (in our case @Risk). The outcome of the simulation is the probabilistic distribution of the output, the manufacturing cost of CNC.

Additional analyses

In addition to the four scenarios evaluated, an assessment of the CNC supply chain is performed. Preliminary calculations of capital and operating costs for drying CNC, compared to gains in transportation costs are done to shed light on the importance of developing drying technologies to trigger CNC commercialization from a financial point of view. However, the need to dry the product is driven by application purposes. Some reported applications for dried nanocellulose are nanocomposites and films.[1,4]

Another analysis includes the impact of increasing hydrolysis reaction yields to provide a more comprehensive view of the process, its limitations and potential for manufacturing cost reduction.

Results and discussion

Mass balance results

Main inflows and outflows for scenario 1 (greenfield with acid recovery) are presented in Table 5. There is a high consumption of makeup water (flow 29), which is mainly used in the liquid–solid separation and CNC concentration steps. Other significant values, besides CNC production (flow 14) are sugar and gypsum generated as by-products (flows 18 and 19).

In scenarios 2, 3, and 4, final product flow is the same, but sulfuric acid (5) and water makeup (29), as well as lime (20) consumption are changed. When acid recovery is not considered (scenarios 2 and 4), the sulfuric acid make-up is substantially higher, and consequently the lime consumed for neutralization. Therefore, gypsum production

Table 5. Main inflows and outflows of CNC mass balance (refer to Fig. 3 for stream numbers).

(Stream number) Stream description→	(1) Dissolving pulp	(5) H_2SO_4 makeup	(7) Sodium chlorite	(11) Caustic soda	(20) Lime	(21) Sodium sulfite	(29) Makeup water[a]
Component↓	(t/day)	(t/day)	(t/day)	(t/day)	(t/day)	(t/day)	(t/day)
Pulp	100.5						
Water	5.3	24.7		12.3		0.035	2,420
Sulfuric acid		45.0					
Sodium chlorite			0.13				
Sodium sulfite						0.035	
NaOH				4.1			
Lime					22.6		
Total	**105.8**	**69.7**	**0.13**	**16.4**	**22.6**	**0.07**	**2,420**

(Stream number) Stream description→	(2) Pulp loss[b]	(14) CNC final product	(18) Sugar solution	(19) Gypsum	(26) Liquid effluent
Component↓	(t/day)	(t/day)	(t/day)	(t/day)	(t/day)
Pulp	0.5				
Water		574.4	129.8	41.5	1,720
CNC		50.0	0.2	0.1	0.4
Sugar		0.1	41.4	13.3	0.9
Gypsum				54.8	
Sodium sulfate and salts		0.5			7.1
Total	**0.5**	**624.9**	**171.4**	**109.7**	**1,728.4**

[a] Water for steam generation not included.
[b] This flow represents the amount of pulp that is lost.

(19) increases by eight-fold. Makeup water (29) increases when the acid recovery section is not available, since the water recovered during acid concentration (17) is zero. Without acid recovery, the sugar solution (18) concentration drops from 24% (wt) to 4% (wt). The co-location option (scenarios 3 and 4) does not change the main flows of material balance when compared to the respective greenfield scenarios (scenarios 1 and 2), but the costs associated with steam and wastewater treatment change. The complete model can be obtained from the main authors upon request.

Capital investment

Estimated capital investments are between USD 95 million and USD 188 million (Fig. 4). These costs do not include the drying section, since the CNC is assumed to be sold as a suspension with 8% (wt) solids concentration. It might be necessary to include a refrigerated storage for CNC suspension; nevertheless, high contingency values (25%) were assumed to cover unexpected costs. In all scenarios, the direct costs represented around 60% of total capital investment. The scenarios in greenfield context (scenarios 1 and 2) account for higher capital investment than the co-location scenarios (scenarios 3 and 4). Additionally, configurations that include an acid recovery section (scenarios 1 and 3) have higher capital investments. Major contributors to the capital investment in the greenfield context are the acid recovery (scenario 1), and the effluent treatment section that will reflect in higher indirect costs, such as contingency and engineering. Likewise, building costs are higher for greenfield scenarios. When the acid recovery section is not considered, capital costs are decreased by 29% and 38% for the greenfield and co-location contexts; however, manufacturing costs will increase.

Manufacturing costs and MPSP

Breakdown of manufacturing costs and MPSP are illustrated in Fig. 5. The costs are for the first year of full production (2020). Depreciation costs are included to show the impact of capital investment, although depreciation is a non-cash cost. Calculated manufacturing costs vary from USD 3632 to USD 4420 / t of CNC (dry equivalent). In all situations, the main cost driver is fiber (between 38% and 45% of total manufacturing costs), followed by depreciation. For configurations without acid recovery, sulfuric acid and lime contribute to about 25% of the manufacturing cost.

MPSP was calculated for all scenarios considering the hurdle rate defined (16%). Scenario 1 (greenfield and acid recovery section) presents the highest MPSP – USD 6070 /t CNC (dry equivalent), which is about 26% higher than scenario 4. The best investment option would be the one with the lowest MPSP. As the difference between MPSP for co-location scenarios is relatively small (around 6%), the best investment would be the one with lower capital investment,

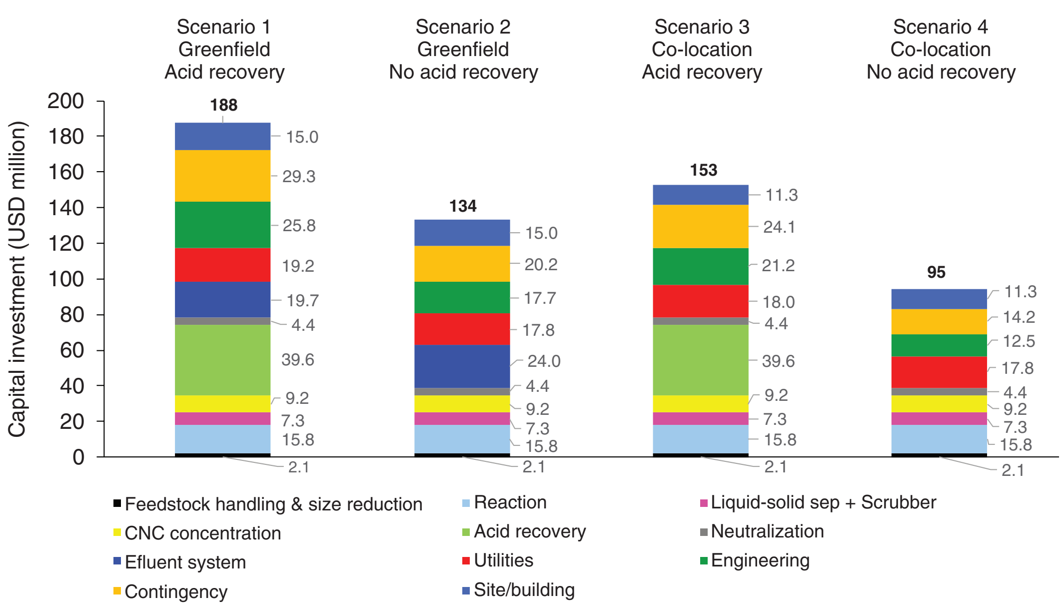

Figure 4. Capital investment comparison for scenarios 1–4.

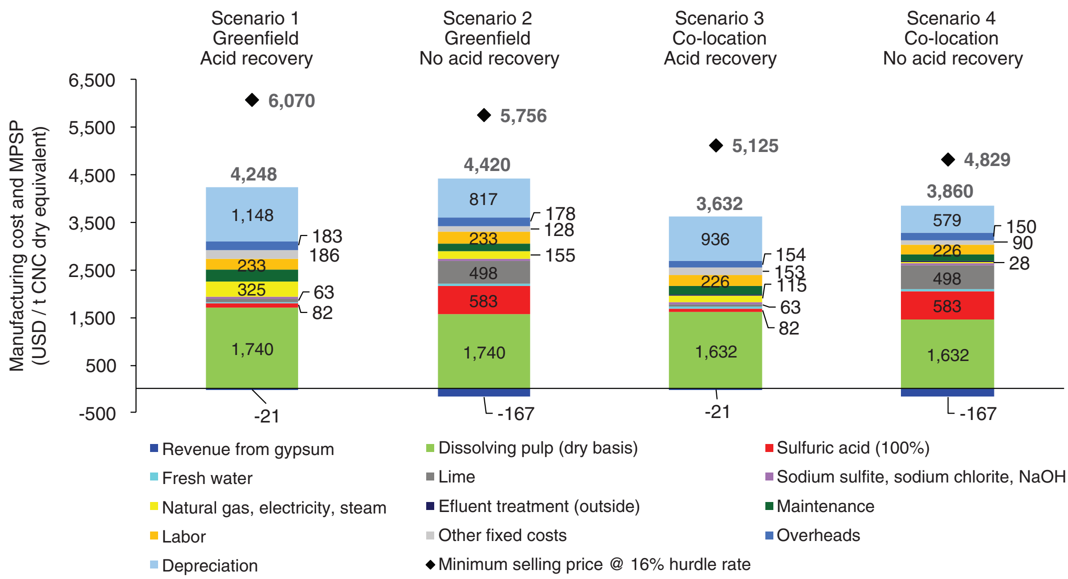

Figure 5. Manufacturing cost breakdown and MPSP for scenarios 1–4, for year 2020.

which is scenario 4. Since less amount of capital is needed, lower payback is achieved in this scenario. Additionally, improvements and new investments in the facility can be done in the future to reduce manufacturing costs.

Return on Investment and payback period

ROI was calculated for all scenarios in each year of operation (Fig. 6), in addition to the payback period (Table 6). However, in all scenarios the CNC price adopted was the lowest MPSP calculated (USD 4829 / t CNC (dry equivalent)).

As the asset is depreciated over the years, ROI values tend to increase for all scenarios over time. By the fifth year of operation (2023), the average ROI was 6.7% for the greenfield contexts and 17.2% for the co-location contexts. However, after year 10, ROI values for greenfield scenarios

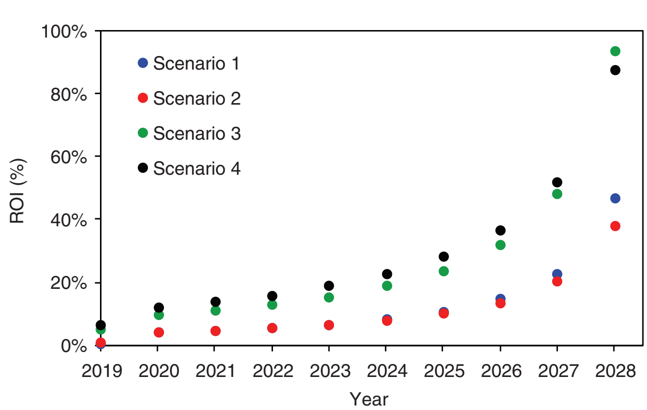

Figure 6. Return on investment (ROI) for scenarios 1–4.

Table 6. Payback period for scenarios 1–4.

	Base-case (Scenario 1)	Scenario 2	Scenario 3	Scenario 4
Payback period (years)[a]	10.2	10.4	8.1	7.6

[a]considering CNC selling price = USD 4829/t of CNC (dry equivalent).

are less than half of estimated ROI for co-location scenarios (average 42% for greenfield and 91% for co-location). Estimated paybacks varied from 7.6 years (scenario 4) to 10.4 years (scenario 2).

Sensitivity analysis

Sensitivity analysis was conducted to identify the inputs variation with higher influence on MPSP. Inputs evaluated were: costs of dissolving pulp, electricity, pulp freight, natural gas, sulfuric acid, lime, caustic soda, fresh water, sodium chlorite, steam, effluent treatment, and sodium sulfide, in addition to the capital investment and gypsum prices. Tornado diagram was chosen due to the high quantity of variables to be assessed. A variation of ±25% on each input was considered for the analysis. The results for scenarios 1 and 4 are presented in Fig. 7 and Fig. 8, respectively. These scenarios were chosen since they present the highest and lowest MPSP.

For both scenarios capital investment and dissolving pulp cost are the inputs with the highest effect on the MPSP. For scenario 1, a 25% increase in capital investment leads to an increase in MPSP of USD 853 / t CNC

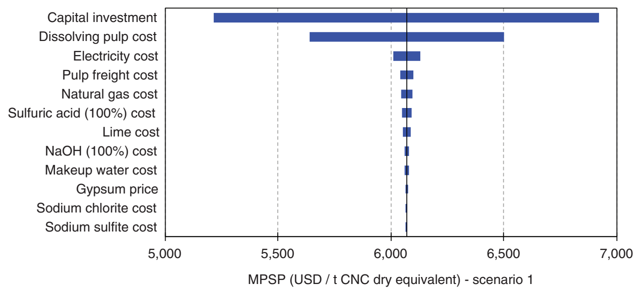

Figure 7. Tornado diagram for scenario 1.

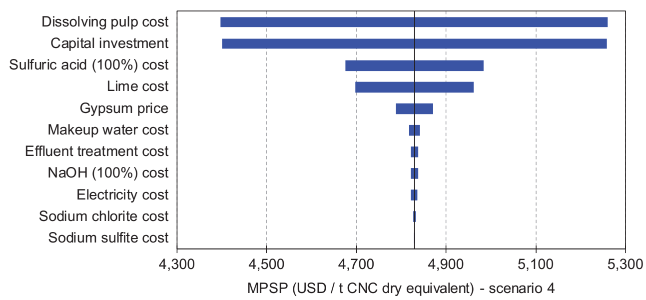

Figure 8. Tornado diagram for scenario 4.

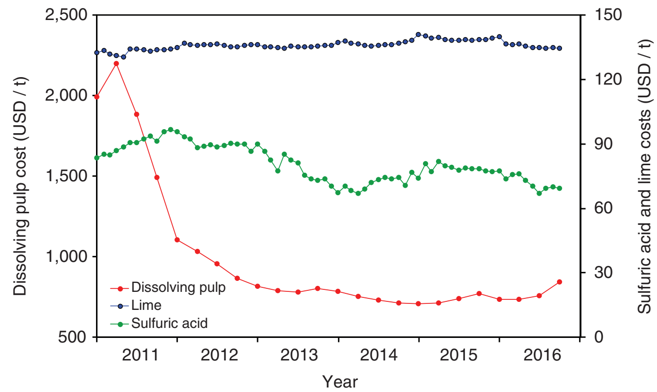

Figure 9. Historical costs for dissolving pulp, sulfuric acid and lime.

(dry equivalent), while the same increase (25%) in dissolving pulp cost impacts the MPSP by USD 431 / t CNC (dry equivalent). Variations of 25% for electricity and other costs have marginal impact on MPSP (1% or lower).

For scenario 4, a 25% increase in pulp cost would increase the MPSP by USD 431 / t CNC (dry equivalent), and if the capital investment is 25% higher, an increase of USD 428 / t CNC (dry equivalent) on MPSP is expected. Acid and lime costs have higher impact on MPSP when compared to scenario 1, due to the absence of the acid recovery section, and consequently an increased consumption of these chemicals. Variation of 25% in acid and lime costs results in a variation of about 3% in MPSP. Electricity is not relevant in this scenario since the effluent is treated outside the plant. It is uncertain that gypsum can be sold as a by-product, however the variation of gypsum prices has an impact lower than 1% in MPSP for both scenarios assessed.

Probability analysis

Probability analysis for manufacturing costs was conducted for scenario 4. This assessment was carried out according to the steps mentioned in the materials and methods section. From Fig. 8, it can be seen that variations in the costs of dissolving pulp, sulfuric acid, and lime, in addition to capital investment are the ones that have the highest impact in the MPSP. Dissolving pulp, sulfuric acid and lime costs are presented in Fig. 9 (2011 to 2016). Historical monthly costs for sulfuric acid and lime were calculated using the respective producer-price index for commodities,[67,68] and then converted to real values using the consumer price index.[69] Probability distribution for capital investment was defined as uniform, based on the accuracy of API estimate (+35%/–20%).

Probability distribution curves were adjusted to functions using @Risk software for the major inputs using historical data (Fig. 10). The blue bars represent the probability distribution of the historical data. The red line is the adjusted function for each probability distribution.

A 5000-iteration Monte Carlo simulation was executed. The simulation output is the probability distribution of CNC manufacturing cost (Fig. 11). Based on the assumptions made for CNC production, there is a 100% chance that the manufacturing costs are below USD 7128 / t of CNC (dry equivalent) for scenario 4. Chances of manufacturing cost below USD 3860 (the deterministic calculated value), are only 12%.This is due to the effect of the inputs variation, which is captured in the probability analysis. We believe that an investor should consider the results from probability analysis as a base estimation for manufacturing costs. Table 7 lists manufacturing costs and proxy values for MPSP at 50%, 75%, 95% and 100% probabilities. It can be noticed that a 5% decrease in probability (from 100% to 95%), changes the maximum calculated manufacturing cost and consequently the MPSP by USD 1300 / t of CNC (dry equivalent), which corresponds to a 15% reduction.

Figure 12(a) illustrates regression coefficients from the probability analysis and Fig. 12(b) shows the descaled values of the coefficients. From Fig. 12(a), the longer the bar, the higher the impact of an input variability on the output. In this case, dissolving pulp variability is the

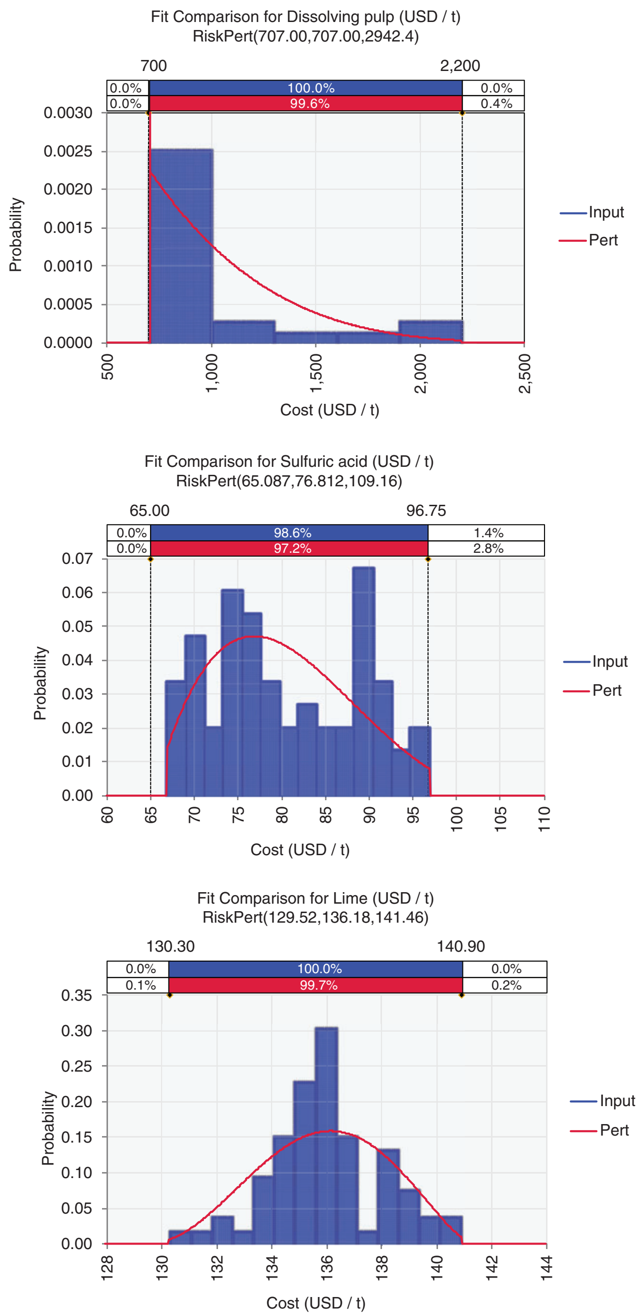

Figure 10. Adjusted distribution probabilities for dissolving pulp, sulfuric acid, and lime costs (USD/t).

major contributor for variability in production costs, followed by the capital investment. Figure 12(b) shows the descaled regression factors. They were calculated by multiplying the regression coefficients by the standard deviation of the output (manufacturing cost) and dividing the result by the standard deviation of each input.[70] The descaled values obtained show by how many units the output varies based on an unit change in the input. It

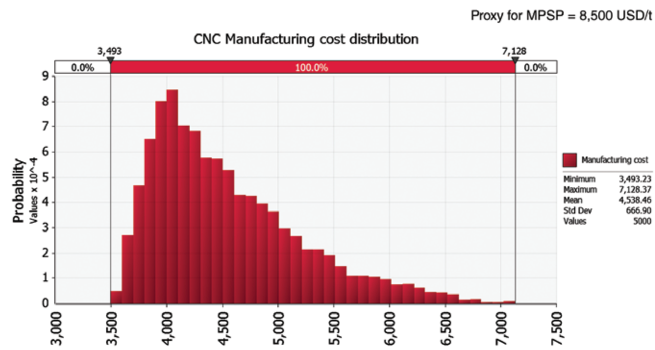

Figure 11. Distribution curve for CNC manufacturing cost (scenario 4).

Table 7. Manufacturing costs and proxy MPSP at different probabilities.

Probability	Manufacturing cost (USD/t CNC dry equivalent)	Proxy for MPSP (USD/t CNC dry equivalent)
50%	≤4,380	≤5,450
75%	≤4,900	≤6,000
95%	≤5,900	≤7,200
100%	≤7,128	≤8,500

can be seen that a change in the capital cost (in this case USD 1 million) will cause a change in the manufacturing cost by USD 8.30 / t CNC (dry equivalent), followed by the sulfuric acid cost (a change of USD 1 in H_2SO_4 cost changes the production cost by USD 6.50 / t CNC (dry equivalent)).

Additional analyses

Some preliminary calculations were performed to identify potential improvements in manufacturing cost and MPSP of CNC. This analysis includes potential savings by increasing reaction yield and the trade-off of drying the final product versus reductions in transportation costs.

Potential savings with increased reaction yields

It can be noticed from Table 2 that reaction yield for the hydrolysis reaction is relatively low (about 50%). The advantages of higher process yields are significant and there are ongoing studies to improve process conditions to reach enhanced CNC yields and minimize acid consumption.[71] However, the maximum yield is limited by the crystalline portion of the material, which for dissolving pulp is expected to be higher than 50%. Additionally, yields of 75% for CNC have been reported for sulfuric acid

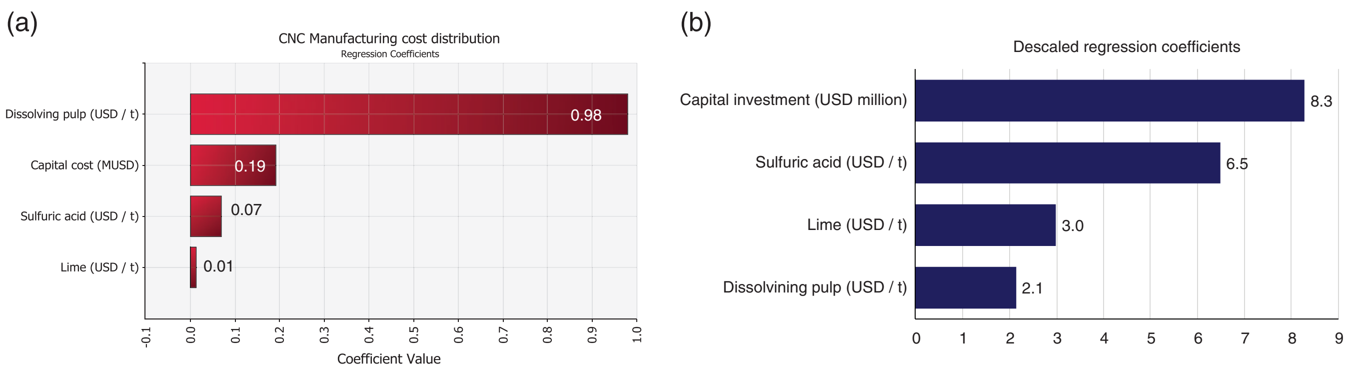

Figure 12. (a) Tornado regression coefficients, (b) Descaled regression coefficients for scenario 4.

hydrolysis (based on bleached eucalyptus pulp).[71] The use of different processes, such as HCl at vapor phase, have shown yields greater than 95% based on cotton cellulose fibers.[72] A preliminary analysis was conducted to calculate the impact of higher yields in the MPSP. The relation between improvement in yield and minimum product selling price is linear for scenarios 1 and 4 (Fig. 13). If the

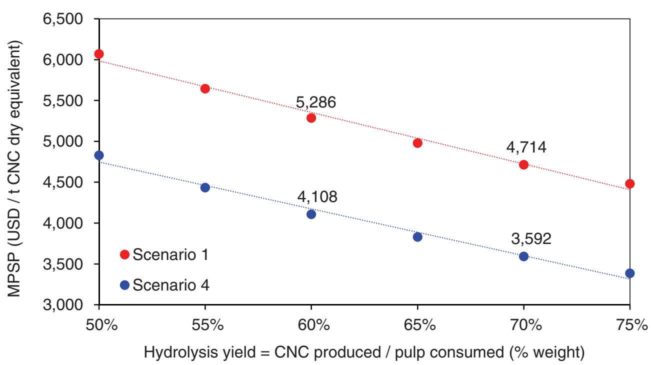

Figure 13. Impact of higher hydrolysis yields on MPSP for Scenarios 1 and 4.

reaction yield increases to 75%, MPSP is reduced by 26% and 30%, respectively.

Impact of CNC drying in project financials

A drying section was added to scenario 4. It was based on apparatus commonly used for CNC spray drying trials.[73] The purpose of this section is not to assess the technical feasibility of the drying process, since it is known that several technical challenges need to be overcome,[73,74] but rather to provide a preliminary analysis on the potential financial impacts of drying CNC. More specifically, the trade-off between potential savings in transportation costs versus the increase in the MPSP due to the addition of the drying section are assessed.

A process diagram showing the main unit operations is illustrated in Fig. 14. This section is fed by the suspension obtained in scenario 4 before full concentration by ultrafiltration. This flow is concentrated from 2% (wt) to 3% (wt) solids, to enable atomization.[38] The suspension is then sent to the spray drying system. The water is

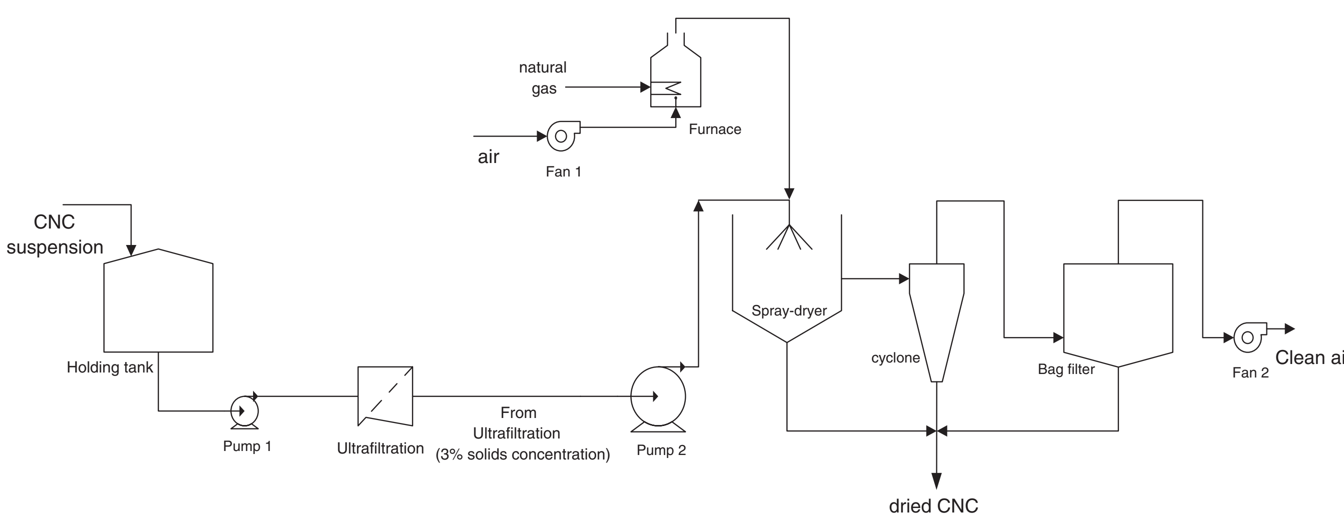

Figure 14. Process scheme of drying process.

evaporated by hot air, and dry CNC is collected in bottom of the spray dryer. A cyclone and a bag filter are also used to separate the dry CNC from the hot air and evaporated water. It was assumed that final CNC product has 5% moisture. Capital investment estimation for drying was based on quotation provided by suppliers and totaled USD 43.7 million.[75] High capital investment in drying is related to the large amount of water that needs to be removed from the suspension, which resulted in a set of five dryers operating in parallel. Operating costs also increased, due to higher consumption of natural gas and electricity for the new system. In addition, transportation costs for both scenarios assumed a 200-mile radius (USD 500/truck of 23 m^3). The density of the CNC suspension was assumed as 1000 kg/m^3 for simplicity, although an 8% (wt) solids concentration suspension may have a slightly higher value, and the density of the dried material was considered to be 1500 kg/m^3.[7]

The assessment of manufacturing and transportation costs is shown in Table 8. The total capital investment increases significantly with the addition of drying section, consequently increasing manufacturing cost and MPSP. The savings in transportation costs (around USD 250/t CNC (dry equivalent)) are not sufficient to overcome the increase in MPSP (USD 1693/t CNC (dry equivalent)). From this preliminary analysis and based on the assumptions previously defined, it can be concluded that the installation of a drying section does not positively affect the financials of the project. In addition, the need for dried CNC will be dependent on product application.

Areas identified for process optimization

The summary of main ideas for optimization aiming to decrease manufacturing costs and MPSP is shown in Table 9. Process areas with higher capital investment are the ones more suitable for optimization, since small changes can make larger differences in total values. A 10% efficiency in pulp cost and capital investment will result in at least 3% reduction in MPSP; while a 10% reduction in sulfuric acid consumption results in less than 2% reduction in MPSP. Focusing efforts in reaction yield and capital investment will have synergistic effect in the MPSP reduction.

Risk profiling of CNC industrial manufacturing

A preliminary risk profiling for CNC manufacturing at industrial scale was performed. Scenario 4 was selected, since it presents the lowest capital investment and MPSP. Current investment payback (using estimated MPSP) is 7.6 years, which can be reduced if the market price of CNC material increases above the MPSP assumed (for instance, payback value drops to 3.8 years if CNC price increases to USD 15 000 / t (dry equivalent)). It should be noticed that CNC prices, as with any other material, will be defined by the market, depending on product supply and demand. It is worth to mention that a relatively low capital investment (USD 95 million) and feedstock availability translate into a low "cost of entry" for new participants, which unless the market size (volume) is big enough would cause CNC prices to drop due to significant additional supply.

Conclusions

This work aimed to estimate the production costs of cellulose nanocrystals from acid hydrolysis, in a greenfield and co-location context. Detailed mass and energy balances, capital investment and manufacturing costs were calculated for each scenario, using data obtained from the USDA Pilot plant, literature, and discussions with experts.

The main conclusion from the analysis are:

- Manufacturing costs for CNC production ranged from USD 3632 to USD 4420/t of CNC (dry equivalent).
- Feedstock cost and capital investment are the major cost drivers for all the scenarios.
- The scenario without acid recovery in a co-location context presented the lowest MPSP. Probability analysis

Table 8. Impact of drying section in capital investment and manufacturing costs for scenario 4.

Scenario→	Without drying section	With drying section	Value difference (% difference)
Capital investment (USD million)	94.5	158.9	64.4 (+68%)
Manufacturing cost (USD/t CNC (dry equivalent))	3,860	4,940	1,080 (+ 28%)
MPSP (USD/t CNC (dry equivalent))	4,829	6,522	1,693 (+ 35%)
Transportation cost (USD/t CNC (dry equivalent))	271.7	15.3	–256.4 (– 94.4%)

Table 9. Main areas identified for optimization of CNC manufacturing costs and MPSP.

Valid for scenario(s)	Areas for improvement	Ideas for improvement	Potential savings
1–4	Minimize pulp consumption	• Optimize reaction conditions aiming higher fiber yields	A 10% decrease in pulp consumption decreases the MPSP by 3–4%
1–4	Decrease pulp cost	• Evaluate the purity of CNC needed according to application – use the most cost efficient feedstock possible	A 10% decrease in pulp cost decreases the MPSP by 3–4%
1, 3	Sulfuric acid recovery section – high capital investment	• Optimize acid consumption in reaction section leading to smaller acid recovery section • Optimize equipment design of acid recovery section	A 10% decrease in acid recovery capital investment decreases the MPSP by 2% A 10% decrease in acid consumption decreases the MPSP by 1.2%
2, 4	Sulfuric acid and lime consumption accounts for 20% of production costs	• Optimize acid consumption in reaction	A 10% decrease in acid consumption decreases the MPSP by 1.9%
1, 2	Effluent system – high capital investment	• Improve reaction yields – less sugars (COD)[a] sent to treatment • Send the effluent to the city treatment station and pay by quantity treated	A 10% increase in reaction yield decreases the MPSP by 7–8%
1–4	Ultrafiltration system – high capital investment (output of liquid–solid separation section has 10% of CNC, which is diluted to 2% CNC before ultrafiltration)	• Check the purity of CNC needed before defining the production process	
1–4	High transportation costs for delivered product (due to high water content)	• Develop technologies for drying CNC keeping its properties	
1–4	Optimize capital investment (entire plant)	• Keep the project scope simple • Design to capacity	A reduction in capital investment by 10% decreases the MPSP by 3–6%

[a]COD = chemical oxygen demand

indicates 50% chances of having production costs lower than USD 4380/t of CNC (dry equivalent) and 95% chances of production costs lower than USD 5900/t of CNC (dry equivalent).

- We believe that main efforts on optimization in CNC production should be done in the reaction yield. Changes in reaction yield will have synergistic effects in the process. From the financial point of view, reduction of dissolving pulp costs (through long term contracts for example), in addition to savings in capital investment will improve the CNC manufacturing costs.

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