ABSTRACT

ABBATI DE ASSIS, CAMILLA. Early-stage Assessment and Risk Analysis for Investments in the Bio-based Industry. (Under the direction of Dr. Ronalds Gonzalez and Dr. Jeffrey Stonebraker).

Programs to drive growth within the bio-based industry (or bioeconomy) have been established in more than 40 countries worldwide, including the United States. Benefits on promoting the development of the bioeconomy sector are widely known, such as revitalization of economically depressed rural areas, reduction of greenhouse gases emissions, and diversification of a nation's industrial base. Investments in the bio-based industry present unique complexities due to the myriad of raw materials available and products that can be manufactured, variation in composition between and within feedstocks, technologies not yet proven at industrial scale, in addition to uncertainties found in any other industry (such as market adoption, pricing, and competition). The challenge resides on the selection of product(s) or technology(ies) for efficient and lower risk investment and/or R&D, without committing significant amount of time and resources in the selection process. Literature review shows a lack of approaches that combine different project aspects (e.g., market, technology), as well as the incorporation of uncertainties at early stages. We hereby present a detailed methodology to evaluate bio-based projects including financial, technical, and market uncertainties at the early stages, when little information is available. Our systematic approach offers the opportunity to evaluate ideas or projects within the bio-based industry in significant shorter time when compared to currently available practices. Three sets of studies were developed to fulfill this goal. The first one involved the bases for investment analysis, through detailed techno-economic and financial risk assessment for investments of three novel bio-based nanomaterials: cellulose nanocrystals, cellulose micro- and nanofibrils and lignin micro- and nanoparticles. Using information from pilot and laboratory-scale facilities, detailed mass and energy balances and capital and operating costs for industrial-scale production were estimated, as well as the minimum product selling price for a given set of financial assumptions. Additional analysis included i) evaluation of the impact of process and cost inputs on the financial feasibility of the investment, ii) process roadmaps for improving project attractiveness, and iii) preliminary screening of potential applications considering financial and market information. Following, an investigation on the use of risk analysis for investment assessment from academic and industrial standpoints was performed. A literature review on risk analysis application for bioeconomy investments was conducted; the risk concept, tools available and major sources of risk were discussed. Next, a field study on the perception and use of risk analysis practices in the bio-based industry was performed, through a survey with 86 decision-makers in this industry segment. It was found that risk assessment is mostly performed in later stages of project, and less complex risk assessment methods, such as qualitative risk analysis and simple deterministic analysis are preferred over probabilistic assessments in general. The last portion of this work combines the concepts previously studied and focus on investment assessment at early stages when no significant resources have been invested and limited project information is available. A methodology is proposed to assess bio-based projects at early stages. It consists of tools to evaluate market, technology, and financial aspects organized in a systematic way, in addition to consideration of uncertainty. Existing approaches to estimate product prices, capital investment, and operating costs at the early stages were evaluated, adapted and included in the methodology, which was validated using the three bio-based nanomaterials case studies. Outcomes from the proposed methodology provide relevant information for investment evaluation, such as a market score, the status of the technology (readiness level), and estimated financial metrics (NPV, IRR, payback) considering main uncertainties. The proposed methodology aims to minimize the use of resources when assessing different project alternatives, standardize their evaluation by providing relevant and systematic information to the decision-maker, and to acknowledge potential risks and uncertainties to be investigated in future project stages.

Early-stage Assessment and Risk Analysis for Investments in the Bio-based Industry

by
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A dissertation submitted to the Graduate Faculty of
North Carolina State University
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DEDICATION

I dedicate this work to the honor of God, in the name of Jesus Christ, for his love and grace, for being my motivation, strength, and shelter in challenging times.

I am thankful to God for this opportunity and for using this journey to show me his infinite love.

"For we are God's masterpiece. He has created us anew in Christ Jesus, so we can do the good things he planned for us long ago." Ephesians 2:10, NLT

BIOGRAPHY

Camilla was born in 1984 in São Paulo, Brazil. She lived with her parents and brother until 2002, when she moved to the city of São Carlos to pursue her undergraduate degree in Chemical Engineering, at the Federal University of São Carlos. After her graduation she moved to Campinas to work for a chemical industry as process engineer. In the following 10 years, while working for Rhodia/Solvay Group, Camilla had the opportunity to interact with fantastic mentors, went to two international missions in US and France, got her master's degree in Chemical Engineering from the University of Campinas, and got married. The work and situations faced as a process engineer aroused Camilla's interest in the disciplines of capital investment, financial analysis, and decision-making, culminating with the will to connect business and technical knowledge for improving engineers' day-to-day lives.

After being apart from her husband since mid-2014 who was pursuing his masters at NCSU, thanks to a scholarship from the Brazilian government, Camilla decided to quit her dream job and moved to Raleigh to pursue her PhD at NCSU starting on January 2016. There was no regret in this decision. Here she learned many different things, met and became friends with awesome people, and grew personally, intellectually, and most importantly, in her relationship with God. After graduation, she will move to Connecticut to work for a consulting company, starting a new and exciting step of her life.

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1 INTRODUCTION

The bioeconomy is defined as a "set of economic activities related to the invention, development, production, and use of biological products and processes" [1]. It is a sector that fosters economic development and sustainability [2] while bringing several benefits. These benefits include revitalization of rural economies [3], [4], reduction of greenhouse gases emissions [5], generation of value-added products from wastes, and diversification of the industrial base [4].

More than 40 countries have established national and international programs focused to drive growth within the bioeconomy [6], and all G7 members have incorporated the bioeconomy in their strategic plans [7]. Some examples include the *Innovating for Sustainable Growth* program in the European Union [3], [8]–[11] and the *Biopreferred* program in the United States [12]. The Bioenergy Technologies Office (BETO) in the United States recently issued a strategic plan for a sustainable bioeconomy and proposes to combine technical knowledge, financial assessment, and risk analysis to evaluate projects [10].

In practice, the bioeconomy includes agricultural activities and industries that use bio-based feedstock sources (bio-based industries). Examples of bio-based industries are forestry, energy, chemicals, materials, and textiles production [4], [13], [14]. Successful cases of bio-based industries are sugar cane mills in Brazil (producing sugar, ethanol, and power), corn ethanol plants in the U.S., and pulp and paper facilities worldwide [15]. The consumer interest in renewable and sustainable products has increased in recent years, and the industry has started to respond to this demand. Wood pellets, bio-based plastics, and bio-based solvents are examples of current commercial products that demonstrate the potential to develop and grow the bio-based industry [4], [16]–[18].

Despite several opportunities available, there are unique complexities that may hinder the bio-based industry expansion. These complexities include inconsistent feedstock supplies, variabilities in chemical composition between and within feedstocks (leading to different reaction yields), development of conversion technologies, and noncompetitive processing costs [3], [19]–[21]. Two examples of recently failed projects include Range Fuels Inc. due to technology complications and Kior Inc. due to technical and market issues; both exemplify the common hurdles the new bio-based industry faces.

With many project alternatives available to expand the bio-based industry and limited budgets and resources, the challenge resides in selecting the most promising alternatives to devote efforts. The Department of Energy (DoE), for example, emphasizes the importance of using techno-economic assessments as a driving force to guide research efforts [15]; indeed, a dozen of techno-economic reports for biorefinery technologies were published over the past 10 years, providing relevant process and financial information for the research community [22]. It is known that significant amounts of time and resources were invested to perform these assessments. Despite the importance of the information provided in these reports, it is rare for many organizations investing in the bio-based industry to have the resources and the availability to invest in detailed techno-economics.

Therefore, there is a clear need for tools and methodologies capable of perform assessments in a systematic and extensive way at early project stages. These tools should provide relevant information for project decision-making, and use less information, time, and resources than detailed and traditional techno-economic analyses. The term early stage refers to the initial phases of a project lifecycle when the project conceptualization and initial planning are performed [23]. Project assessment at early stages helps in defining the project goal, identifying and screening potential alternatives, and evaluating the impacts of uncertainties on different project options. As illustrated in Figure 1-1, decisions made at early stages highly affect project cost, schedule, and resources consumed [24].

Previous research efforts for early stage assessment of bio-based projects have mostly targeted product screening by comparing simple financial metrics (revenue – feedstock costs), market aspects (e.g., market size, market interest), or technology conditions (e.g., amount of research reported, industrialization status) [12], [15], [20], [25]–[30]. Most of the assessments used qualitative criteria, and few studies considered the financial aspects and uncertainty. Another group of assessments focused on the selection of technologies or process configurations. Although the authors define these analyses as early stage, they consist of complex simulations using detailed process and financial information [31]–[34], which makes very difficult their application at initial project steps. Existing methodologies aimed at new product development for other industries were also investigated; overall, they evaluated product attractiveness by considering multiple criteria, such as financial metrics, market landscape, necessary research and development efforts, technology fit to an organization, and the organization's ability to manufacture the product [35]–[38]. However, these methodologies used information that is usually not available during early stages and failed to detail practical methodologies that can be used to estimate inputs. Uncertainty analyses and probabilistic risk analyses were not considered for these assessments.

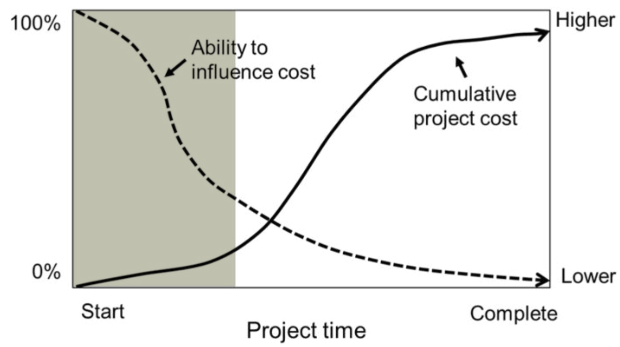

Figure 1-1: Cost-influence curve in a project lifecycle (adapted from Rocque, 2003). [39]

Literature review shows a lack of a methodology to assess bio-based investments at early stages, to include different project aspects, and to conduct uncertainty assessment.

The present work aims to fill this gap, by proposing a methodology to evaluate projects at early stages in a systematic way, considering the technical, market, and financial aspects, as well as the impact of uncertainties through probabilistic assessment. A simple and practical methodology is proposed, which aims to save considerable time and resources in the analysis process (a typical analysis can have the execution time reduced from a couple of months to weeks); ultimately aiding research institutes, industries, and government agencies in efficient R&D guidance and selection of the most promising projects.

To build the technical foundation for this work, this dissertation was structured in nine chapters (Figure 1-2). Chapter 1 comprises the introduction to the bioeconomy concept, motivations, goals of the present work, and thesis structure.

Chapters 2, 3 and 4 are systematic assessments of three novel bio-based materials: cellulose nanocrystals (CNC), cellulose micro- and nanofibrils (CMNF), and lignin micro- and nano-particles (LMNP), respectively. Although the research community has committed significant research efforts on production processes and applications of CNC and CMNF, no assessment on the financial feasibility of these materials had been published. Detailed techno-economic and risk assessment on the industrial production of these materials was performed, using information from pilot scale facilities at the USDA Forest Products Laboratories and the University of Maine. The assessment performed elucidates the major contributors to manufacturing costs, the impact of process modifications on production costs, and how uncertainties would affect both manufacturing costs and estimated minimum product selling price. These analyses provide relevant business intelligence information to guide R&D studies, to assess applications, and to aid on decisions concerning industrialization of these materials. The assessment for LMNP used information from laboratory experiments performed at Aalto University. A techno-economic assessment of potential manufacturing costs of LMNP using different lignin types and solvents, as well as an estimate of minimum product selling price was performed. Additionally, major cost drivers and scalability constraints were discussed. An assessment of potential LMNP applications from a financial perspective was performed and the most promising product applications based on market value and manufacturing costs were identified. This study aims to establish a knowledge base for application development, to provide guidance on R&D and industrialization efforts for new biomaterials, consequently fostering bio-based industry development.

Chapter 1	**Introduction**
Chapters 2, 3 and 4	**Evaluation of emerging biobased technologies** • Detailed techno-economic and risk assessment for CNC (cellulose nanocrystals), CMNF (cellulose micro- and nanofibrils), LMNP (lignin micro and nanoparticles) • Additional analyses: evaluation of major contributors to manufacturing costs, scale up assessment, and preliminary assessment of potential applications.
Chapters 5 and 6	**Investigation of risk analysis practices** • Literature review comprising the risk concept, existing tools, and published literature on financial risk assessment for the bio-based industry • Survey with decision-makers investigating common risk analysis practices, sources of risks considered, and impact of risk analysis in decision-making
Chapter 7	**Methodology to assess investments at early stages** • Revision, adaptation, and integration of investment assessment tools for early stage assessment, including technical, financial, and market aspects • Inclusion of quantitative risk assessment
Chapter 8	**Suggestions for future work**
Chapter 9	**References**

Figure 1-2: Structure of present work.

Considering the important role of risk assessment in investment evaluation, chapters 5 and 6 investigated the use of risk analysis on bio-based investment assessment and decision-making from academic and organizational standpoints. Chapter 5 is a literature review on financial risk assessment for investments in bioeconomy. This study examined the risk concept, the tools available, and the published literature on financial risk assessment for bio-based projects. Chapter 6 consists of a survey performed with decision-makers from bio-based companies, which investigate risk assessment practices, main sources of risks considered in the analysis, and how risk assessment is considered for investment decision-making. Outcomes from literature review and survey provided valuable insights into the development of a methodology for investment assessment at early stages.

Finally, chapter 7 shows a proposed methodology to assess investments in bioeconomy at early stages, aiming at industrialization and commercialization. Concepts previously studied (techno-economic assessments, financial risk analysis, preliminary market assessment, and project evaluation) were used to construct the methodology. Contrary to the case studies in chapters 2 to 4, the methodology assumes that no detailed information is available for the assessment, which is a typical situation for projects at early stages. The methodology is composed of tools to evaluate market and technology status, tools to estimate capital and operating costs when no flowsheet or detailed process information is available, and a cash flow assessment to investigate project financials including risk analysis. Four case studies are used to validate the methodology and outcomes are compared to detailed assessments previously performed. Advantages of the proposed methodology include i) the use of few information to perform the assessment, ii) the evaluation of market, technical, financial, and common bio-based project risks since the initial project phases, iii) the inclusion of quantitative risk assessment to investigate the impact of project uncertainties, and iv) the significant reduction of time and efforts invested for analysis and screen of investments at early stages.

Suggestions for future works and references are presented in Chapters 8 and 9, respectively.

2 CONVERSION ECONOMICS OF FOREST BIOMATERIALS: RISK AND FINANCIAL ANALYSIS OF CNC MANUFACTURING [1]

2.1 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 5,900 / 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.

2.2 Introduction

Cellulose is the most abundant biopolymer available in nature [40], obtained mainly from wood and plants, but also synthesized by algae, tunicates, and bacteria [41]. Its notable characteristics, such as biodegradability, optical and mechanical properties, have led to several studies of this material in its nanoscale form (nanocellulose) [42]. 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

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[1] The material in this chapter has been published as:
de Assis CA, Houtman C, Phillips R, Bilek T (E. M.), Rojas O, Pal L, et al. Conversion Economics of Forest Biomaterials: Risk and Financial Analysis of CNC Manufacturing. *Biofuels, Bioprod Biorefining* 11:682–700, 2017.

obtained by acid hydrolysis, and consist of crystalline particles with 3–5 nm width and 50–500 nm length. [40], [43] 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. [43], [44] Wood is the preferred source of cellulose due to its availability and high cellulose content [45]. BC is produced by micro-organisms, with typical dimensions of 6–50 nm width by several micrometers in length [43], [46].

According to the Web of Science database, there are more than 5,000 publications on nanocellulose (1994 to 2016) [47], with a significant increase in interest in the last decade. Patents granted during the same period, according to Google Patents database [48], totaled more than 500 (Figure 2-1). However, these publications are mainly related to technical assessments of production pathways [41], [42], [49], evaluation of properties [43], [44], strategies for nanocellulose surface modifications [50], and its applications [51], [52]. 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 1,000 kg / day (dry equivalent) [53]. 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 sup-ply chain for CNC manufacturing are assessed. In this work, we narrowed the analysis to the conversion process through sulfuric acid hydrolysis.

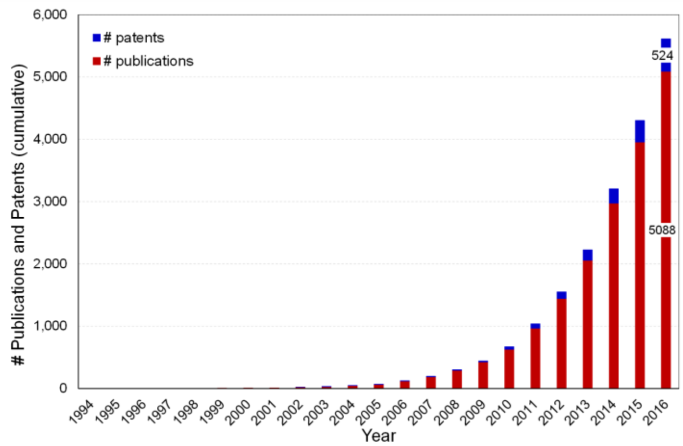

Figure 2-1: Cumulative number of patents and publications with the keywords nanocellulose, cellulose nanocrystal(s), cellulose nanofibril(s), cellulose nanowhisker(s) and nanocrystalline cellulose, from 1994 to 2016.

2.3 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 [54], [55]. 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 [56].

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 [56]. 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 [57]. Main potential markets for nanocellulose include paints and coatings, cement manufacturing, automotive parts, and paper and paper packaging. [55], [57], [58] Some examples of specific applications of nanocellulose are: (i) viscosity modifier for paints [58], [59], (ii) reinforcing material for cement and polymers [57], [58], [60], (iii) additive to improve barrier performance in coatings [61], and (iv) wet-end additive to enhance strength and improve dewatering of paper [62]. 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 [63], [64].

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 [65]. 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.

2.4 Literature review

2.4.1 Nanocellulose production processes

The processes to manufacture CNC and CNF are illustrated in Figure 2-2. 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) [41], [66], [67]. 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 [41], [45]. 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 [68]. Common mechanical treatments are homogenization, microfluidization, and microgrinding [50]. Other treatments comprise cryocrushing, high-intensity ultrasonication, disk refining, and steam explosion [69]–[71]. Several pre-treatments have been proposed in order to reduce energy consumption and modify nanocellulose surface [41]. Examples of those are: TEMPO mediated oxidation (2,2,6,6-tetramethyl-piperidine-1-oxyl radical) [72], [73], enzymatic hydrolysis [74], carboxymethylation, treatment with electrolyte solution, cryocrushing, acetylation [75], and treatment using micro-emulsions [76]. 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 [44]. We will cover the economics of CNF in a future publication.

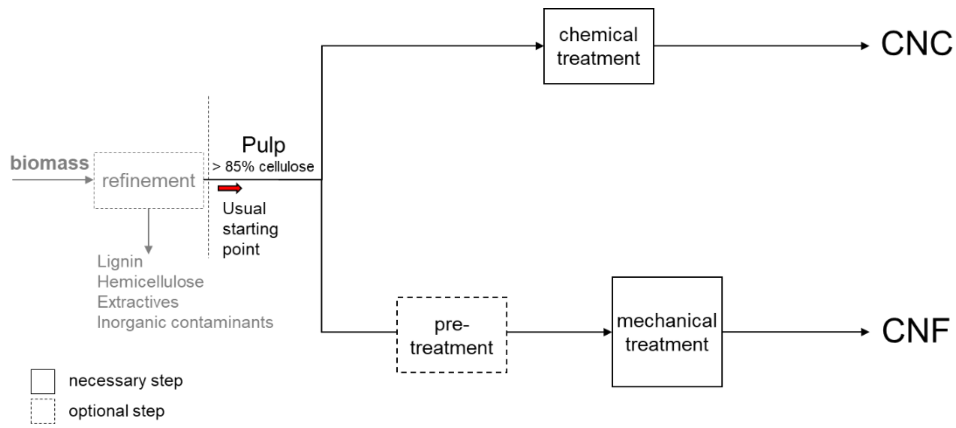

Figure 2-2: Production processes for CNC and CNF.

CNC are produced by the chemical treatment of pulp. Acid hydrolysis can be applied to dissolve the amorphous regions of the fibrils [46], [66]. Sulfuric acid is one of the most common used acids for hydrolysis [41], [45], due to its low cost and better stability of the CNC suspensions. [46] CNC can be also obtained from microcrystalline, micro-fibrillated, or nanofibrillated cellulose [41], [46]. 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 pretreated 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 [66]. In R3™ technology, CNC is produced from agricultural and forestry bio-mass, through an oxidative process involving hydrogen peroxide and citric acid [77], [78]. Other products obtained are specialty cellulose and microcrystalline cellulose (MCC) [153]. Reported yields for CNC production from acid hydrolysis are usually low, between 30 % and 50 % based on pulp [79], and between 15 % and 30 % based on wood (assuming 50 % cellulose content in dry wood [80], and 90 % cellulose content in pulp) [81]. However, there has been ongoing research aiming to minimize cellulose losses during the process. An example is the integrated production of CNC and CNF [79], [82].

CNC is usually obtained as a water-dispersed material, with concentrations varying from 3 % to 11 % [66]. Drying this material can be challenging due to the tendency of CNC to aggregate and cellulose's hydrophilic nature [41], [83], but these issues need to be overcome to reduce transportation costs and enhance additional applications [45]. 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 [66], [69] Other processes studied include oven drying, supercritical drying, and drying at room temperature [83], [84].

2.4.2 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 2,210 / t) were taken into consideration in the analysis [85]. In addition, few information is available on the manufacturing costs of CNC. Cowie (2015) has estimated manufacturing costs to increase from USD 4,000 / t to USD 16,000 / t when depreciation of equipment is considered [86]. However, no additional information on the manufacturing process and input values have been disclosed. Others have estimated production costs between USD 2,000 / t and USD 15,000 / t [87]. Once more, there is no available information on how the cost estimation was performed, and no information on mass and energy balances.

2.5 Materials and methods

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

2.5.1 Feedstock

Dissolving pulp, viscose grade (> 90 % cellulose content) [81], is used as feedstock.

2.5.2 Base-case scenario description

CNC manufacturing process is similar to the one avail-able 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) [53], [88] 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 2-3 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 ultra-filtration (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 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.).

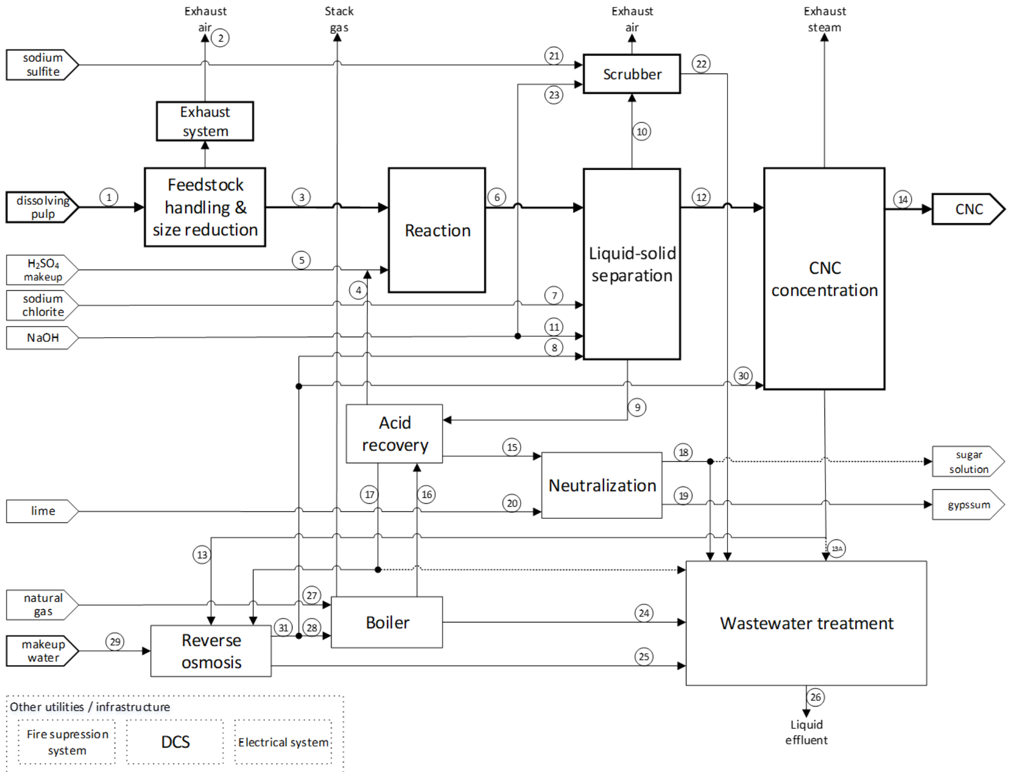

Figure 2-3: Block diagram for CNC manufacturing - scenario 1.

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.

2.5.3 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 2-1). 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. As previously described, the base-case scenario (scenario 1) contemplates a greenfield facility to produce CNC via acid hydrolysis, including an acid recovery section.

Table 2-1: 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

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) [89]. 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 com-pared 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.

2.5.4 Process information

Table 2-2 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 [88], [90]. Other sources of information are literature, experimental results from USDA laboratory trials [88], and information kindly supplied by companies [91], 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.

Table 2-2: Major process information used for mass balances.

Process information	Unit	Value adopted	Reference
CNC production	t / d (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 make-up	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	% (in weight)	10	Lab result [d]
CNC concentration after ultrafiltration	% (in weight)	8	Pilot plant [a]

[a] Pilot plant process data from trials at USDA Forest Product Laboratories (Madison, WI) [88].
[b] With acid recovery.
[c] Without acid recovery.
[d] Data from experiments ran at USDA Forest Product Laboratories (Madison, WI).

2.5.5 Cost information

Major cost information used to run the analysis are listed in Table 2-3. 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 [92], [93]. All cost values were corrected to the start-up year (2019), using an inflation rate of 1.2 % (average from 2012 – 2015, according to U.S. Treasury data) [94]. 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 [95]. For all scenarios, tap water is used as water makeup.

Table 2-3: Major cost information for CNC production.

Input	Value (2019)	Unit	Reference
Dissolving pulp (viscose grade)	763	USD / t (FOB in pulp mill)	RISI database [96]
Sodium sulfite	342	USD / t	FisherSolve™
Sulfuric acid (100 %)	90	USD / t	ICIS website [92]
Sodium chlorite (crystals, 80 %)	5,004	USD / t	ICIS website [92]
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 [97]
Electricity	69.5	USD / MWh	U.S. Energy Information Administration [93]
Effluent treatment	0.6	USD / t treated	Ulrich and Vasudevan (2006) [95]
Gypsum	9.5	USD / t (FOB)	U.S. Geological Survey (2015) [98]
Freight for pulp	50	USD / t	Expert info - 500 miles radius (additional to pulp cost)

2.5.6 Financial assumptions

Financial assumptions for this study are listed in Table 2-4. 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 [99], and have been compared to other sources [100], [101]. 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 % [102].

Table 2-4: Financial assumptions.

Input	**Value (2019)**	**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) [102]
Depreciation schedule, straight line	10	years	assumed
Working capital	10 %	% of sales of next year	assumed
Tax rate on EBIT	35 %	%	NREL[99]
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

2.5.7 Financial metrics

Main financial metrics used in this work are briefly explained.

Net Present Value (NPV) is the sum of the all dis-counted cash outflows and inflows of the project [103]. 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 [104].

Return on Investment (ROI) is calculated by dividing the after-tax profit by the capital employed (working capital + asset value) year by year [103].

Minimum product selling price (MPSP) is the mini-mum 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 [105]. It is calculated as the number of years needed for the cumulative free cash flow to become positive.

2.5.8 Capital investment

Capital investment was based on information provided by American Process Inc. (API) [91]. 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 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).

2.5.9 Block diagrams

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

2.5.10 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).

2.5.11 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.

2.5.12 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 [40], [43].

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.

2.6 Results and discussion

2.6.1 Mass balance results

Main inflows and outflows for scenario 1 (greenfield with acid recovery) are presented in Table 2-5. 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 (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.

Table 2-5: Main inflows and outflows of CNC mass balance (refer to Figure 2-3 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	69.8	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.

2.6.2 Capital investment

Estimated capital investments are between USD 95 million and USD 188 million (Figure 2-4). 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 con-text (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.

2.6.3 Manufacturing costs and MPSP

Breakdown of manufacturing costs and MPSP are illustrated in Figure 2-5. 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 3,632 to USD 4,420 / 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 6,070 / 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, 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.

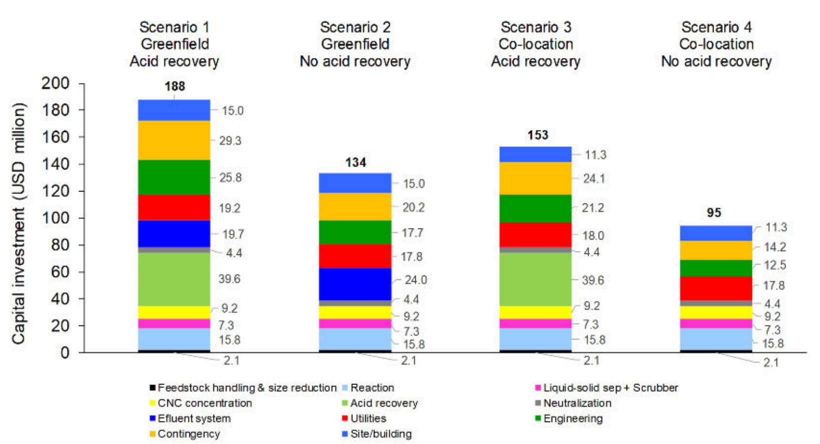

Figure 2-4: Capital investment comparison for scenarios 1–4.

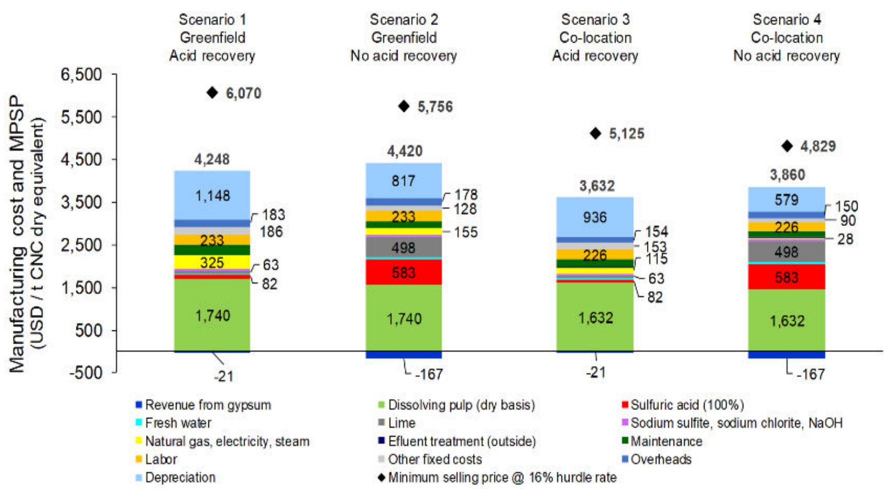

Figure 2-5: Manufacturing cost breakdown and MPSP for scenarios 1–4, for year 2020.

2.6.4 Return on Investment and payback period

ROI was calculated for all scenarios in each year of operation (Figure 2-6), in addition to the payback period (Table 2-6). However, in all scenarios the CNC price adopted was the lowest MPSP calculated (USD 4,829 / t CNC (dry equivalent)).

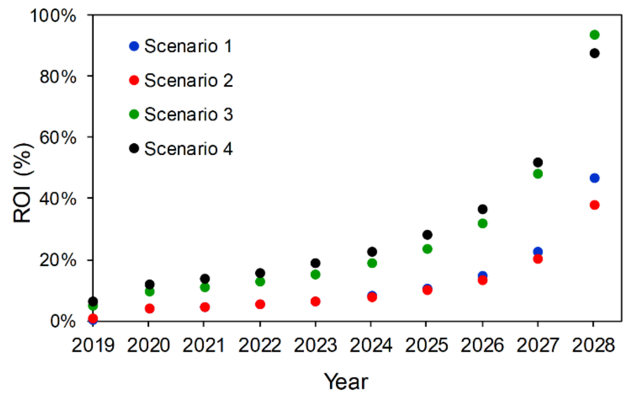

Figure 2-6: Return on investment (ROI) for scenarios 1–4.

Table 2-6: 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 4,829/t of 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 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).

2.6.5 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 Figure 2-7 and Figure 2-8, respectively. These scenarios were chosen since they pre-sent 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 (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.

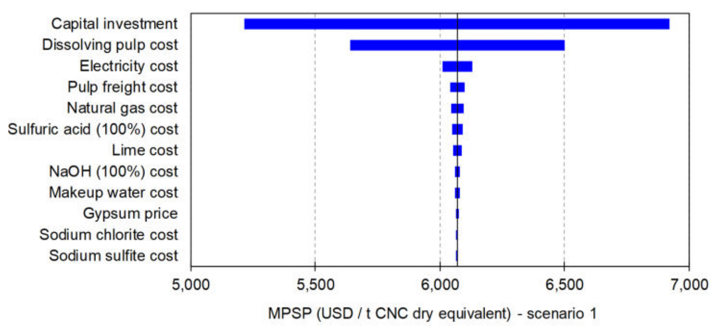

Figure 2-7: Tornado diagram for scenario 1.

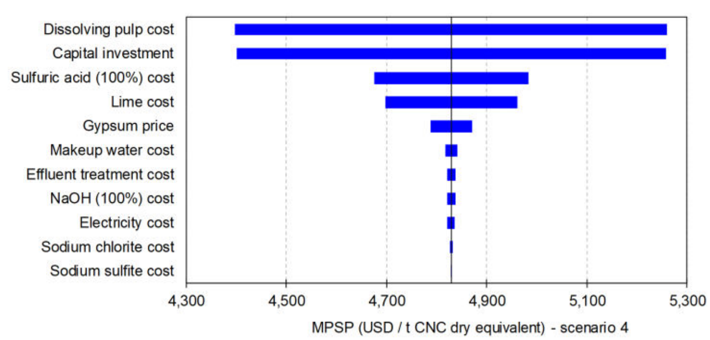

Figure 2-8: Tornado diagram for scenario 4.

2.6.6 Probability analysis

Probability analysis for manufacturing costs was con-ducted for scenario 4. This assessment was carried out according to the steps mentioned in the materials and methods section. From Figure 2-8, 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 Figure 2-9 (2011 to 2016). Historical monthly costs for sulfuric acid and lime were calculated using the respective producer-price index for commodities [106], [107], and then converted to real values using the consumer price index [108]. Probability distribution for capital investment was defined as uniform, based on the accuracy of API estimate (+ 35 % / – 20 %).

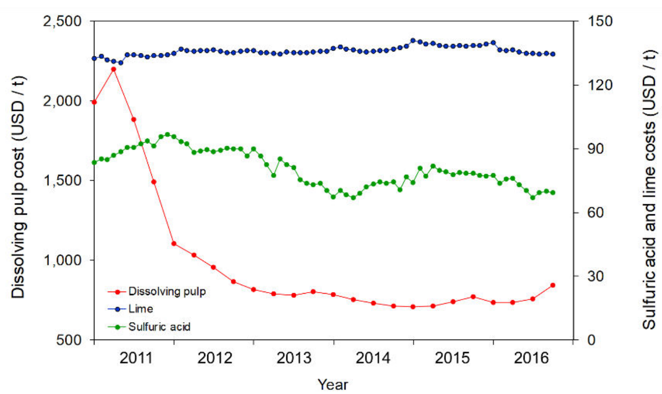

Figure 2-9: Historical costs for dissolving pulp, sulfuric acid and lime.

Probability distribution curves were adjusted to functions using @Risk software for the major inputs using historical data (Figure 2-10). The blue bars represent the probability distribution of the historical data. The red line is the adjusted function for each probability distribution.

A 5,000-iteration Monte Carlo simulation was executed. The simulation output is the probability distribution of CNC manufacturing cost (Figure 2-11). Based on the assumptions made for CNC production, there is a 100 % chance that the manufacturing costs are below USD 7,128 / t of CNC (dry equivalent) for scenario 4. Chances of manufacturing cost below USD 3,860 (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 2-7 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 1,300 / t of CNC (dry equivalent), which corresponds to a 15 % reduction.

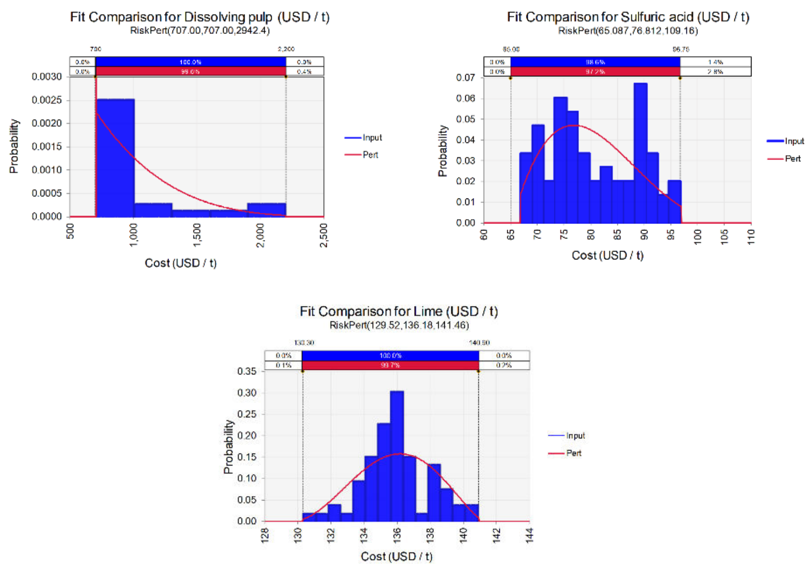

Figure 2-10: Adjusted distribution probabilities for dissolving pulp, sulfuric acid, and lime costs (USD / t).

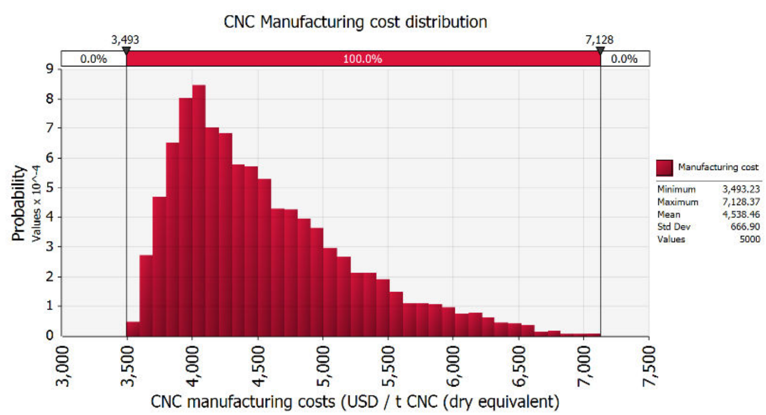

Figure 2-11: Distribution curve for CNC manufacturing cost (scenario 4).

Table 2-7: 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

Figure 2-12(a) illustrates regression coefficients from the probability analysis and Figure 2-12(b) shows the descaled values of the coefficients. From Figure 2-12(a), the longer the bar, the higher the impact of an input variability on the output. In this case, dissolving pulp variability is the major contributor for variability in production costs, followed by the capital investment. Figure 2-12(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 [109]. The descaled values obtained show by how many units the output varies based on a unit change in the input. It 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)).

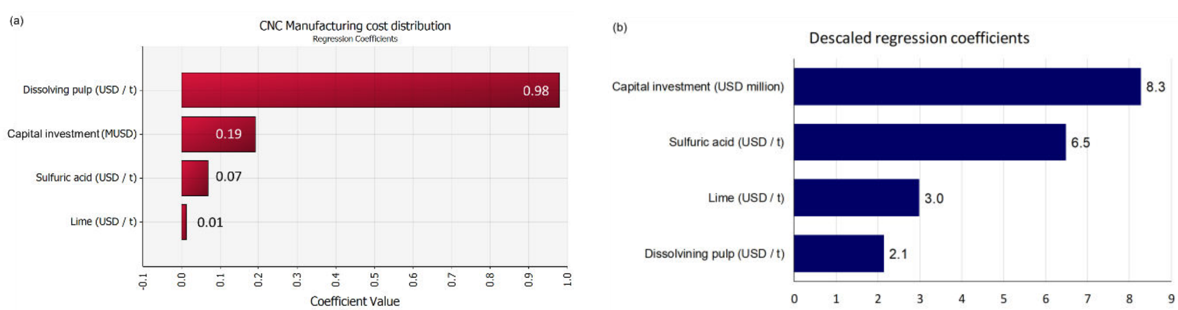

Figure 2-12: (a) Tornado regression coefficients, (b) Descaled regression coefficients for scenario 4.

2.6.7 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.

2.6.7.1 Potential savings with increased reaction yields

It can be noticed from Table 2-2 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 [110]. 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 hydrolysis (based on bleached eucalyptus pulp) [110]. The use of different processes, such as HCl at vapor phase, have shown yields greater than 95 % based on cotton cellulose fibers [111]. 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 (Figure 2-13). If the reaction yield increases to 75 %, MPSP is reduced by 26 % and 30 %, respectively.

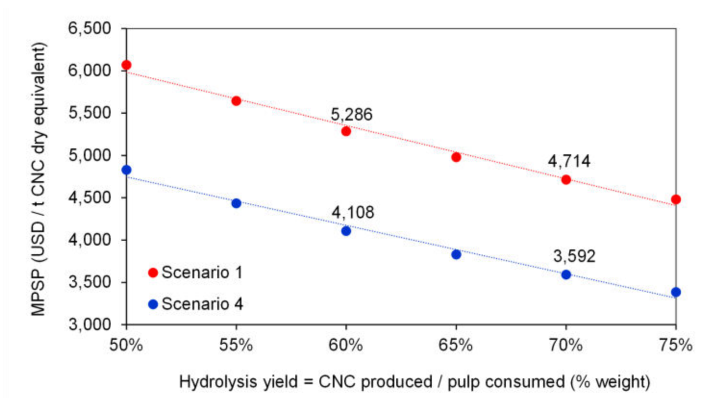

Figure 2-13: Impact of higher hydrolysis yields on MPSP for Scenarios 1 and 4.

2.6.7.2 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 [112]. 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 [112], [113], 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 Figure 2-14. 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 [77]. The suspension is then sent to the spray drying system. The water is 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 [114]. 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 1,000 kg / m3 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 1,500 kg / m^3 [46].

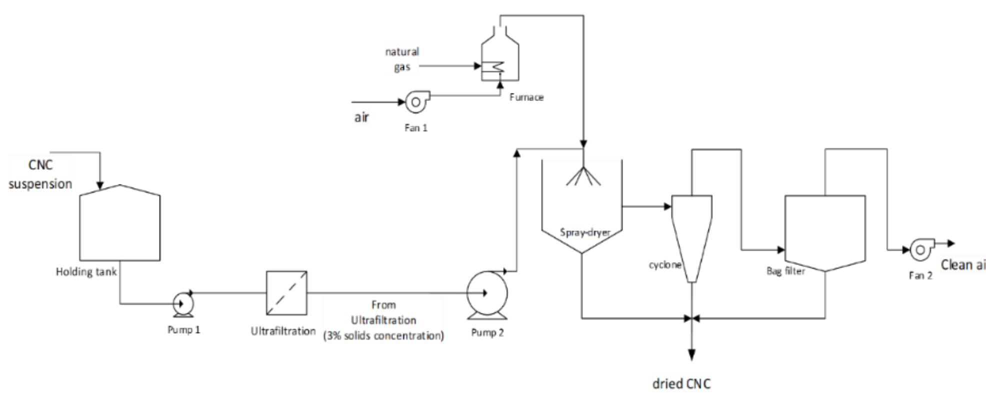

Figure 2-14: Process scheme of drying process.

The assessment of manufacturing and transportation costs is shown in Table 2-8. 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.

2.6.8 Areas identified for process optimization

The summary of main ideas for optimization aiming to decrease manufacturing costs and MPSP is shown in Table 2-9. 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.

Table 2-8: 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 2-9: 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 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 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 MPSP by 2 % A 10 % decrease in acid consumption decreases 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 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 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 MPSP by 3 – 6%

[a] COD = chemical oxygen demand

2.6.9 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.

2.7 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 3,632 to USD 4,420 / 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 indicates 50 % chances of having production costs lower than USD 4,380 / t of CNC (dry equivalent) and 95 % chances of production costs lower than USD 5900 / t of CNC (dry equivalent).
- We believe that main eff orts 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.

3 CELLULOSE MICRO- AND NANOFIBRILS (CMNF) MANUFACTURING – FINANCIAL AND RISK ASSESSMENT [2]

3.1 Abstract

Conversion economics, risk, and financial analyses for an industrial facility manufacturing cellulose micro- and nanofibrils (CMNF) from wood pulp is presented. Process data is based on mass and energy balances from a pilot facility in the University of Maine. Here, CMNF is produced from untreated wood pulp by using disk refining, with an assumed production capacity of 50 t (dry metric ton equivalent) per day. Stand-alone and co-location manufacturing facilities were simulated and assessed. Minimum product selling prices (MPSP, estimated to achieve a 16 % hurdle rate) for different scenarios ranged from USD 1893/t CMNF to USD 2440/t CMNF (dry equivalent). Pulp and energy consumption were identified as major cost drivers. Consequently, it was found that the use of alternative feedstock, in addition to co-location configuration, can reduce MPSP by 37 %. Since estimated MPSP of CMNF is lower than cellulose nanocrystals (CNC) – both estimated to achieve a 16 % hurdle rate, we believe market adoption of CMNF in the near term is more promising, regardless of specific applications. This study provides state of the art business intelligence information on the conversion economics, risk, and financial analyses for CMNF manufacturing. Thus, the data represents valuable information to entrepreneurs, R&D scientists, and product developers who plan to adopt CMNF in their processes and products.

3.2 Introduction

3.2.1 Cellulose micro- and nanofibrils

There is significant research interest in developing applications for micro- and nanocellulosic materials based on their extremely high surface area, nanostructure, notable mechanical properties, and renewability. The focus of the present study is cellulose micro-

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[2] The material in this chapter has been published as:
de Assis CA, Iglesias MC, Bilodeau M, Johnson D, Phillips R, Peresin MS, Bilek T (E. M.), Rojas O, Venditti R, Gonzalez R. Cellulose micro- and nanofibrils (CMNF) manufacturing - financial and risk assessment. *Biofuels, Bioprod Biorefining* 12:251-264.

and nanofibrils (CMNF). Before describing the CMNF manufacturing process, it is important to pro-vide definitions on material nomenclature and main characteristics, since there is no wide consensus in the literature [43], [44].

Cellulosic materials with at least one dimension in the nanoscale can be categorized as nanocelluloses [44]. The main differences between cellulose nanocrystals (CNC) and cellulose nanofibrils (CNF) or nanofibrillated cellulose (NFC) include physical and surface proper-ties, composition, and manufacturing process employed. For CNC manufacturing, acid hydrolysis treatment is applied and the amorphous regions are dissolved to obtain individual, high crystalline cellulose, which can be also named cellulose nanowhiskers [74]. CNF are produced mainly via mechanical treatments whereas crystal-line and amorphous regions of the cellulosic chains are maintained. CNF are known for their flexibility and high aspect ratio, with diameters smaller than 100 nm and lengths from 500 nm to several microns [43], [44], [50]. The terms microfibrillated cellulose (MFC) and cellulose microfibrils (CMFs) have been also used for materials with diameters < 100 nm and lengths in the microscale [44], [75], [115], [116]. There has been interest in developing international standards for nanocellulose terminology [117]; however they are not available yet. For the purpose of this study, the final product analyzed will be named cellulose micro- and nanofibrils (CMNF), since the material presents diameters in the micro- and nanoscale. For the literature review, the terminology used will follow the respective publication nomenclature.

CMNF has several potential applications and it may benefit from lower manufacturing costs when compared to CNC. Market reports estimate the potential demand for CMNF to be five times bigger than CNC in the next 2–7 years [55]. Estimated commercial prices for CMNF range from USD 9000 to USD 221,000 / t, depending on process scale, pre-treatment and mechanical treatment applied [66]. As a result of the growing interest in developing and researching applications for CMNF [70], [118], [119], several companies have already begun to use this material at industrial scale. For instance, Mitsubishi Pencil Co., Ltd is using CNF as a rheology modifier for pen inks [64]. Nippon Paper Industries Co. uses CNF for manufacturing sheets with incorporated metal ions that confer deodorant and anti-bacterial properties [63]. Automotive oil and air filters manufacturers, such as Cummins and Baldwin Filters Inc., are also using CNF for the manufacturing of filter media; such CNF-based filters are said to display enhanced filtration properties and retention of very small particles (up to 2 μm) [120].

As it has been described by de Assis et al. in a recent publication on the economics of CNC [121], there are more than 5,000 publications and 500 patents on nanocellulose. To the best of our knowledge, a detailed conversion economics (along with mass and energy balance) of CMNF is not publicly available. The purpose of this work is to provide state-of-the-art business intelligence information on the conversion economics, risk, and financial analyses for CMNF manufacturing, providing valuable information to entrepreneurs, R&D scientists, and product development practitioners regarding manufacturing cost, minimum product selling price (MPSP), and detailed mass and energy balances over the CMNF manufacturing process.

3.2.2 Processes to obtain CMNF

Herrick et al. [122] and Turbak et al. [123], [124] have pioneered the production of microfibrillated cellulose (MFC), through mechanical separation of cellulose fibers by high-pressure homogenization. Due to the high energy consumption of the mechanical process, alternative technologies and pre-treatments have been developed over the years.

The starting point for CMNF manufacturing is cellulose pulp, usually bleached pulp, with most of the non-cellulosic materials removed [115]. Studies have shown that CMNF can also be manufactured from unbleached fibers [67], [125]. Typically, the pulp is dispersed in water to a solids content between 0.5 % and 2.5% in weight [126]. The cellulose suspension can be subjected to pre-treatments such as chemical or enzymatic, and then mechanical treatment is applied. The final product forms a hydrogel, even at such low CMNF concentration (2 % wt.), due to the increase in surface area and consequently extensive hydration and water coupling [50].

Possible pre-treatments and mechanical treatments for CMNF manufacturing are illustrated in Figure 3-1. The most common mechanical treatments are homogenization, microfluidization, and microgrinding. During homogenization, the pulp suspension passes through a small channel, pushed by a piston; high shear forces defibrillate the material [69]. Pressure drops can be as high as 550 bar [115]. Although homogenizers are ordinarily used in industry (such as dairy and pharmaceutical) [127], there are risks of equipment clogging when cellulosic nanomaterials are processed [41]. In microfluidization, the pulp suspension passes through a chamber with a specific geometry, where high shear forces and pressure (around 2,760 bar) are applied [115], resulting in the fragmentation of the fibers into smaller sizes. CMNF produced by microfluidization present more uniform size distribution [75]; however, several passes in the equipment are needed to reach nanoscale dimensions. In addition, the throughput is typically lower than homogenization and pre-treatments are necessary to prevent high energy consumption and equipment clogging [76]. For microgrinding, the suspension passes through two special disks with a narrow gap clearance, which imposes shearing stress into the material (rotation speeds are around 1,500 rpm) [75], [115], [128]. Disk refining technology, similar to microgrinding, allows higher production rates and will be further detailed.

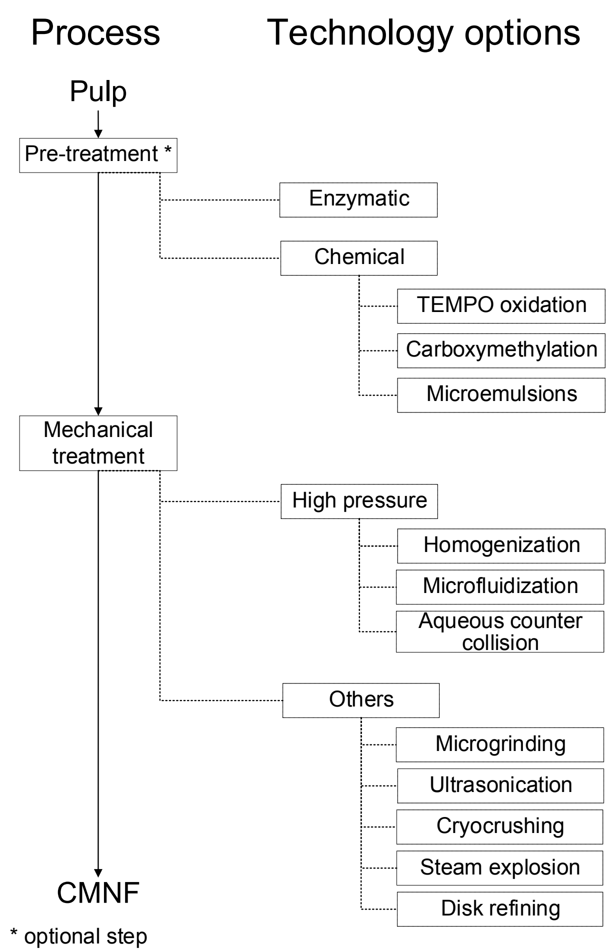

Figure 3-1: List of pre-treatments and mechanical treatments for CMNF production.

Other mechanical treatments for CNF manufacturing, although not widely used, are aqueous counter collision, high-intensity ultrasonication, cryocrushing, and steam explosion [69], [129]. Aqueous counter collision (ACC) consists of the ejection of cellulose aqueous suspensions through two nozzles. The collision between the two jets produces CNF [129]. Ultrasonication is a laboratory-scale method where fiber at low solid concentration (0.2 – 0.5 % wt.) is exposed to high-intensity ultrasound waves [115], [116]. Cryocrushing consists of immersing the pulp in liquid nitrogen and crushing it with a cast iron mortar and pestle [115]. Resulting fibers include diameters between 0.1 μm and 1 μm [115]. Finally, steam explosion has been reported to be an effective method to obtain CNF, where high-pressure steaming and subsequent decompression are applied to the cellulosic material. During decompression, flash water evaporation produces the rupture of the material allowing the cellulose reduction into smaller particles [130].

Pre-treatments commonly used to manufacture CMNF can be classified as enzymatic or chemical. During enzymatic pre-treatments, the cellulose fibers are modified by an enzyme (endoglucanase is commonly used) which reduces the molecular weight of the polymer aiding defibrillation [115], [116]. Concerning chemical pre-treatments, TEMPO-oxidation, initiated by Saito and Isogai [72], [73], has been the most studied [75]. In this method, 2,2,6,6-tetra-methylpiperidine-1-oxyl is used as oxidizing agent. The C-6 hydroxyl groups are converted to carboxylate groups, which allow repulsive forces to facilitate fibers separation. Another common chemical method is carboxymethylation, where hydroxyl groups are substituted by carboxymethyl groups, which block hydrogen bonding [44], [115]. Microemulsions have been also used as agents to reduce hydrogen bonding [76].

Pre-treatments are usually performed to reduce energy consumption of mechanical treatments and to modify the cellulose surface for specific applications [69]. The draw-backs of chemical pre-treatment include additional waste generation; for enzymatic pre-treatments time and energy requirement for enzyme separation may increase production costs [49].

CMNF are currently produced in pre-commercial and commercial scale by companies such as Stora Enso, Nippon Paper, American Process, Borregaard, and UPM [53], [131]–[133]. Exilva, Borregaard’s microfibrillated cellulose, is the first commercial production facility in the world, with 1,000 t / yr (dry basis) capacity [133], [134].

Our study aims to provide a better understanding of CMNF conversion economics at industrial scale, considering stand-alone and co-location scenarios. Major cost drivers for each scenario will be identified, and assessment of conversion economics using more cost-efficient feedstocks will be discussed. It is our intention to provide meaningful information to the R&D community about CMNF lowest manufacturing cost pathway and help in the assessment of CMNF products adoption for different applications. This will provide essential business intelligence information to stakeholders in the bioeconomy.

3.2.3 Techno-economic assessments on CMNF

Few techno-economic assessments are available in the literature, and they consider only major inputs for the calculation of manufacturing costs. Additional factors, such as indirect costs and capital investment, have not been considered. For instance, preliminary cost estimations for CNF used for paper reinforcement have been performed based on costs of chemicals, enzymes, and energy [118]. The estimated manufacturing costs varied from 2.25 € / kg to 205.73 € / kg, mainly driven by energy costs. TEMPO-mediated oxidation, soft acid hydrolysis, enzymatic treatment, and mechanical beating were considered. Similarly, preliminary manufacturing costs for MFC manufacturing from different feedstocks and mechanical treatments were compared [135]. The values, based only on energy and raw material costs, ranged from USD 445 / t to USD 1,960 / t (using bleached and unbleached kraft hardwood pulp as raw materials).

3.3 Materials and methods

A detailed mass and energy balance and a financial analysis for CMNF manufacturing were developed; details on the materials and methods are described herein.

3.3.1 Feedstock

Feedstock used for simulation purposes is northern bleached soft wood kraft pulp (NBSK), from northeast United States and Canada. This is the same material used in the pilot facility at the University of Maine [70].

3.3.2 Production rate

The production rate considered for the base-case scenario is 50 t CMNF/day (dry equivalent). It was assumed that the facility operates 340 days/year, thus annual production rate is 17,000 t CMNF / year (dry equivalent).

3.3.3 Process description

The University of Maine nanomaterial pilot facility is used as a reference for the industrial-scale process [136], [137]. Although there are different technologies available to manufacture CMNF, disk refining was chosen due to the vast experience that the University of Maine has with the equipment, in addition to the ease of scale-up and relatively low energy requirements when compared to other technologies. The installed capacity of the disk refiner in the University of Maine is 1,000 kg/day (dry equivalent).

The process to manufacture CMNF via disk refining is illustrated in Figure 3-2. Mechanical treatment is performed without pre-treatment and the process runs in batch mode. NBSK pulp (1) and tap water (2) are mixed in a hydropulper to 3 % (wt.) solids concentration. The suspension (3) is pumped to a buffer tank. Then, the suspension is recirculated through the disk refiner until it achieves 90 % fines (in number). Fines are defined as particles with lengths below 0.2 mm. A heat exchanger is located in the recirculation loop to cool down the suspension if needed (due to high abrasion in the disk refiner), although it has been rarely used in the pilot facility. The final CMNF product (4) at 3 % (wt.) solids concentration has a gel-like nature and is packed in drums and sold as a suspension. There is no need to refrigerate or to use biocides to prevent the growth of microorganisms. The estimated shelf life of the final product is one year. The process to manufacture CMNF does not generate liquid or gaseous wastes.

At the University of Maine, the quantity of fines in the slurry is measured using a Techpap Morfi analyzer. Although the Techpap Morfi device is able to measure particles above 5 µm in length, results from scanning electron microscopy (SEM) of CMNF slurry (at 90 % fines) have shown that the material has dimensions at the nanoscale, with widths between 20 and 100 nm and lengths from several to tenths of micrometers. For CMNF currently produced at the University of Maine, measurements using Techpap Morfi equipment allow a consistent indication of product quality, and the same principle is being considered for the industrial facility simulated.

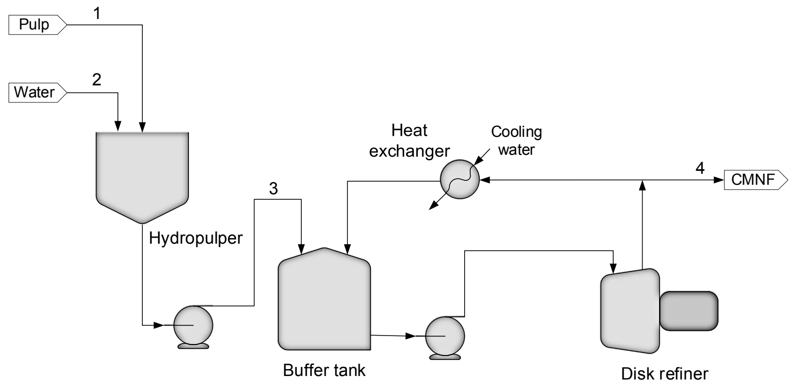

Figure 3-2: Process sketch for CMNF manufacturing at industrial scale.

The disk refiner available at the University of Maine was manufactured by GL&V [71]. Disk refiners are based on standard pulp and paper refining technologies and can present single or double disk configurations. An example of a dual disk configuration is illustrated in Figure 3-3. The suspension enters the upper part of the equipment and passes between the disks. For CMNF production, the refined pulp passes several times between the disks until the desired particle size is achieved. To achieve 90 % fines, different types of plates might be necessary. One option is to change the plates at some stage of the operation; another option is to install refiners with different plates in series. Due to high abrasion, it is necessary to change the plates after some time of operation. Based on our discussions with the disk refiner supplier, we have assumed disk replacement costs as part of maintenance costs, which are a percentage of the total investment.

3.3.4 Scenarios evaluated

Scenario 1 considers a stand-alone (from now on greenfield) facility. By greenfield it is meant that the project starts from bare ground. Scenario 2 considers the CMNF manufacturing facility to be co-located within a mill that produces NBSK pulp. The final CMNF product is sold to different clients. The following modifications are considered for scenario 2 (in relation to scenario 1): (i) NBSK pulp is supplied at 3 % (wt.) solids concentration from the pulp mill, which implies no need to either install a hydropulper or to dilute the raw material; (ii) NBSK pulp has a lower cost, since freight and drying costs are not necessary; (iii) land cost is considered to be zero, and (iv) fewer employees are needed, reducing labor cost. An additional scenario, named on demand co-location (scenario 3) is considered in the analysis. In this scenario, CMNF production rate is at 50 % of scenarios 1 and 2 (i.e., 25 t / day of CMNF (dry equivalent)), and it is assumed that the final product is used within the mill. Additional cost savings on labor are possible in scenario 3. Examples of applications related to papermaking include addition of MFC and CNF into paper [139], [140], addition of CNF layers as the core of the paper sheet [141], and the application of CNF to improve barrier properties for packaging [61], [142]. Solids concentration of final CMNF dispersion is 3 % (wt.) for all three scenarios assessed.

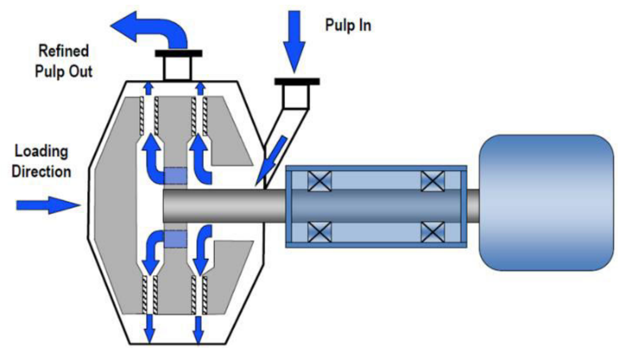

Figure 3-3: Illustration of a disk refiner (dual disk) [138].

3.3.5 Process data

Main process data for CMNF production are summarized in Table 3-1. Data have been collected from the University of Maine and equipment suppliers (personal communication with GL&V - disk refining capital investment estimate) [136]. Production rate for scenarios 1 and 2 was chosen in order to be comparable with previous CNC study [121]. Electricity consumption for the disk refining system is based on data from the pilot plant at the University of Maine and from an equipment supplier (personal communication with GL&V - disk refining capital investment estimate). For the hydropulper, energy consumption is based on equipment sup-plier information [143]. No losses are considered for the simulation, although it is known that very small amounts of material may be lost due to spills and equipment cleaning.

Table 3-1: Main process data for CMNF production.

Process input	Scenario 1 Greenfield	Scenario 2 Co-location	Scenario 3 On demand co-location
CMNF production (t CMNF / day – dry equivalent)	50	50	25
Feedstock used	NBSK pulp[a]	NBSK pulp[a]	NBSK pulp[b]
Initial feedstock solids content (% wt.)	90 %	3 %	3 %
Process yield 2	100 %	100 %	100 %
Electricity consumption - hydropulper (kWh / t pulp dry equivalent)	333	333	333
Electricity consumption - disk refiner (kWh / t CMNF dry equivalent)	2,500	2,500	2,500

[a] NBSK = northern bleached softwood kraft

[b] Process yield is the ratio between disk refiner mass outflow and inflow

3.3.6 Cost data

Major cost information is presented in Table 3-2. It was initially expected that fiber cost would be lower for NBSK pulp, when compared to dissolving pulp (used for CNC production), since market pulp has lower cellulose content than dissolving pulp. However, the data collected from RISI (www.risiinfo.com) has shown that NBSK pulp can be 20 % to 45 % more expensive than dissolving pulp. These discrepancies are mainly related to a specific cur-rent supply and demand situation. The demand for market pulp has increased in the last years, especially for tissue production, which would be the major driver for the price increase. Pulp costs for the assessment are the average values for the past 2 years, while for electricity the variation over the last 3 years has been considered. Tap-water costs are from 2004, and were corrected to the assessment date (2019) using an average annual inflation rate of 1.2 % [94].

Table 3-2: Major cost drivers for CMNF manufacturing.

Input	**Value (2019)**	**Units**	**Reference**
NBSK pulp cost (freight included)	1,016	USD / t	RISI database [a]
Tap water cost	0.66	USD / t	EPA [97]
Electricity cost	71.9	USD / MWh	Energy Information Administration [93], [144]
Freight for pulp [b]	50	USD / t pulp dry	Expert info - 500 miles radius
Drying costs [b]	35	USD / t pulp dry	Assumption

[a] http://www.risiinfo.com/.

[b] For co-location scenarios, freight and drying costs are subtracted from NBSK pulp cost.

3.3.7 Capital investment

Capital investment estimates were based on a quotation provided by GL&V for the disk refining system and hydropulper (personal communication). Equipment cost estimates for ordinary equipment, such as pumps and tanks, were derived from CNC capital investment data [121]. Installation costs and indirect costs were estimated using literature references [145]. A contingency of 18 % on direct costs was considered for all scenarios. Capital investment for scenario 3 was based on higher throughput equipment quotations and considers a scaling factor of 0.6.

3.3.8 Financial assumptions

Financial assumptions for the simulated facility are illustrated in Table 3-3. The financial horizon is assumed as 10 years. The assembly time for this facility was assumed to be 2 years, and production in first year of operation (2019) is 80 % of nominal plant capacity. Straight-line depreciation (10 years) is assumed and facility terminal value is 5 times the EBITDA (earnings before interest, taxes, depreciation, and amortization) in the last year of operation. The hurdle rate considered was 16 %, based on pulp & paper and specialty chemical industry statistics [102]. The number of employees was estimated for each scenario based on authors' industrial experiences. As previously mentioned, replacement of the disks of the refiner is included in the yearly maintenance costs (maintenance costs represent 2 % of the replacement asset value).

Table 3-3: Main financial assumptions for all scenarios.

Input	Value	Units
Project start	2017	year
Financial evaluation horizon	10[a]	years
Production on year 0 (2019)	80 %	% of plant capacity
Production on year 1	100 %	% of plant capacity
% of CAPEX spent in year -2 (2017)	50 %	% of investment
% of CAPEX spent in year -1	50 %	% of investment
Depreciation schedule, straight line	10	years
Working capital	10 %	% of sales of next year
Hurdle rate	16 %	%
Tax rate on EBIT	35 %	%
Terminal value in year 10	5	multiple of EBITDA
Operating days / year	340	days / year
Maintenance cost	2 %	% of RAV [b]
Capital reinvestment	1 %	% of RAV [b]
Hourly and administrative staff	18	scenario 1
	8	scenario 2
	2	scenario 3
Overhead costs	3 %	% of sales
Other fixed costs (insurance, property taxes, and emissions)	1.5 %	% of RAV [b]

[a] After project starts / [b] Replacement asset value

3.3.9 Modeling and financial analysis

Process flowsheets were built using Microsoft Visio® and mass and energy balances were performed using Microsoft Excel® spreadsheets. Results of mass and energy balances were integrated in the financial model (performed using also Microsoft Excel® spreadsheets), in addition to cost data, capital investment estimations, and financial assumptions. Manufacturing costs were estimated and a cash flow analysis was performed to estimate MPSP. MPSP is defined as the price that sets the project net present value (NPV) of the investment to zero at the hurdle rate assumed. Other financial metrics calculated for each scenario are return on investment (ROI) and payback. More details on these metrics can be found in our previous analysis on CNC conversion economics [121].

3.3.10 Financial risk analysis

Financial risk analysis was performed for each scenario. Sensitivity analysis was initially performed using Microsoft Excel® spreadsheets in order to identify inputs with higher effect on the output (in this analysis, the MPSP) by varying the initial input values assumed. Cost of feedstock, water, electricity, and capital investment were varied by ± 25 %, and the value of the output was recorded. Sensitivity analysis data are illustrated using a spider plot. Those parameters in which variation has higher impact on the output are considered for probability analysis. More information on risk assessment tools can be found elsewhere [65].

Probability analysis was performed using the software @Risk and using probability distributions of selected input parameters. The variation of each parameter was based on available information. More specifically, variation in feed-stock and electricity costs was based on historical values and variation on capital investment is based on the estimate accuracy (± 30 %). The main outcome of this analysis is the probability distribution of CMNF manufacturing cost. In addition, proxy values for MPSPs were estimated, so the probability of having a specific MPSP can also be assessed.

3.4 Results and discussion

3.4.1 Mass and energy balances results

Mass and energy balances were calculated for each scenario. Main flows for scenario 1 and 2 are listed in Table 3-4 and Table 3-5. The flowrates for scenario 3 are half of the values for scenario 2. Stream numbers are indicated in Table 3-2. The process is very simple, and only water and pulp are used as raw materials. Water for cooling was not considered, since it is not a continuous flow. According to equipment suppliers and the University of Maine experience, there is no need to constantly cool down the material during recirculation. Energy consumption for the three scenarios is listed in Table 3-6. Electricity consumption consists mainly of the hydropulper and disk refiner usage. An additional 25 % electricity consumption was added for pumps, lights, ventilation, and instrumentation. Energy consumption ranges from 156 MWh / day to 177 MWh / day for scenario 1 and 2, each at a

50 t CMNF / day (dry equivalent) production rate, and drops to 78 MWh / day for scenario 3 with a 25 t CMNF / day (dry equivalent) production.

Table 3-4: Mass balance for scenario 1 - greenfield.

Stream	**1**		**2**		**3**		**4**		**5**
Descrip-tion	**Pulp**		**Water**		**Pulp suspension to CMNF tank**		**Final CMNF product**		**Losses**
	t/day	%wt	t/day	%wt	t/day	%wt	t/day	%wt	t/day
Cellulose Pulp	50	90 %		0 %	50	3 %	50	3 %	0
Water	5.6	10 %	1,611.1	100 %	1,616.7	97 %	1,616.7	97 %	0
Total	**55.6**	**100 %**	**1,611.1**	**100 %**	**1,666.7**	**100 %**	**1,666.7**	**100 %**	**0**

Table 3-5: Mass balance for scenario 2 - co-location.

Stream	**1**		**2**		**3**		**4**		**5**
Descrip-tion	**Pulp**		**Water**		**Pulp suspension to CMNF tank**		**Final CMNF product**		**Losses**
	t/day	%wt	t/day	%wt	t/day	%wt	t/day	%wt	t/day
Cellulose Pulp	50	3 %			50	3 %	50	0 %	0
Water	1,616.7	97 %	0		1,616.7	97 %	1,616.7	100 %	0
Total	**1,666.7**	**100 %**	**0**		**1,666.7**	**100 %**	**1,666.7**	**100 %**	**0**

Table 3-6: Energy consumption for scenarios 1–3.

Equipment	**Scenario 1**	**Scenario 2**	**Scenario 3**
	kWh / day	**kWh / day**	**kWh / day**
Hydropulper	16,667	0	0
Disk refiner	125,000	125,000	62,500
Others	35,417	31,250	15,625
Total	177,083	156,250	78,125

3.4.2 Capital investment

The breakdown of the capital investment for the greenfield and co-location scenarios is illustrated in Figure 3-4. Capital investment values vary from USD 18.5 million to USD 37.7 million. In Figure 3-4, hydropulper and disk-refining system values represent direct costs, which include equipment erection, instrumentation and controls, piping, electrical system, buildings, yard improvements, service facilities, and land. For scenario 1, investment cost is mainly related to the disk-refining system, which is higher than scenario 2 due to costs related to buildings, yard improvements, and land for the greenfield facility. Indirect costs (project management, basic engineering, detailed engineering, and contingency) increase proportionally to equipment costs. Although the production rate for scenario 3 is 50 % of scenario 2, capital investment is only 34% lower due to diseconomies of scale.

It may be possible to reduce capital investment on CMNF manufacturing by using a retrofitted refiner. However, this option was not considered in this study since the modifications may vary and will depend on availability of existing equipment.

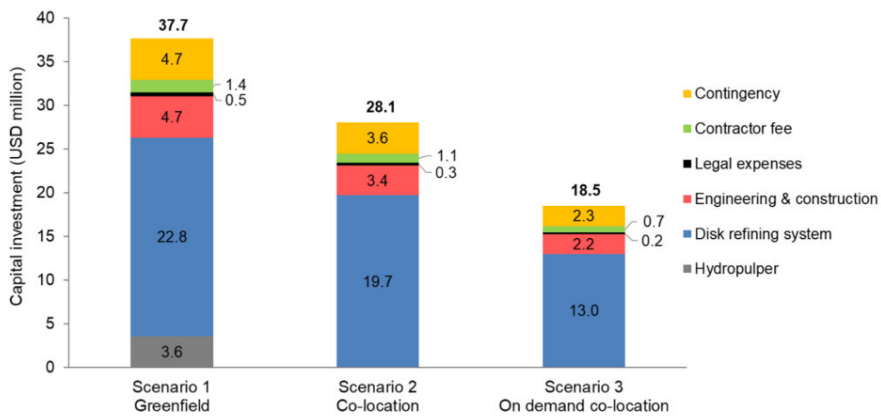

Figure 3-4: Breakdown of capital investment for scenarios 1–3.

3.4.3 Manufacturing cost and MPSP

CMNF manufacturing costs in 2020 (when facility reaches 100% capacity) vary from USD 1493 / t to USD 1899 / t CMNF (dry equivalent), as illustrated in Figure 3-5. Pulp represents more than 60 % of the total manufacturing cost, for all scenarios. Electricity is the second largest cost driver, accounting for about 15 % of the manufacturing cost, followed by depreciation, which accounts for 12 % to 14 % of the total manufacturing cost. The manufacturing costs for scenario 2 (co-location) are ca. USD 400 / t lower than greenfield (scenario 1) due to lower pulp, electricity, and labor costs.

MPSP was calculated for all scenarios using cash flow analysis, and values ranged from USD 1893 / t CMNF to USD 2440 / t CMNF (dry equivalent). The lowest MPSP was found for scenario 2 (co-location). In addition to the lower manufacturing cost, the lower capital investment per metric ton of material produced for scenario 2 results in a MPSP lower than USD 2000 / t of CMNF (dry equivalent).

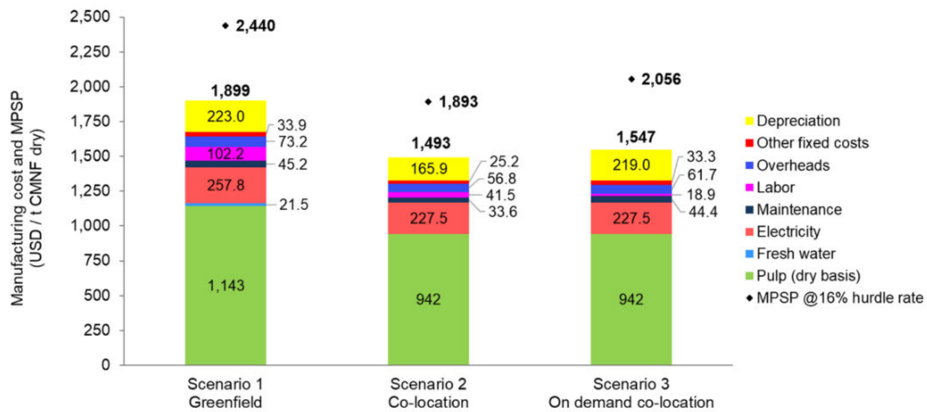

Figure 3-5: Manufacturing cost estimation and MPSP for scenarios 1–3 (for 2020).

3.4.4 Payback and return on investment

Payback periods for the three scenarios were calculated using a selling price of CMNF equal to the lowest MPSP (USD 1893 / t CMNF (dry equivalent)). Payback periods were 12.9, 5.7, and 6.7 years for scenarios 1, 2, and 3, respectively. ROIs were estimated for all scenarios, considering the scenario 2 MPSP, and are illustrated in Figure 3-6. The ROI value for the greenfield scenario (scenario 1) is much lower than in co-location options, due to higher capital investment as well as higher manufacturing cost. scenario 3 has a lower ROI than scenario 2 since the negative impact of diseconomies of scale is greater than savings in labor costs. From this analysis, it is clear that the co-location scenario has advantages over the greenfield one. A firm starting greenfield CMNF production may be easily displaced by competitors entering the market with co-located facilities, since co-location offers lower manufacturing cost, lower capital investment, and consequently lower MPSP. Clearly, a more detailed analysis should include product delivered.

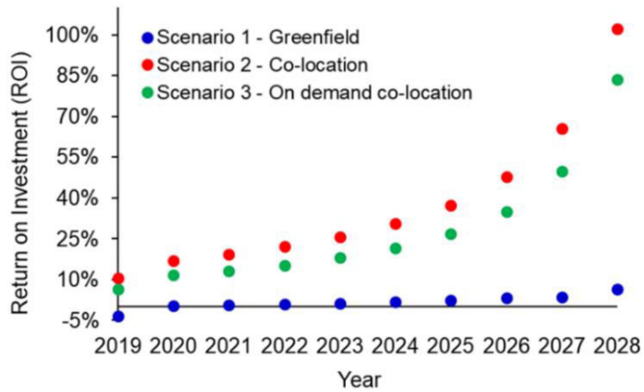

Figure 3-6: ROI for scenarios 1–3, considering CMNF price as USD 1893/t (dry equivalent).

3.4.5 Financial risk analysis

Sensitivity analysis was conducted for all scenarios. Capital investment and costs of pulp, electricity and water were varied by ± 25% and MPSP was recalculated. Sensitivity analysis results for scenarios 1 and 2 are illustrated in spider plots (Figure 3-7). For all scenarios, the MPSP is more sensitive to variations in pulp cost, capital investment, and electricity. Although the water consumption is relevant in the greenfield scenario (scenario 1), changes in its price affect the MPSP by less than 1 %.

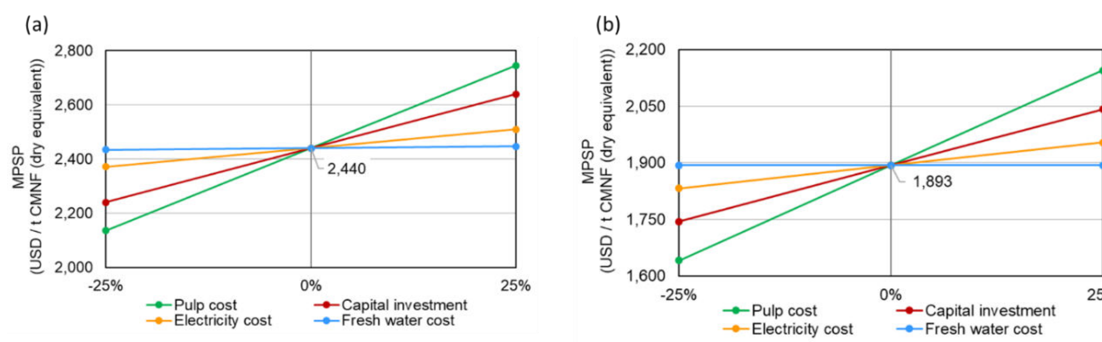

Figure 3-7: Results of sensitivity analysis for scenario 1 - greenfield (a) and scenario 2 - co-location (b).

Probabilistic risk analysis was performed for scenario 2, considering the probability distributions of capital investment and costs of pulp and electricity. The distributions' fits are illustrated in Figure 3-8. A uniform distribution was adjusted for the capital investment, considering equal chances of capital investment falling between USD 19.7 million and

USD 36.5 million (± 30% of initial estimate). Triangular distributions were adjusted for pulp and electricity costs based on 2- and 3-year historical data, respectively. The probability distribution of CMNF manufacturing cost for scenario 2 is illustrated in Figure 3-9.

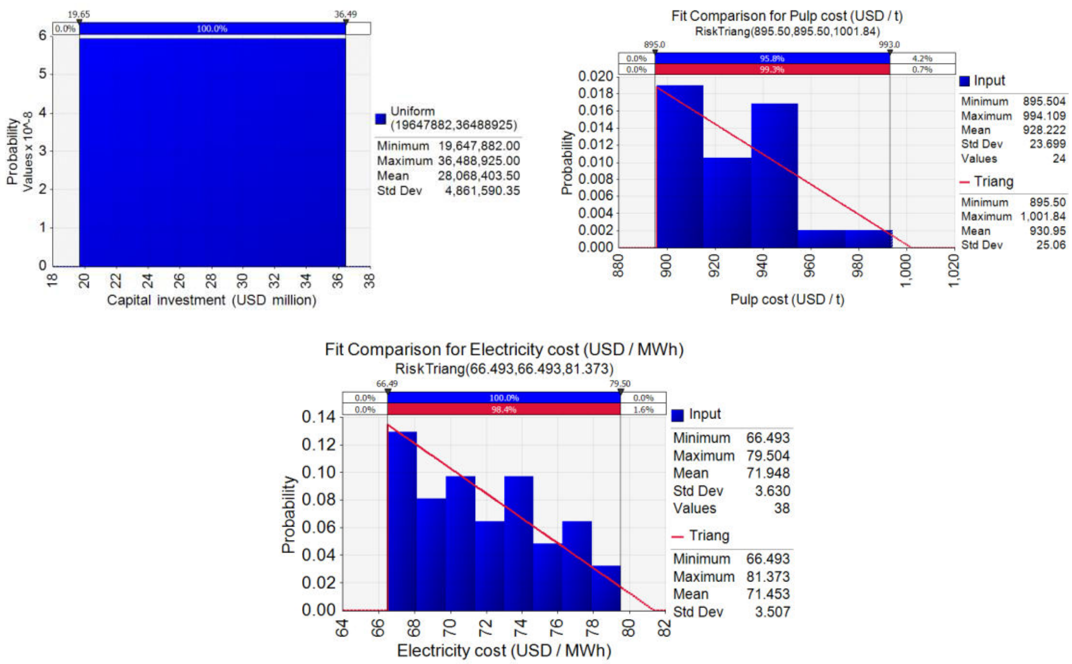

Figure 3-8: Distribution fits for capital investment (uniform), pulp cost (triangular), and electricity cost (triangular) (scenario 2).

When uncertainties are considered, estimated manufacturing cost range from USD 1,375 to USD 1,630 / t CMNF (dry equivalent). There is about 52 % probability of manufacturing cost being lower than the deterministic value of USD 1493/t CMNF (dry equivalent). Table 3-7 shows the proxy values for MPSP for scenario 2. These MPSP values were calculated by changing the inputs until the defined manufacturing cost is reached. The selected MPSP value for investment decision-making will depend on the risk appetite of the investor; we believe it is safer to consider values around USD 2050 / t CMNF, which represent around 95 % probability of occurrence. MPSP at 100 % probability are about 11 % higher than deterministic value, due to low variability of pulp costs, the major cost driver for CMNF manufacturing.

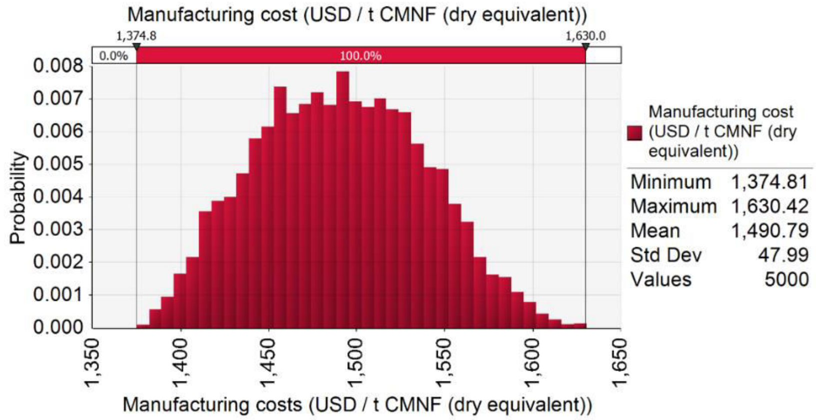

Figure 3-9: Probability distribution of CMNF manufacturing cost for scenario 2 - co-location.

Table 3-7: Probability of manufacturing cost and MPSP values for scenario 2 - co-location.

Probability	**Manufacturing cost (USD / t CMNF dry equivalent)**	**Proxy for MPSP (USD / t CMNF dry equivalent)**
50 %	≤ 1,490	≤ 1,900
75 %	≤ 1,525	≤ 1,930
95 %	≤ 1,570	≤ 2,050
100 %	≤ 1,630	≤ 2,110

3.4.6 Comparison with CNC manufacturing cost

From a process engineering and a financial point of view, in the short term, CMNF manufacturing seems to be established commercially more likely than CNC. Several reasons can prompt fast track commercialization. For instance, lower capital investment is needed to start CMNF manufacturing, and if no pre-treatment is applied, the process to obtain CMNF is relatively simple, using raw materials already available in a mill, with almost no effluent generated.

CMNF manufacturing cost can be much lower than CNC, which can reach around USD 7000 / t (dry equivalent) [121]. Although electricity consumption for CMNF manufacturing is higher, CNC production uses larger quantities of chemicals and requires higher capital investment for same production capacity. In addition, the high complexity of the CNC production facility intensifies labor and maintenance costs.

3.4.7 Suggested improvements to reduce CMNF manufacturing cost and MPSP

From the analysis presented herein, it is observed that any pulp cost reductions will lower manufacturing cost and MPSP. Since pulp cost accounts for about 60 % of manufacturing cost, an assessment was performed by changing feedstock type and cost for scenario 2, with results illustrated in Figure 3-10. If pulp cost can be as low as USD 600 / t, such as bleached eucalyptus kraft pulp – BEK (http://www.risiinfo.com/ and personal communication), CMNF manufacturing cost can be as low as USD 1150 / t CMNF (dry equivalent), with MPSP around USD 1540 / t CMNF (dry equivalent). If the selling price is the same as MPSP from scenario 2 (USD 1893 / t CMNF (dry equivalent)) and manufacturing cost ~ USD 1150 / t CMNF (dry equivalent), the calculated payback period drops from 5.7 to 4.2 years. Another option to be considered is the use of (agricultural) wastes and recycled fibers or sludge as feedstocks, which might be more cost-efficient [135]. However, it should be noticed that the use of different feedstocks can yield different product properties and a different configuration of disk refiners might be necessary. None of these aspects were assessed in this study. We do believe that characterization of CMNF from different types of pulp (soft wood, hardwood, agricultural residues) is of paramount importance to understand the trade-off between (i) fiber cost, (ii) effect on process operation and cost (how easy the feedstock can be refined), and (iii) the intrinsic features of CMNF from different feedstocks.

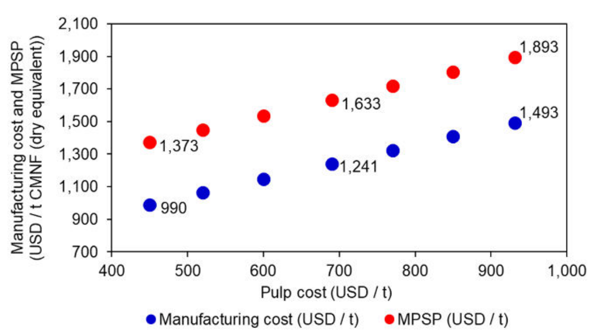

Figure 3-10: Impact of reduced pulp costs on CMNF manufacturing cost and MPSP (scenario 2 - co-location).

3.5 Conclusions

The current study aimed to estimate manufacturing cost and MPSP for CMNF produced at industrial scale. Considering a 50 t / day (dry equivalent) facility using disk refining technology, calculated manufacturing cost can be as low as USD 1493 / t CMNF (dry equivalent), with MPSP of USD 1893 / t CMNF (dry equivalent). The major cost driver for CMNF production is pulp, which represents more than 60 % of manufacturing cost for greenfield and co-location scenarios. Co-location provides a lower MPSP, with savings possible due to lower capital investment, cost of pulp, electricity, and labor. When uncertainties are considered, the MPSP for co-location scenario can be up to 11 % higher than deterministic value. Due to high costs of market pulp (specifically NBSK), MPSP was assessed considering lower feedstock costs. If bleached eucalyptus kraft pulp is used as feedstock, for example, operating costs can be as low as USD 1150 / t (dry equivalent) and MPSP drops to USD 1540 / t (dry equivalent) for the co-location scenario.

Due to process simplicity, lower manufacturing cost and MPSP, it is expected that CMNF could be the starting point for industrial development of cellulosic nanomaterials. However, the commercial price of CMNF are cost and supply driven. Whether or not markets will support these or higher prices will depend on the use of these materials, which will be strongly dependent on market adoption and improved properties, when compared to the current technologies available.

4 TECHNO-ECONOMIC ASSESSMENT, SCALABILITY, AND APPLICATIONS OF AEROSOL LIGNIN MICRO- AND NANOPARTICLES [3]

4.1 Abstract

Lignin micro- and nanoparticles (LMNPs) synthesized from side-streams of pulp and paper and biorefinery operations have been proposed for the generation of new, high-value materials. As sustainable alternatives to particles of synthetic or mineral origins, LMNPs viability depends on scale-up, manufacturing cost, and applications. By using experimental data as primary source of information, along with industrial know-how, we analyze dry and spherical LMNPs obtained by our recently reported aerosol/atomization method. First, a preliminary evaluation toward the commercial production of LMNPs from industrial lignin precursors is presented. Following, we introduce potential LMNPs applications from a financial perspective. Mass and energy balances, operating costs, and capital investment are estimated and discussed in view of LMNPs scalability prospects. The main potential market segments identified (from a financial perspective) include composite nanofillers, solid foams, emulsion stabilizers, chelating agents, and UV protection. Our technical, financial, and market assessment represent the basis for R&D planning and efforts to lower the risk related to expected industrialization efforts. Manufacturing costs were estimated between 870 and 1,170 USD/t; also, minimum selling prices varied from 1240 and 1560 USD/t, depending on raw materials used. Sensitivity analysis indicated that manufacturing cost can be as low as 600 USD/t, depending on the process conditions considered. Finally, based on the financial assessment, potential applications were identified.

4.2 Introduction

Lignin naturally occurs in woody and nonwoody plants, representing from 15 % to 30 % by weight of the total dry mass, depending on the source [146]. Lignin has a complex structure originating from hydrogenative polymerization of three basic precursors, namely, p-

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[3] The material in this chapter has been published as:
de Assis CA, Greca LG, Ago M, Balakshin MY, Jameel H, Gonzalez R, Rojas OJ. Techno-Economic Assessment, Scalability, and Applications of Aerosol Lignin Micro- and Nanoparticles. *ACS Sustainable Chemistry & Engineering* 6 (9), 11853-11868, 2018.

hydroxyphenyl (H), coniferyl (G), and sinapyl (S) alcohols. The resulting macromolecule contains various functional groups and its monomeric phenylpropane units (or C9-unints) are linked by different ether and C−C linkages (Figure 4-1a) [147]–[150]. The huge opportunity for securing vast quantities of lignins from the forest products industry, economically and at large scale, is concurrent with developments in biorefineries and bioproduct mills that integrate biomass conversion processes. At present, the primary production sources of industrial lignin are the organic-rich streams generated during biomass digestion (wood pulping), which contains mainly dissolved lignin, carbohydrates and their degradation products and extractives, as well as cooking inorganics. The latter components are usually recovered from solution while the remaining material, the ligninic fraction, is normally used for energy generation [151]. This current low-end use of lignin can be seen as a starting point for the future bioeconomy, as an alternative to fossil resources that do not compete with food supply.

Due to its diverse functional groups, lignin can find other uses [15], such as absorbents, emulsifiers, dispersants, and as chelating agents [152]–[155]. Additionally, a wide range of chemicals and products, such as adhesives, can be produced from lignin [156]–[158]. Moreover, it can be used for the production of bioplastics, as well as for controlled and slow release of fertilizers [159]. Carbon fibers can be obtained from lignin [160], which in turn can be used as component in supercapacitors and energy storage devices [149], [160], [161]. Nevertheless, several challenges exist to facilitate value-added applications of lignin. They include relatively low reactivity, low compatibility in many polymer blends, the chemical structure variability (which depends on the feedstock and extraction conditions), broad molecular weight distributions, inconsistency in composition profiles, and tendency to repolymerize after fragmentation, among others [158], [162]. In addition to the complexity of the lignin structure in the plant biomasses, all biorefinery processes result in dramatic increase in complexity and chemical heterogeneity of the structures of technical lignins [158], [163].

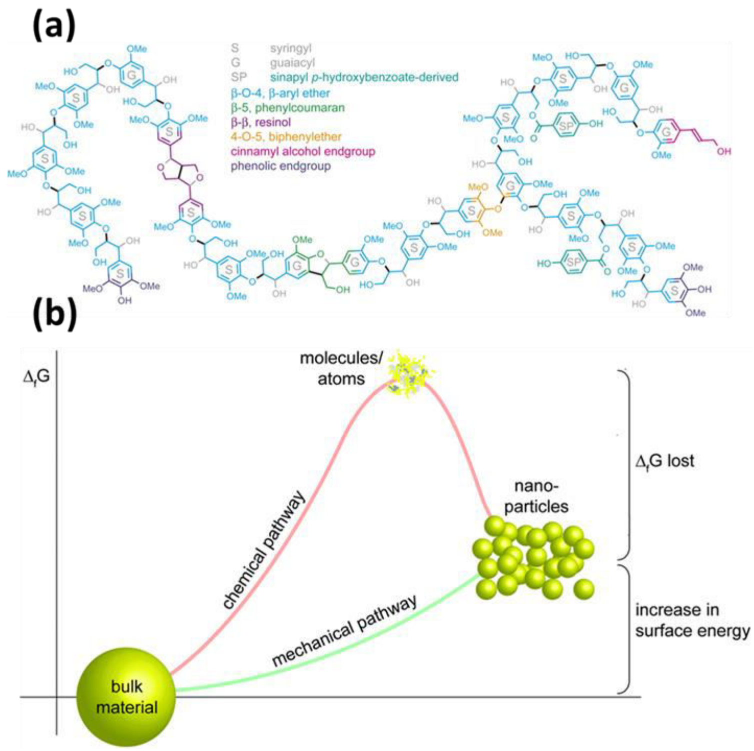


Figure 4-1: (a) Plausible structural model of a lignin fragment showing various functional groups and interunit linkages.

Reprinted in part with permission from ref. [164] (Copyright 2010 American Society of Plant Biologists). (b) Energy profile (Gibbs free energy) along with chemical or mechanical nanoparticle preparation. The chemical pathway presents an unnecessary diminution step (high intermediate ΔG) since the atomic/ionic or molecular intermediates are then again combined to nanosized particles. Reprinted in part with permission from ref [165] (Copyright 2015 The Royal Society of Chemistry).

4.2.1 Lignin micro- and nanoparticles (LMNPs)

A remarkable behavior of lignins, when subjected to specific conditions, is their tendency to form small particles within the plant cell walls [151], [166]. In this work, lignins from pulp and paper processes are used as feedstock for the manufacture of colloidal lignin or lignin micro- and nanoparticles (LMNPs). LMNPs represent a toolbox toward property development that can be quite attractive for practical applications. These can be exemplified in current efforts to supply materials with color, thermal, and light stability as well as strength [167]. Moreover, improved or new functions can be achieved from multiple components integrated in the form of particles [165]. In general, the isolation of particles via mechanical pathways is less energy demanding than chemical routes. This is a direct result of the surface energy that is lower compared with typical chemical manufacturing enthalpies, such as dissolution, reduction, and others (Figure 4-1b) [165]. Thus, small and chemically inert particles can be used, for example, in pigments, as polymer fillers or in surface finishing [165]. In the specific case of lignin particles, there is great promise as emulsion stabilizers, antioxidants, and agents for UV protection [151], [168]–[170].

The field of polymer nanoparticles is quickly expanding and playing a pivotal role in a broad spectrum of areas [171]. This fact can be realized from the ever-increasing number of publications, as depicted in Figure 4-2a. This trend is based on the properties of polymer particles, which meet a wide range of applications and market needs. To some extent, the same can be said for those derived from lignin, a subset of polymer particles, Figure 4-2b. The use of lignin micro- and nanoparticles to produce added value materials can open an important pathway for the development of new applications and consequently contribute to fostering the future bio-based industry [151], [172].

4.2.2 LMNPs formation mechanism and synthesis

At given conditions, lignin tends to form spherical particles [151], [166]. Prior studies have proposed that LMNPs are formed in situ when biomass is subjected to temperatures higher than the lignin phase transition (~175°C) [151], [166]. Formation of particles with different shapes and sizes, between 5 nm to 10 μm, have been reported. The mechanisms proposed for the formation of these particles includes: (i) a coalescence phase, when temperature is above lignin softening point, allowing it to expand and move within the cell wall matrix; (ii) a migration phase, when lignin migrates to the cell surface, and finally (iii) particle formation and extrusion from the cell wall, as cellulose microfibrils are exposed and consequently attached to each other by hydrogen bonding [151], [166]. Lignin can be separated from other wood components by well-known processes (such as kraft pulping), although particular conditions are needed for the generation of respective particles at the micro- and nanoscale [168].

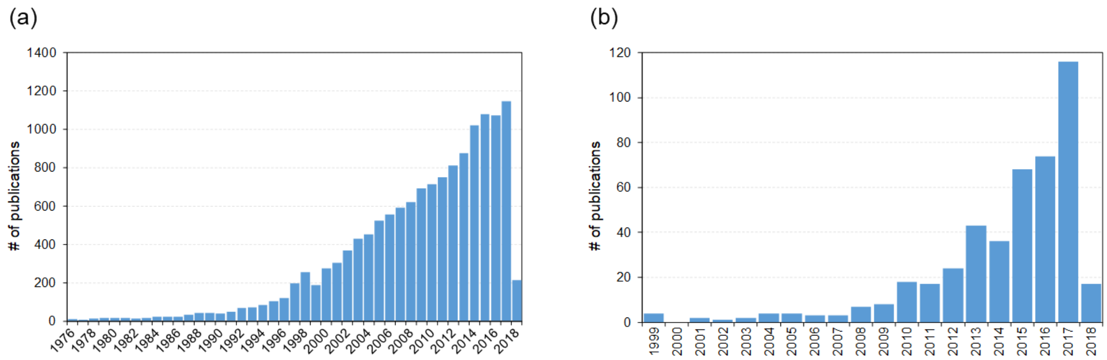


Figure 4-2: (a) Number of publications per year according to a search with Web of Science (March 2018).
using the search terms "TI = (polymer* or biopolym* or biomacrom*) and TI = (particle* or nanoparticle* or microparticle* or bead* or microbead* or nanobead* or capsule* or microcapsule* or nanocapsule* or microsphere* or nanosphere*) and refined by TOPIC: (production or isolation or synthesis or development or separation). (b) Number of publications per year according to Web of Science (March 2018) using the search terms "TI = (Lignin*) and TI = (particle* or nanoparticle* or microparticle* or bead* or microbead* or nanobead* or capsule* or microcapsule* or nanocapsule* or microsphere* or nanosphere*) NOT TS = (particleboard* or board*). Field tags: TI = title, TS = topic.

Biomass pretreatments may indeed change the lignin structure and generate different types of materials [162], [173]. For lignin characterization purposes, various analytical procedures including ball milling (followed or not by enzymatic treatments) have been used to isolate lignins from biomass without significantly modifying its structure [150]. The drawbacks of these processes include the very high energy demand and limitations in scaling up, making them industrially unrealistic. At the industrial scale, lignin is isolated from the wood by different processes, such as kraft, soda, and sulfite pulping, generating kraft lignin, alkali lignin, and lignosulfonates, respectively [158], [168], [174]. On the basis of pulp production, the kraft process is the most commonly used to separate lignin from wood, generating about 78 million metric tons of lignin world-wide [158], [174]–[176]. While this lignin is used in energy cogeneration, there is a potential to recover between 5% to 10% of the total kraft lignin production without negative impacts on mills' operations and finance (depending on pulp mill production limitations). The current recovery of pulping lignins is only 2%of the industrial production, where the majority of commercial lignin is sourced from the sulfite process, with a total production close to 1.1 million metric tons/year of lignosulfonates as of 2015 [158], [168], [174], [177], [178].

Lignin particles with various sizes and shapes, hollow or solid, have been reported by using different processes, such as solvent or pH shifting, cross-linking/polymerization, mechanical treatment, ice-segregation, template-based synthesis, electrospinning, CO_2 antisolvent, and aerosol processing [168]. A description of these processes can be found in recently published reviews [151], [162], [168]. In the solvent shifting process, the lignin is dissolved in a water-miscible organic solvent. The solution is then mixed with excess water, generating the LMNPs due to the reduced solvency [168]. In pH shifting, lignin is diluted in a solvent (e.g., ethylene glycol) or water at a high pH, followed by addition of an acidic solution (e.g., HCl), allowing the formation of LMNPs [179]. Cross-linking and polymerization have been used for the synthesis of LMNPs, which may include the use of surfactants and cross-linking agents [168]. Mechanical treatments, such as homogenization and sonication, were applied to reduce particle size of lignin to the nanoscale [180], [181]. In the ice-segregation method, an aqueous lignin solution was rapidly frozen, followed by ice sublimation, thus generating a network of lignin nanofibers [182]. Template-based synthesis, as suggested by its name, uses a template (e.g., alumina membrane) to shape the lignin into a desired form, such as nanotubes [183], [184]. Electrospinning of lignin solutions has been demonstrated in the presence of poly(ethylene oxide) or poly(vinyl alcohol) in the solution [185]. Carbon dioxide antisolvent is a technique that uses CO_2 at supercritical conditions for lignin precipitation [186]. Finally, LMNPs have been produced from kraft lignin solution (tetrahydrofuran and water) by evaporating the solvents and redispersing the solids obtained in water [187].

Solvent shifting, CO_2 antisolvent, aerosol, and dissolution/evaporation pathways have presented the highest yields reported. The main drawbacks of solvent shifting and CO_2 antisolvent are the low solids concentration in final product and high operating pressures, respectively. The dissolution/evaporation process, despite the high yields, needs multiple steps. Mechanical treatment for the manufacturing of LMNPs seems promising, given the similarities to existing pulp and paper operations and the absence of hazardous solvents; however, the broad range of particle sizes obtained may prevent applications of the final product (due to nonuniformity). Most relevant for any practical use, most of the above methods are highly intensive in solvent use. In contrast, previous efforts demonstrated the possibility of aerosol processing, in one step, to obtain dry lignin particles with sizes ranging from 30 nm to 2 μm and with various surface energies (wettability), depending on the source and process conditions [172]. Moreover, in situ development of surface features on the particles is possible, such as wrinkling, which is attractive in advanced applications [188]. A comparison of the processes previously discussed including the types of lignin used, yields, advantages, and disadvantages is presented in Table 4-1. Due to ease of scale-up and relatively high yields, the aerosol process was selected in our techno-economic study.

Due to the relative novelty of LMNPs and the recent dates associated with the reports and advances in the manufacturing processes, to our knowledge, no techno-economic studies on LMNPs manufacturing process are available, although some studies indicate potential for scale-up [172], [187]. We hereby propose a preliminary assessment for LMNPs manufacturing at industrial scale. The selected process (aerosol method) is described and discussed along with estimated capital and operating costs. Additionally, the impact of different process conditions on project financials is evaluated through sensitivity analyses. Finally, an evaluation of potential applications is provided. The collective information and methodologies used are expected to help in directing LMNPs development efforts to the most promising opportunities.

Table 4-1: Comparison of different LMNP isolation methods (based on Beisl *et* al., 2017). [168]

Technology	**Lignin types used**	**Reported yield**	**Advantages**	**Disadvantages**
Solvent shifting	AL, KL, OS, EHL	33% - 90.9%	simple process; yields solid and hollow particles	low solids content (~ 1%)
pH shifting	AL,KL, EHL	10%		high solvent demand; low yields (10%)
Cross-linking / polymerization	KL, AL, LS		controlled size of particles [189]	
Mechanical treatment	AL, KL	-	process known in pulp and paper industry; simple process; does not use hazardous solvents [162]	non-uniformity of particle size broad particle distribution range
Ice segregation	AL			
Template-based synthesis	AL, other lignins		controlled shape characteristics [183], [184]	
Electrospinning	KL, OS, LS, PL		low solvent usage	
CO_2 antisolvent	KL, OS	51% - 88%	controllability of morphology, size and size distribution; CO_2 is non-flammable and non-toxic	high operating pressure
Aerosol processing	AL, KL, OS	> 60 %	single step process; absence of liquid byproducts; high yields	
Dilution followed by solvent evaporation and redispersion [187]	KL	85%	possibility to scale-up; simple process	several steps needed; final product is dispersed in water

AL = alkali lignin, KL = kraft lignin, OS = organosolv lignin, EHL = enzymatic hydrolysis lignin, LS = lignosulfonate, PL = pyrolytic lignin.

4.3 Materials and methods

4.3.1 Synthesis of LMNPs

Different types of lignins were used at the laboratory scale for the aerosol flow process. The precursors included soda, organosolv, and kraft lignins [172]. In the first generation of this process, a lignin solution (e.g., alkaline solution for alkali lignin, and dimethylformamide for organosolv or kraft lignin) was prepared in an agitated vessel. The solution was then sent to a collison-type jet atomizer with nitrogen that generated small droplets. The droplets were carried to a heated reactor at a given temperature (e.g., 100 °C for water or 153 °C for DMF), and the solvent was evaporated. The reactor outflow consisted of a mixture of lignin particles and solvent in the vapor phase. This outflow was sent to a Berner-type low-pressure impactor, where LMNPs were collected and the vapor was exhausted. A second, larger version of the unit was developed for the benefit of this study to increase the capacity, which included a nebulizer and a cyclone collector (Figure 4-3). In this larger version, the cooling water in the solution source is necessary to prevent overheating of the ultrasonic nebulizer during extended operation periods. Figure 4-4 illustrates LMNPs that can be produced with this system.

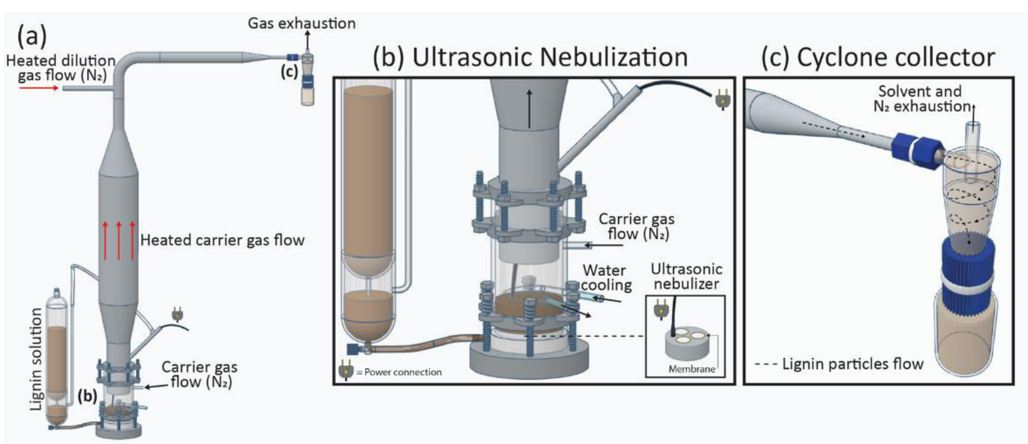


Figure 4-3: Laboratory-scale setup used for LMNPs synthesis in this study: (a) general scheme for the aerosol flow reactor; (b) ultrasonic nebulizer assembly; and (c) cyclone collector assembly.

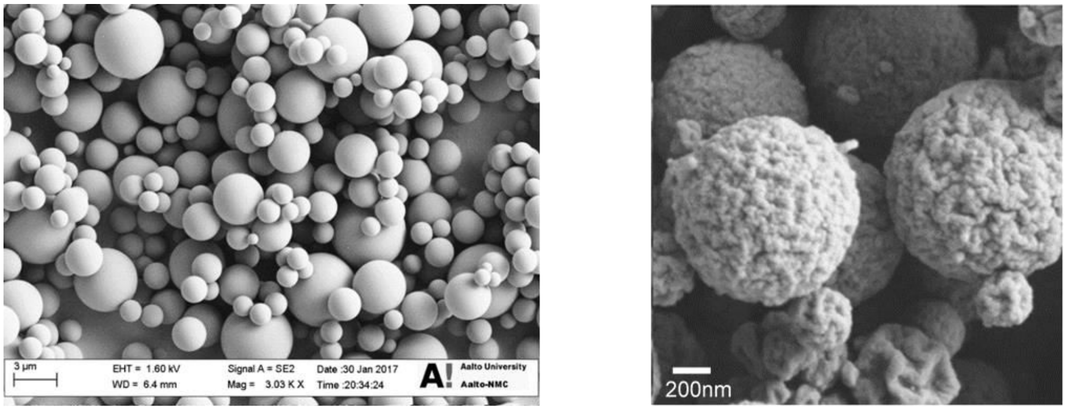


Figure 4-4: Example of LMPNP produced by the aerosol flow system shown in Figure 4-3.

On the left, spherical, dry, and smooth lignin particles with sizes in the micrometer range (scale bar = 3 μm). On the right, a SEM image of LMNPs (scale bar = 200 nm) showing surface wrinkling, which can be produced by adjusting the operation conditions in the unit. Adapted with permission from ref [188] (Copyright 2018 The Royal Society of Chemistry).

4.3.2 Techno-economic analysis of LMNPs manufacturing at industrial scale

The steps used to perform the techno-economic analysis for LMNPs manufacturing are illustrated in Figure 4-5. Initially, information from the laboratory scale process was collected to identify the main streams and processes (e.g., reaction, separation, heating, etc.). Using this information, and based on industrial experience, a block diagram was constructed. Process areas and major equipment needs were defined, as well as main process streams. Process information from the laboratory scale was collected (such as production yields, raw materials, and energy requirements), and adjusted for mass and energy balances at the industrial scale. Production flow rates were estimated, and the main equipment (tanks, pumps, atomizer and separator) were designed.

The following step aimed to link the technical and financial models. Ordinary equipment costs were estimated using Peters and Timmerhaus' cost estimation tool and Matches' databases [190], [191]. The cost for atomization and separation equipment was based on previous quotations from equipment suppliers. The overall capital investment was estimated by multiplying the sum of equipment costs by factors that account for equipment erection, piping, electrical systems, instrumentation and controls, buildings, yard improvements, service facilities, land, as well as indirect costs (engineering, construction and legal expenses, contractor fees, and contingency); factors used were based on information available in literature [145]. To estimate direct operating costs, calculated process flow rates were combined with unitary costs of feedstocks and utilities. Other operating costs (maintenance, labor, depreciation, overheads, and other fixed costs) were based on direct operating costs and capital investment values, in addition to wages information used in previous assessments [121], [192]. Finally, a simplified cash flow modeling was executed and the minimum product selling price (MPSP) was estimated for a set of financial assumptions that will be described later. MPSP is the estimated product price for the investment to achieve Net Present Value (NPV) zero at a specified hurdle rate (the minimum rate expected when investing in a project). The assessment was then supplemented by a sensitivity analysis, where main process and financial parameters were varied and their impact on the project financials were evaluated [65]. Microsoft Visio was used to create block and process diagrams at the laboratory and industrial scales. Microsoft Excel was used for mass and energy balance calculations, as well as financial assessment and sensitivity analysis of the industrial process.

4.3.3 Feedstock

Kraft lignin and lignosulfonate were selected as the precursors for the industrial scale process, due to their commercial availability. For experiments at the laboratory scale process, kraft lignin, DMF and ammonium hydroxide (25 % aqueous) were purchased from Sigma-Aldrich; they were used without further purification. For the industrial process, bulk-scale feedstocks and chemicals were assumed. Suitable solvents for lignin precursors were defined: water for the lignosulfonate and dimethylformamide (DMF) and ammonium hydroxide solution (14 % wt.) for kraft lignin. DMF was used in the initial experiments with kraft lignin [172] and ammonium hydroxide was considered given its lower cost. The three solvents were selected to establish a comparison of their effect in the economic feasibility and considering that they easily dissolve the respective lignin for the aerosol flow process, at 5 % solids concentration.

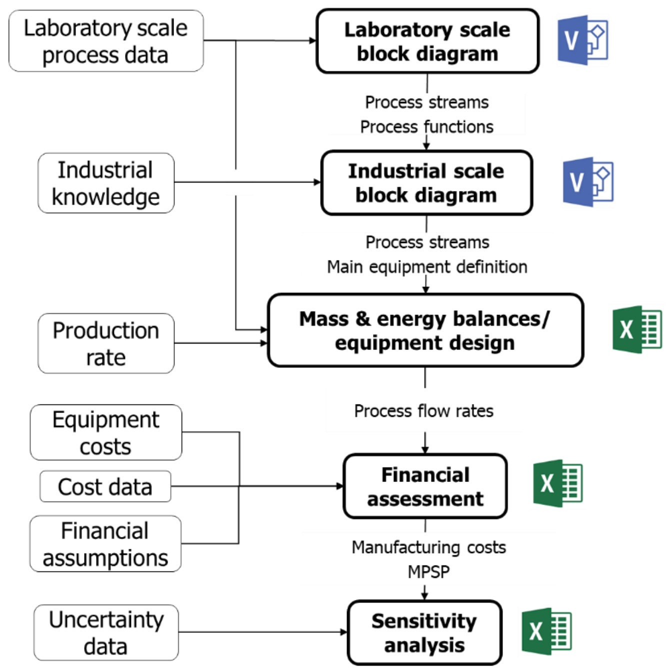


Figure 4-5: Steps to perform techno-economic analysis of LMNPs manufacturing.

4.3.4 Technology selected and scenarios assessed

As indicated previously, the techno-economic analysis of the aerosol technology was performed. It is worth noting that the atomizer and separation technologies were used for the cost modeling of LMNPs manufacturing at the industrial scale. Additional bench scale analyses, pilot testing, as well as discussions with equipment suppliers were carried out to confirm the adequacy of this technology from a technical perspective. Three scenarios were selected (Table 4-2). All scenarios considered the LMNPs facility co-located with a pulp mill, which was assumed to supply dried lignin to the new facility. Note, however, the possibility of using lignin solutions generated directly in the process, avoiding drying, which would entail a considerable benefit in the economics of the process. In our calculation we assumed that lignin was delivered in dry form, making it more cost-demanding. Despite this added cost, it is reasonable to still expect a lower cost compared to alternative processes to obtain lignin particles, such as solvent or pH shifting. Not only they require the lignin solution feed but also other solutions (anti-solvent or acid solutions) that ultimately are to be removed by drying.

Table 4-2: Summary of scenarios assessed.

Scenario	Lignin precursor	Solvent
1	kraft lignin	dimethylformamide (DMF)
2	kraft lignin	ammonium hydroxide (14 % wt. in water)
3	lignosulfonate	water

4.3.5 Description of simulated industrial scale process

The first step to simulate the nth plant for LMNPs manufacturing was to construct a block diagram of the laboratory-scale process, and to adapt it to the industrial scale. For the laboratory scale facility (Figure 4-3), four main unit operations were identified (dissolution, atomization, drying, and vapor–solid separation). The block diagram of the proposed industrial scale process for LMNPs manufacturing is illustrated in Figure 4-6, top. While one can assume that the lignin is sourced as a solution from the actual process, in situ, here we adopt the most challenging situation where the lignin feed is obtained as a dry powder. Such dried lignin was then diluted in the given solvent using an agitated vessel. Afterward the solution was sent to the atomizer and separation systems. This equipment was able to generate small solution droplets, followed by the evaporation of the solvent using hot air that flowed countercurrent in a drying chamber. The stream consisting of dried particles and the vapor phase of the solvent was sent to a device where the vapor–solid separation was performed. A cyclone and bag filter were assumed for separation. The particles were collected at the bottom of the cyclone, and the vapor phase passed through a bag filter to collect the remaining particles. The solids collected from cyclone and bag filter are the final product, LMNPs. The vaporized solvent in the separation step was drafted from the system using a fan and recovered in the solvent recovery section. In the solvent recovery section, the solvent was condensed in a heat exchanger. The recovered solvent was mixed with fresh solvent and fed back to the dissolution step. Solvent losses were accounted in the simulation, due to possible residual solvent within the final product (LMNPs) and the very small losses through venting systems, which were calculated using EPA guidelines [193]. The impact of solvent losses is further evaluated in this work. A flowsheet for the proposed industrial process is presented in Figure 4-6, bottom.

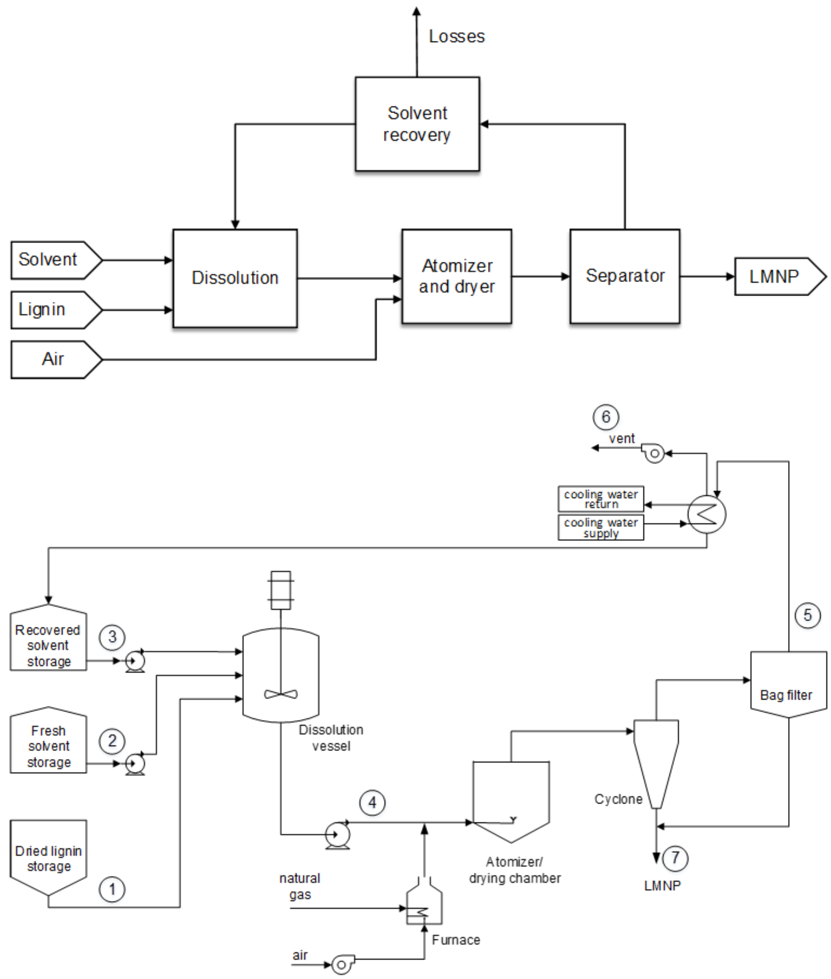


Figure 4-6: Simplified block (top) and process (bottom) diagrams for industrial scale manufacturing of LMNPs.

4.3.6 Process assumptions

The main process assumptions for the industrial process are included in Table 4-3. The production rate was defined based on Culbertson (2017) [30], which assumed that 5.2 % of lignin liquor can be extracted as lignin product from a kraft pulp mill with a capacity of 440,000 air-dry metric ton/yr. The yields for LMNPs reported by Ago *et* al [172] were > 60 %; such relatively lower yields at the laboratory scale, in absence of a bag filter, are mainly attributed to particles retained in the drying chamber and losses in the solvent exhaustion system. It is expected that for the industrial facility these issues would be controlled, generating no product losses. Thus, we assumed negligible lignin losses in the industrial scale manufacturing. A separator efficiency was defined for the industrial process, which means that the solids that could not be separated in the cyclone and bag filter were sent to the solvent recovery system together with the solvent and then reprocessed. A typical mass balance is presented in Table 4-4.

Table 4-3: Main process assumptions for LMNP manufacturing at industrial scale.

Input	**Value**	**Unit**	**Reference**
Production rate	150	metric ton/day	Culbertson, 2017 [30]
Facility type	collocated within a pulp mill		Assumed
Lignin concentration in solution	5 %	% wt.	Ago *et* al., 2016 [172]
Lignin losses to the environment	0 %	% wt. of input flow	Assumed
Losses of solvent to atmosphere	0.001 %	% wt. of recirculating solvent	Based on EPA [193]
Solvent concentration in final product	0.5 %	% wt.	Assumed
Separation efficiency	99 %	wt. solid out / wt. solid in	Assumed
Cooling tower temperature difference	10	°C	Assumed
Cooling water makeup	2 %	based on recirculating flow	Assumed
Overall equipment efficiency	95 %		Assumed

Table 4-4: Typical mass balance for industrial manufacturing of LMNPs (for stream numbers refer to Figure 4-6, bottom).

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Description	**Lignin, t/day**	**Fresh solvent, t/day**	**Recovered solvent, t/day**	**Solution to atomizer, t/day**	**Vapors to recovery, t/day**	**Losses to vent, t/day**	**LMNP, t/day**
Lignin	150.0		1.5	151.5	1.5		150.0
Solvent		0.8	2878.0	2878.8	2878.0	0.03	0.8
Total	**150.0**	**0.8**	**2879.5**	**3030.3**	**2879.6**	**0.03**	**150.8**

4.3.7 Scalability assessment

4.3.7.1 Feedstock

For the proposed techno-economic analysis, we assumed that the kraft and lignosulfonate lignins used were not of high purity. Lignin may contain ash and carbohydrates, which are not soluble in organic solvents. Although not considered in the current analysis, additional filtration equipment might be necessary for separating insoluble impurities from the lignin solution. In addition, it was assumed that a less pure lignin does not affect negatively the LMNPs quality for the intended applications. The consequences of using an industrial grade feedstock should be assessed by laboratory and pilot trials before scaling up the process.

4.3.7.2 Process configuration and equipment.

The production of LMNPs at the laboratory scale process was performed in semibatch mode. The dissolution phase was in batch, and atomizing and drying steps were performed continuously. To ease operation and consequently produce LMNPs in a cost-effective manner, the industrial process was assumed to run in continuous mode; this prevents equipment idle time and ensures their efficient utilization. Nevertheless, it was assumed that the facility would operate 95 % of the year (Overall Equipment Efficiency-OEE-of 95 %) to account for maintenance and facility downtime (Table 4-3).

The nebulizer in the laboratory scale process was defined as an atomizer and separator system, which can be easily designed and scaled up for capital cost estimation. In addition, the particle drying system at the laboratory scale (oven) used electrical resistance to evaporate the gases. In the industrial scale, air was assumed to be heated in a furnace using natural gas as fuel (Figure 4-6, bottom).

4.3.7.3 Utilities and infrastructure

Considerations about infrastructure and utilities are necessary for the simulation of an industrial facility. For example, the laboratory scale process used nitrogen as carrying gas between process equipment. The transport of particles at industrial scale considered a fan to draft air and consequently carry the particles. It was assumed that the solvents were recovered by a condensing system and recirculated back to the dissolution step.

4.3.8 Major costs and financial assumptions

Major raw materials and energy costs are presented in Table 4-5. Reported kraft lignin value vary between 250 and 500 USD/t [30], [178]. For the current assessment, we considered USD 250/t based on Culbertson (2017) [30]. Lignosulfonates values range from

300 to as high as 2700 USD/t, depending on purity [15], [178]. For LMNPs, we assumed that there is no requirement on lignosulfonate quality. Using the literature review and industry quotations, we adopted the value reported of 300 USD/t. DMF costs were retrieved from ICIS database (2000) and adjusted to current values using the PPI (producer price index) reported by the Bureau of Labor Statistics [194], [195]. The PPI used was for crude petroleum and natural gas extraction−primary products, since DMF is manufactured from methanol. Ammonium hydroxide costs were based on average anhydrous ammonia prices reported by Fertecon [196], and calculated as indicated by Airgas, an ammonium hydroxide supplier [197]. Water was assumed as tap water. Natural gas and electricity costs were retrieved from FisherSolve and EIA (U.S. Energy Information Administration) [93] databases, respectively.

Table 4-5: Major costs considered for LMNPs process.

Input	**Value (2019)**	**Unit**	**Reference**
Kraft lignin	250	USD / t	Culbertson (2017) [30]
Lignosulfonate	300	USD / t	Holladay *et*. al (2007) [15]; Miller *et*. al (2016) [178]; industry contacts
Dimethylformamide (DMF)	1,530	USD / t	ICIS (2000) [92]
Ammonium hydroxide (14% wt)	72.7	USD / t	Fertecon [198] and AirGas [197]
Tap water	0.66	USD / m^3	EPA[(a)] (2004) [97]
Natural gas	4.5	USD / MMBTU	Fisher*Solve*
Electricity	69.5	USD / MWh	EIA[(b)] (2016) [93]

[a] EPA − Environmental Protection Agency, USA. [b]EIA − Energy Information Administration, USA

Table 4-6 illustrates financial assumptions for the techno-economic analysis of LMNPs industrial manufacturing. These assumptions are similar to the ones considered in previous bionanomaterial assessments [121], [192]. The hurdle rate considered (16 %) is approximately twice the average cost of capital reported for pulp and paper and chemicals (specialty) industry segments [102]. The construction time considered for the LMNPs facility is two years, although we acknowledge that additional savings are possible if the construction time is reduced to 1.5 years.

Table 4-6: Financial assumptions.

Input	Value	Unit	Reference
Project start	2017		assumed
Production year 0 (2019)	80 %	% of plant capacity	assumed
Production year 1 (2020)	100 %	% of plant capacity	assumed
Project life (after start-up)	10	years	assumed
% of CAPEX spent in year -2	50 %		assumed
% of CAPEX spent in year -1	50 %		assumed
Depreciation schedule, straight line	10	years	assumed
Working capital	10 %	% of sales next year	assumed
Maintenance cost	2 %	% of RAV[a]	assumed
Capital reinvestment	1 %	% of RAV[a]	assumed
Hourly and administrative staff	12	employees	assumed
Overhead costs	3 %	% of sales	assumed
Other fixed costs (insurance, property taxes, and emissions)	1.5 %	% of RAV[a]	assumed
Inflation	1.2	% / yr.	U.S. Treasury [94]
Taxes on EBIT	35 %	%	NREL [99]
Hurdle rate	16	%	Damodaran (2017) [102]
Project terminal value (at year 10)	5	times EBITDA	assumed

4.3.9 Assessment of LMNPs market value and potential applications

A product price may be defined by its manufacturing cost, as well as by the market, which is driven by supply and demand. Additional analyses were proposed to assess the potential market value of LMNPs. The market value of LMNP was assessed systematically (Figure 4-7). In brief, a literature search was carried out to identify characteristics of LMNPs and investigate potential applications. Following, a preliminary evaluation of products in current use was performed, identifying potential ones where LMNPs can be used as a substitute. Estimated manufacturing costs for LMNPs were compared to potential market prices of materials that can be substituted by LMNPs. Applications where the manufacturing costs were higher than market prices were screened out. The most promising applications were the ones with higher market prices, in addition to the ones with broad market availabilities. When available, the use of a substitution ratio is recommended (i.e., the amount of lignin needed for a given application divided by the amount of existing product used for the same application). In the absence of information, a ratio of 1:1 was considered.

The information generated are proposed as a guide to screen the most promising applications, aiming commercialization.

4.4 Results and discussion

4.4.1 Capital investment for LMNPs manufacturing

The estimated capital investment for LMNPs manufacturing is shown in Figure 4-8. For the three scenarios assessed, the total investment was estimated at about USD 160 million, with atomizer and separation system representing approximately 65 % of the capital investment, followed by engineering and construction expenses. A similar capital investment was expected for the three scenarios, since the atomizer and separation systems costs are based on the flow rate of the liquid evaporated. The scenarios considering water-based solvents present higher solvent recovery capital investment due to the higher energy demand (the heat of vaporization of water is approximately four times that of DMF) and consequently require larger heat exchanger areas.

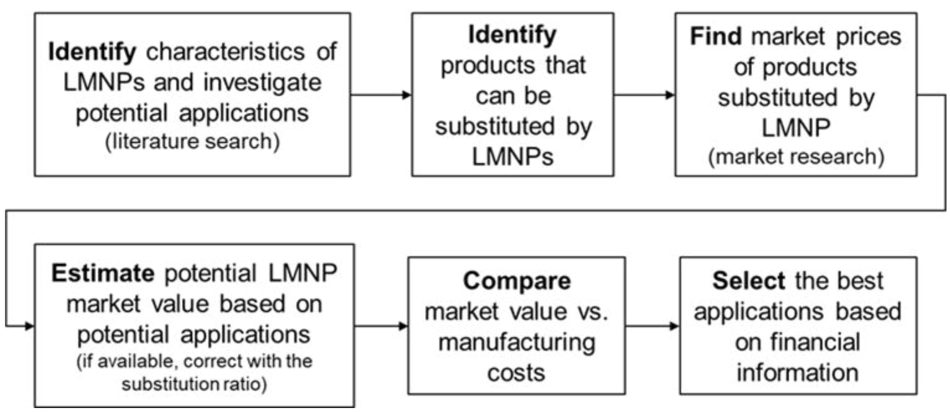


Figure 4-7: Steps for preliminary assessment of LMNPs economic potential.

4.4.2 LMNPs manufacturing cost

The estimated manufacturing cost for LMNPs using the aerosol technology are illustrated in Figure 4-9. The manufacturing costs vary between 871 and 1168 USD/t, depending on the scenario selected. In addition, the estimated minimum product selling prices to achieve NPV zero at 16 % hurdle rates vary from 1241 to 1559 USD/t.

For all scenarios, major costs are related to lignin, utilities, and depreciation. The scenario where DMF was used as a solvent presented significant lower utility costs. As the heat of vaporization of DMF is approximately four times lower than water (137 kcal/kg vs. 540 kcal/kg) [199], [200], less energy is needed to vaporize the DMF used as solvent and consequently lower costs related to natural gas are expected. However, solvent makeup costs for the scenario that uses DMF are higher due to its relatively higher cost, although solvent makeup is not a significant portion of manufacturing cost.

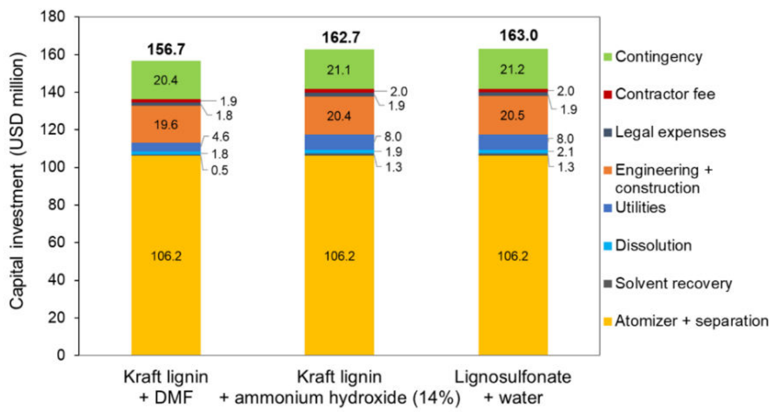


Figure 4-8: Estimated capital investment for LMNPs manufacturing.

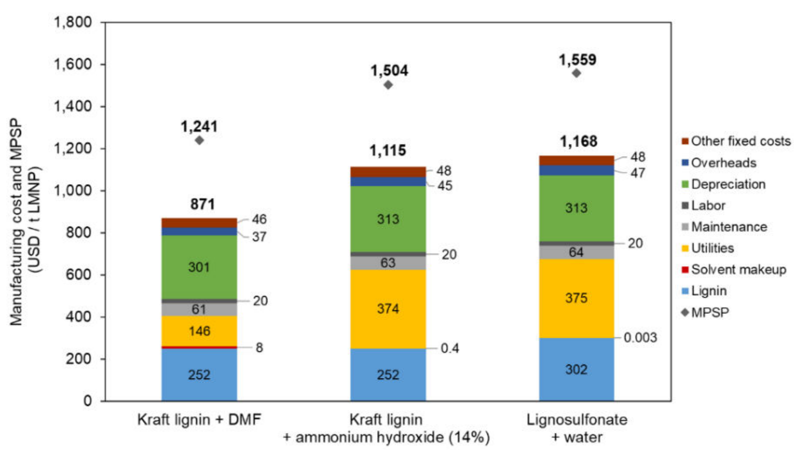


Figure 4-9: Estimated costs for LMNPs manufacturing.

On the basis of the manufacturing cost information and knowledge of the process, changes in process conditions were proposed to reduce costs. For instance, a higher concentration of lignin in the solution that feeds the atomizer would allow for less solvent vaporization and recirculation in the system. Consequently, solvent makeup and natural gas consumptions can be reduced, as well as capital investment. Other aspects to be investigated are the impact of lignin costs, production rate, and solvent losses on manufacturing costs. In addition, the use of other (not yet commercial but promising) lignin/solvent combination (e.g., organosolv lignin and acetone) was preliminarily examined. Using sensitivity analysis, the impacts of these propositions were quantified and discussed in the following section.

4.4.3 Sensitivity analysis

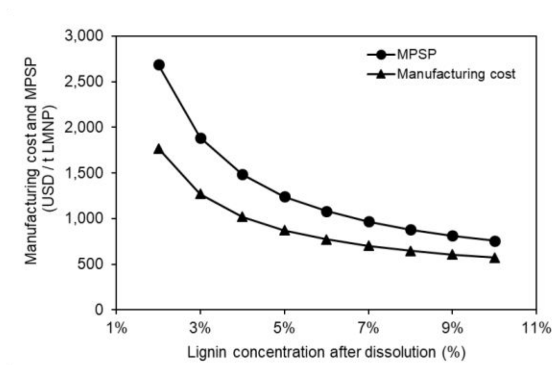
4.4.3.1 Impact of initial lignin concentration on project financials

As previously discussed, lignin concentration in the precursor solution markedly affects energy and capital investment for LMNPs manufacturing. For scenario 1 (kraft lignin/DMF), the manufacturing cost significantly decreased when lignin concentration in the initial solution increased (Figure 4-10a). For low lignin concentrations, the difference between manufacturing cost and MPSP increased substantially due to the increase of evaporative capacity and higher capital investment. The manufacturing cost decreased by approximately 35 % if lignin concentration was 10 % (wt.) or more, when compared to the 5 % (wt.) lignin concentration scenario. If the lignin concentration drops to 2 %, then the manufacturing costs will be double of that determined for the base case scenario (5 % wt.). Ultimately, the manufacturing cost of LMNPs are very sensitive to the initial lignin concentration in the precursor solution, and should be carefully evaluated for further work.

4.4.3.2 Impact of production rate in project financials

The production capacity selected for the current study considered a feasible scenario of a kraft lignin manufacturing facility co-located with a pulp mill, where the lignin is extracted from the black liquor (see Culbertson, 2017). [30] Since LMNPs may be classified as a specialty material, which is added in small quantities to enhance product and material properties, the product demand may be lower than the reference scenario (150 t/day). The impact of facility scale on manufacturing cost is illustrated in Figure 4-10 (scenario 1 - kraft lignin/DMF). From a financial perspective, for LMNPs productions over 100 t/day, the impact of scale in manufacturing costs was minor: if the production is doubled, from 100 to

200 t/day, then the manufacturing costs and MPSP decrease by about 3.6 %. However, higher production rates may imply better contracts for raw materials and energy supply, which were not accounted in this assessment and may benefit potential producers. It is worth noting that additional factors might be considered when investing in a LMNPs facility, such as the market demand and competition, which were not in the scope of this work. The most expensive equipment in the LMNPs manufacturing facility was the atomizer and separation system, which presents modular capital investment for capacities over the base case scenario (150 t/day), not extensively affected by economies of scale. If the LMNPs production rates were below 50 t/day, then the impact of economies of scale starts to take effect. For a 25 t/day production rate, for example, the estimated manufacturing costs and MPSP were nearly 15 % higher than the base-case.



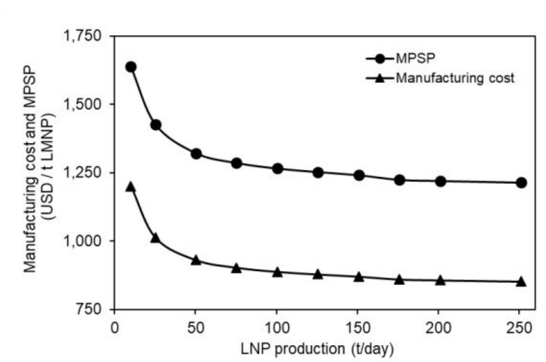


Figure 4-10: (a) Impact of lignin concentration on manufacturing cost and MPSP. (b) Impact of production rate on manufacturing cost and MPSP. Both cases apply to scenario 1 (kraft lignin/DMF).

4.4.3.3 Impact of lignin cost on manufacturing cost and MPSP

For the initial assessment, the lowest cost possible of lignin was considered for all scenarios. Nevertheless, as described previously, kraft lignin and lignosulfonate costs can vary widely. Figure 4-11 illustrates how lignin costs affect manufacturing cost and minimum product selling prices (MPSP) of LMNPs. For the scenarios assessed (scenario 1, kraft lignin/DMF and scenario 3, lignosulfonate/water), the range of costs considered for lignin precursor is between 250 USD/t to 500 USD/t for kraft lignin and 300 USD/t to 2,700 USD/t for lignosulfonate. When the highest kraft lignin cost reported (500 USD/t) is considered, the

LMNPs manufacturing cost is moderately increased by 30 %, and MPSP by 20 %. Lignin costs varies between 29 % and 45 % of manufacturing costs.

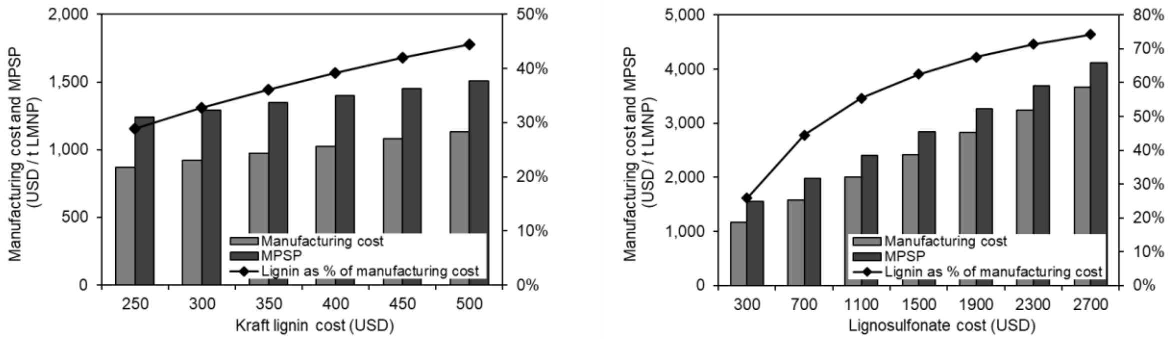


Figure 4-11: Impact of lignin cost on LMNPs manufacturing cost and MPSP (left: scenario 1−kraft lignin/DMF, right: scenario 3 - lignosulfonate/water).

Given the broader ranges of reported costs for lignosulfonates, it can be noticed that the MPSP can be as high as 4100 USD/t when higher-grade lignosulfonates are used. For the highest lignosulfonate cost situation, lignin accounts for 74 % of manufacturing cost, versus 26 % when lignosulfonate prices of 300 USD/t are considered. For an average cost of lignosulfonate (1500 USD/t), estimated LMNPs manufacturing cost is 2414 USD/t, which is about two times the manufacturing cost when lignin is 300 USD/t. As lignin costs are significant in LMNPs manufacturing, lower grades and cheaper lignin precursors are preferred from a financial perspective.

4.4.3.4 Impact of solvent losses in project financials

Solvent losses were considered minimal in the simulated scenarios (around 0.03 % of recirculating flow rate). As the solvent losses during processing in industrial scale (e.g., as purge) or losses of solvent to final product have not been investigated in detail, we believe that an assessment on the impact of solvent losses in product manufacturing cost is valuable at this initial stage. Figure 4-12 illustrates the impact of solvent losses in manufacturing cost. The impact of solvent loss in LMNP manufacturing cost is more pronounced when DMF is used as a solvent (scenario 1). DMF prices are higher than ammonium hydroxide; consequently, increased solvent losses affect LMNP from kraft lignin and ammonium hydroxide to a lesser extent. An interesting outcome of this analysis is that either minimizing solvent losses or selecting a low cost solvent, when losses are inevitable, contribute to important reductions in LMNPs manufacturing cost.

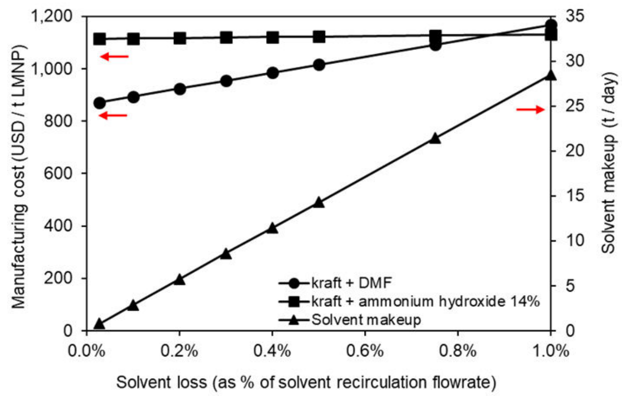


Figure 4-12: Impact of solvent losses on LMNPs manufacturing cost for kraft lignin/DMF (scenario 1) and kraft lignin/ammonium hydroxide 14 % wt. (scenario 2).

4.4.3.5 Use of acetone as a solvent and a biorefinery lignin as a feedstock

The manufacturing costs and minimum product selling prices previously calculated considered lignin precursors that are commercially available (kraft lignin and lignosulfonates). However, additional lignin precursors can be potentially used for LMNPs manufacturing. For instance, lignin can be efficiently extracted from the crude biorefinery residues with approximately 90 % acetone solution in water [201] and, after separation of residual cellulose-rich solids, directly sent to the atomizer without lignin isolation from the solution. This inexpensive feedstock should dramatically reduce manufacturing cost. The heat of vaporization for the acetone solution was calculated as 180 kcal/kg, using the software Aspen Plus v8.2, considering the thermodynamic model NRTL-HOC. The heat of vaporization of the acetone solution is slightly higher than the DMF value; indeed, there are no energy savings when compared with scenario 1 (kraft lignin/DMF). If, alternatively, pure acetone is used (heat of vaporization of 120 kcal/kg), [202] then small cost reductions are possible. Assuming a lignin cost of 100 USD/dry t (fuel value), [15], [158] acetone cost of 1200 USD/t (based on ICIS and adjusted for current values), [92] initial lignin concentration of 5 % (wt.), and the same assumptions for previous scenarios, the calculated LMNPs manufacturing cost is 747 USD/t and the minimum selling price is 1119 USD/t (14 % and

9 % lower than kraft lignin/DMF scenario). Most of the savings are due to the reduced cost of lignin. The breakdown of manufacturing cost for the lignin biorefinery scenario is shown in Figure 4-13. As for previous scenarios, lignin feedstock, energy (natural gas and electricity), and depreciation are the major contributors to the manufacturing cost.

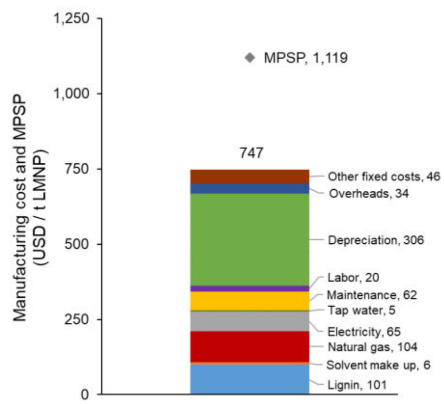


Figure 4-13: Breakdown of manufacturing cost and MPSP for biorefinery lignin and acetone as solvent.

4.4.4 Potential applications of LMNPs

A preliminary assessment of LMNPs properties and potential applications was performed. Initially, the specific characteristics of LMNP and potential applications were identified by a literature search. It is worth noting the broad range of LMNPs applications, such as in the food industry, pharmaceutical, materials, and agriculture. Table 4-7 correlates the potential applications with distinct characteristics of lignin particles. Detailed information can be found in recently published reviews on LMNPs applications [168], [203].

Table 4-7: LMNPs properties and potential applications.

Property	Application	Ref.	Comments
Resistance to decay and biological attacks	Veneer protection	[204]	Use of derivatized lignin (epoxidation)
	Films for active packaging (drug delivery, tissue engineering, wound healing)	[205]	
UV absorbance and antioxidant activity	Cosmetics (skin care, sunscreens)	[170]	
UV absorbance	Pesticide protection	[170]	Lignin used for UV protection of microbial agents that act against insect pests
Capsule formation	Pesticide encapsulation	[206]	Use of acetylated lignin to allow spheres formation
High stiffness	Polymer reinforcement	[168]	
Low toxicity, non-cytotoxicity, small size, capsule formation	Drug-delivery	[168], [206]–[213]	
Stable behavior of nanoparticles	Emulsion stabilizer	[214], [215]	Application in oil well drilling
pH dependent stability	Pickering emulsions for polymerization	[216]	Polystyrene preparation.
Possible to electrospun	Feedstock for carbon fiber production	[217]	Diameter of carbon fibers between 400 nm and 1 µm
Shape tenability, high interfacial area, UV absorbance, antioxidant effect, high stiffness, miscibility with polymer matrix, thermal stability	Composite and polymer filler	[151], [203], [204], [218]	Lignin at nanoscale allows uniform distribution in composite
Low density, non-conducting material, light color	Natural rubber filler	[219]	
Low density, reinforcing properties, large availability	Phenolic foam reinforcement	[220]	
Affinity of Lignin with TNT (2,4,6-trinitrotoluene)	Substrates for TNT detection	[221]	

A literature research on the materials in current use for the potential applications was performed. The purpose was to exemplify what type of materials LMNPs could substitute. As no information was available, a substitution ratio of 1:1 was considered. Note that additional assessments for the substitution of current materials are necessary, such as the

LMNPs substitution ratio and the impacts on final product performance. The most promising applications were identified from a financial perspective, by comparing existing products prices and the estimated LMNPs manufacturing cost and MPSP. In addition, when available, the existing market volume for the materials is provided. A summary of the findings is illustrated in Table 8. Suggestions on potential market for LMNPs were done by comparing the lowest estimated manufacturing cost (871 USD/t) and MPSP (1241 USD/t) of LMNPs, specifically for kraft lignin and DMF as precursors, with prices of potential substitutes. In most cases, the use of spherical lignin nano- and microparticles for the given application bears a significant advantage compared to the respective (amorphous) powder. This assessment reveals that some uses of LMNPs seem unfeasible from a financial perspective (such as displacing carbon black). The relatively low price of carbon black used for these applications makes the adoption of LMNPs more difficult in these markets, if only a financial perspective is considered. Nevertheless, this scenario can change if the manufacturing costs are reduced, as illustrated by our previous sensitivity analyses. From this initial assessment, replacement of some emulsion stabilizers (gum arabic and Grinsted), UV protection products, chelating agents (such as nitriloacetic acid), nanofillers (other than carbon black), and composites reinforcements were economically attractive and therefore were identified as potential candidates for further technical investigation. These categories present substitutes with high prices, but relatively limited market sizes. Other categories of potential applications includes phenol-formaldehyde resins, foams, bactericides, other emulsion stabilizers, and other chelating applications. Some of these products represent a large market size, which makes it very attractive for lignin product commercialization. However, prices of potentially replaced products (from 1500 to 3000 USD/t) are close to the MPSP estimated for LMNPs. Therefore, further assessments should include market perspective and technical feasibility of each specific application.

Table 4-8: Preliminary assessment of the economic potential of LMNPs.

Category	Examples of material currently used	Price (USD/t)	Source for synthesis	Volume (t/y)
Emulsion stabilizers	Gum Arabic	1,500 – 3,000 [222]	Acacia trees	60,000 [223]
	Glycerol monostearate	1,900 [224]	Glycerol	
	Grinsted (DuPont)	3,800 [224]	Vegetable oils and algae	
	Hydrogenated castor oil	1,500 [225]	Hydrogen + castor oil	15,000 [225]
	Cetyl alcohol	2,000 [226]	Palm oil	
Foams raw materials	Polyols	2,700 [227]	Glycols (e.g., ethylene glycol, propylene glycols)	7.5 million [228]
Chelating agents	Ethylenediaminetetraacetic Acid (EDTA)	1,200 [92]	Acetic acid + ethylene diamine	
	Nitriloacetic acid (NTA)	10,000 [229]	Ammonium, formaldehyde and sodium cyanide	
	Diethylenetriaminepentaacetic Acid (DTPA)	2,500 [226]		
UV protection	2-ethyl hexyl-4-methoxy cinnamate	10,000 [226]	Oil (propylene)	
	Benzophenones	4,000 [226]	Methane and benzene	
	Phenolic benzotriazoles	20,000 [226]	Nitrobenzenes	12,000 [230]
Bactericide & carrier	Silver nanoparticle	1,500,000 [226]	Silver	
	Titanium dioxide (TiO_2)	1,500 - 2,500 [231]	Mineral	14 million [232]
	Zinc oxide (ZnO)	1,500 - 2,000 [226]	Mineral	1.4 million [233]
Carbon filler	Carbon nanotubes	10,000,000 [234]	Carbon dioxide, acetylene	Few hundreds [234]
	Graphene	200,000 [235]	Carbon	
	Carbon black	500 - 700 [236]	Petroleum	12 million [236]
Raw material for phenol-formaldehyde resins	PF resin	1,200 [237]	Petroleum	2.5 million (phenol to resin) [238]
Reinforcement for composites	Glass fiber	800 – 2,500 [226]	Mineral	4.5 million [240]
	Aramid	26,000 [239]	Petroleum	78,000 [241]

4.5 Conclusions and future prospects

While the Life Cycle Assessment was not the focus of this work, converting lignocellulosic streams has been shown to be quite attractive. Particularly, valorization of lignin has been identified as a key factor to reach environmental benefits. [30] With this in mind, the present study dealt with a techno-economic analysis and market assessment of LMNPs. Preliminary manufacturing costs using different types of lignins (kraft lignin and lignosulfonates) and solvents (DMF, water, and ammonium hydroxide) were estimated between 870 and 1170 USD/t, depending on raw materials used and processing conditions. Major cost drivers for LMNPs manufacturing include lignin, utilities, and depreciation. Estimated manufacturing costs can be as low as 600 USD/t if higher lignin concentration in the solution feed is used. Sensitivity assessment showed that if higher grades of lignin are utilized, the manufacturing cost can increase considerably, reaching 1100 USD/t (for kraft/DMF scenario) and 3660 USD/t (for lignosulfonate/water scenario).

The current work shows a potential feasibility for the applications of LMNPs in replacement of high value products, such as some emulsion stabilizers, UV protection products, chelating agents and polymer nanofillers. Additionally, there is the possibility of using LMNPs in applications targeting large size markets, such as composites and formaldehyde resins. Special mention is the case of particulate coatings, which can be quite promising given the excellent packing of LMNPs in coating layers, as demonstrated recently.[216] In all cases, the utilization of LMNPs as bio-based component is beneficial from the point of view of the inherent properties of spherical micro and nanoparticles, which are different than those in other forms as well as the fact that they are environmentally benign. Observing the difference between the estimated LMNPs minimum product selling prices and the market price of large-scale lignin substitutes, it is important to develop manufacturing pathways to reduce LMNPs manufacturing cost. Additionally, it is suggested a better understanding of the substitution ratios for specific applications, as well as the impact of LMNPs use in final product properties and performance. On the basis of the financial evaluation herein discussed, important elements contributing to LMNPs production costs are (i) the cost of the lignin feedstock, (ii) the energy required to evaporate the solvent, (iii) the lignin concentration in the solvent, and, likely, (iv) the solvent price. Thus, it is suggested to target future research on:

- The technical feasibility of using potentially lower cost feedstock, such as lower grade industrial lignins and crude biorefinery lignins.

- The use of low cost solvents with low heat of vaporization, such as aqueous acetone and ethanol, which are well suitable for dissolution of some grades of lignin.
- The effect of higher concentration of lignin starting solution on LMNPs properties and application performance.
- The reduction of solvent losses and improvement of solvent recovery, especially on studies aiming the scale-up of LMNPs manufacturing.

We believe the outcomes of this study are relevant for LMNPs industrialization and fast-track commercialization.

5 REVIEW: RISK MANAGEMENT CONSIDERATION IN THE BIOECONOMY [4]

5.1 Abstract

In investing in a new venture, companies aim to increase their competitiveness and generate value in scenarios where volatile markets, geopolitical instabilities, and disruptive technologies create uncertainty and risk. The bio-based industry poses additional challenges as it competes in a mature, highly efficient market, dominated by petroleum-based companies, and faces significant feedstock availability and variability constraints, limited technological data, and uncertain market conditions for newly developed products. Thus, decision-making strategies and processes for these investment projects must consider solid risk estimation and mitigation measures. Focusing on the bio-based industrial sector, this paper critically reviews state-of-the-art probabilistic and deterministic methodologies for assessing financial risk; discusses how a complete risk analysis should be performed; and addresses risk management, listing major risks and possible mitigation strategies.

5.2 Introduction

5.2.1 Problem statement

Investing in new ventures is a pathway to increase a company's wealth and create long-term value [242], [243]. Selecting among the most promising and robust alternatives increases the chances of the financial success of an investment. Furthermore, if the risks, uncertainties, and ever-changing circumstances associated with investment decisions are not fully addressed, [244], [245] the likelihood that a high-risk and/or financially unsuccessful project is chosen increases [246], [247]. The inherent complexities associated with the bio-based industry and bioeconomy, [248], [249] such as dynamic geopolitics, market conditions, and innovations in feedstock handling and processing technologies, exemplify the important role that risk management has when designing investment strategy. In this work, we refer to bio-based industry as the industry that uses predominately renewable feedstocks that are

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generally a substitute for petroleum based products [14]. The term bioeconomy refers to the 'set of economic activities related to the invention, development, production and use of biological products and processes' [250]. Another definition considers bioeconomy as the sustainable utilization of renewable resources for economic, environmental, social, and national security benefits [4].

Investments in the bioeconomy unveil promising opportunities for the development of local and global economies. As an example, the implementation of bio-based industries can trigger job creation, develop rural areas, and consequently local economies [4], [251]. Similarly, the use of renewable materials decreases the dependence on petroleum and reduces greenhouse gas (GHG) emissions [4], [13], [251]. The creation of biorefineries can allow small facilities to generate additional and new bio-based products while using the available feedstock in the region [252]. However, due to inherent innovation and uncertainties associated with the bioeconomy, chances of failure are always present and the application of risk assessment can potentially decrease them.

Although large-scale biorefineries such as corn ethanol in the USA and sugarcane mills in Brazil are well established [253]–[257], as well as the pulp and paper industry, recent failure of ventures using lignocellulosic feedstocks can be attributed in part to an incomplete understanding of risks or the absence of robust risk-mitigation plans [258]. The following examples are for the biofuels industry, since the recent investments in industrial facilities were focused in this sector. For instance, Range Fuels Inc., initiated operations in 2010 with the goal of producing 20 million gallons of biofuel from wood chips; however, in less than one year and after spending $300 million of public and private funding, the company closed its operations due to lack of sufficient pilot plant data to prove the merits of the technology, a poorly functioning main reactor that was initially designed for coal and not properly redesigned for wood, and problems with the gasification catalyst performance [258]–[260]. Similarly, Kior Inc., a biofuels producer that initiated operations in 2012, closed down its facility after approximately one year [261]–[263]. Reactor bottlenecks, low equipment reliability, mechanical issues, poor catalyst performance, and the decrease of final products' market prices were listed as main reasons for the closure [264].

Since investors are risk averse [265], [266], risk awareness and mitigation plans that consider both technological and process design as well as market conditions are essential to the expansion of the bio-based industry. Unfortunately, data scarcity from long-term operations at industrial scale makes the evaluation of new technologies a challenge [267]. Moreover, the equipment and technology used to handle feedstock are often adapted from similar industries (such as pulp and paper and sugarcane mills), leading to unknown operating conditions and difficulties in predicting equipment costs. Other process uncertainties comprise variability between and within the chemical compositions of feedstocks that lead to different reaction yields, conversion technologies that are still under development, scale-up, and chemicals recycling at large-scale production [268]. Market uncertainties, such as feedstock cost and availability, petroleum price instability (that affects biofuels and commodities prices), and unpredictability of new products prices also strongly affect project feasibilities [269]. Finally, geopolitical instability, environmental concerns, societal acceptability issues, and issues associated with the project execution (such as delay in equipment delivery, lack of qualified labor work, among others) persist as with any other industry.

Risk analysis, including the assessment of technology and financial risks, can guide future research and development efforts that in turn minimize the potential for project failure. As techno-economic calculations consume a significant amount of time and resources, risk assessments must be performed at the early stages of project design to reduce costs and screen out the high risk and/or less attractive options. While assessing all associated risks is extremely complex, an analysis that elucidates and examines the primary sources of financial risk is essential for effective business planning because it allows for better mitigation strategies [270]. Despite its importance, numerous feasibility studies do not consider risk analysis and there is no publication that addresses the importance of risk analysis in the bioeconomy [271], the tools available, and detailed analysis around mitigation strategies.

This work critically reviews concepts of uncertainty, risk, and risk analysis and addresses methods and risk evaluation tools used to assess financial risks of an investment. This work intends to fill the gap in the bio-based industry and bioeconomy literature by (i) assessing quantitative risk assessment methods, (ii) elucidating what a complete financial risk analysis should include, and (iii) listing major risks and mitigation strategies.

5.3 Literature review

The first part of this section provides conceptual information on risk, risk analysis, uncertainty, and related concepts, followed by an overview on how financial risk assessment can be executed in the context of capital investment decisions. The second part critically reviews the main tools used for quantitative risk evaluation in projects related to the bioeconomy.

5.3.1 Methodology

Google Scholar, Scopus, and Web of Science were used to search for related literature, using keywords such as risk, risk concept, risk analysis, uncertainty, uncertainty analysis, biofuel, biomass, bioproduct, cellulosic feedstock, Monte Carlo simulation, sensitivity analysis, stochastic analysis, and techno-economic analysis. Studies that performed qualitative risk assessments were not included in this review. The literature search on the definitions was not exhaustive, since its purpose was to provide concepts for ease of comprehension. In addition, publications related to safety and hazards risks were screened out because we understand that this is a separate area of study. The structure of the review is according to the following rationale: identification of final bioproducts and project scopes evaluated with financial risk analysis, investigation of the inputs and outputs assessed, comments on information provided by risk analysis, illustration of the approaches used for risk assessment, discussion on the main gaps identified, and finally, a description of the tools used for quantitative risk analysis, including a case study example.

5.3.2 Main definitions

The concepts of risk and uncertainty are not consistent in literature [272]–[274], generating confusion even among specialists. Compilations of definitions can be found in several sources [275]–[278]. Some authors equate risk with uncertainty, showing how uncertainty can lead directly to negative impacts [245], [279], [280]. Others believe that the concepts are quite different, showing that risk relates to the confidence in the input parameters used for a cost estimation while uncertainty relates to the imprecision of the calculation in a model. Authors have related risk to probability distributions and claim that uncertainty exists when it is not possible to allocate probabilities to the results [247], [272], [281]. Others think that the concept of risk can be thought of as progressing from a narrow perspective of probability to a broader perception involving events, consequences, and uncertainties [274], [282]. Considering the context of investment evaluations and decision-making processes, the following definitions are suggested. Figure 5-1 illustrates how these concepts are related in the context of capital investment decisions and

Figure 5-2 presents the stepwise process for executing an investment analysis.

- Uncertainty (A) designates both the existence of more than one value or the absence of information and is also related to randomness [275], [283]. Since uncertainty is intrinsic in any system, its characterization and interpretation is an essential element of the risk analysis [284].
- *Risk* is a random event that negatively affects a company's goals [273], [275], [279]. If the impacts are positive, it is categorized as an opportunity [273], [279].
- *Risk analysis (or risk assessment)* (B) is a methodology used to estimate how often an event may happen and the extent of its consequences [285]. It comprises the identification of the source of uncertainty, uncertainty quantification, the formulation of uncertainty for risk analysis, and finally the risk quantification [268]. Risk analysis can be conducted with either qualitative (C) or quantitative (D) methodologies.
- *Qualitative risk analysis* methods (C) classify the uncertainties that describe each scenario in terms of costs and benefits [268]. The risk evaluation is based on uncertainties assessment and usually contemplates prior experience, analogous situations, or even instincts or gut feelings [285]. An example of a well-known qualitative risk analysis methodology is the SWOT analysis. [5]

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[5] SWOT stands for Strengths, Weaknesses, Opportunities, and Threats. In this methodology the issues of a project, for example, are listed in the four quadrants of the SWOT analysis grid, helping to comprehend how the strengths can be monitored to achieve opportunities and how the weaknesses can evolve to threats [444].

- *Quantitative risk analysis* methods (D) use numeric scales to quantify the uncertainties in a model [268]. The models for quantitative risk analysis can be deterministic – single output (E) or probabilistic – multiple outputs (F) [284].
- *Sensitivity analysis* (G) is a deterministic risk analysis method used to estimate the changes in model's outputs based on inputs variations [244], [268], [283], [286]–[288]. The impact of changes are evaluated one input at a time and, consequently, the effect of simultaneous changes in two or more inputs cannot be assessed [244], [268]. Tools to perform sensitivity analysis include tornado charts, spider plots, and switching value tables. Sensitivity analysis is widely used by the forestry industry [289], probably due to its simplicity and easy interpretability of results.
- *Probability analysis* (or stochastic analysis) (F) is executed to estimate the probability distribution of the output values, based on the probability distributions of the inputs [245], [283], [286]. Although probability analysis is also identified as risk analysis or uncertainty analysis in the literature [244], [245], [279], [283], [284], [290], [291], we believe that risk analysis is a broader concept that includes sensitivity and probability analysis methods, as shown in Figure 5-1. Sampling methods for stochastic analysis include Monte-Carlo and Latin Hypercube, which will be discussed in detail later.
- *Risk management* (H) is a process that includes risk identification and analysis, development of mitigation strategies, and the monitoring of new events categorized as risks and opportunities [273].

Profitability calculations are usually performed to provide information regarding the financial feasibility of a venture. Techno-economic models (L) have been used for this purpose, and use the best set of inputs (K), selected from inputs that are both certain (J) and uncertain (A). Due to associated uncertainties (A) of some inputs and unknown future circumstances, the investment can still follow a risky pathway that may lead to a less profitable output. To identify, understand, reduce, and mitigate potential threats, it seems reasonable to perform investment risk analysis (B) and risk management (H) during the capital investment evaluation process. The outputs from techno-economic model, risk analysis and risk management (M) can provide a better understanding of the investment profitability outcomes, possible risks related to the venture and the possible mitigation plans.

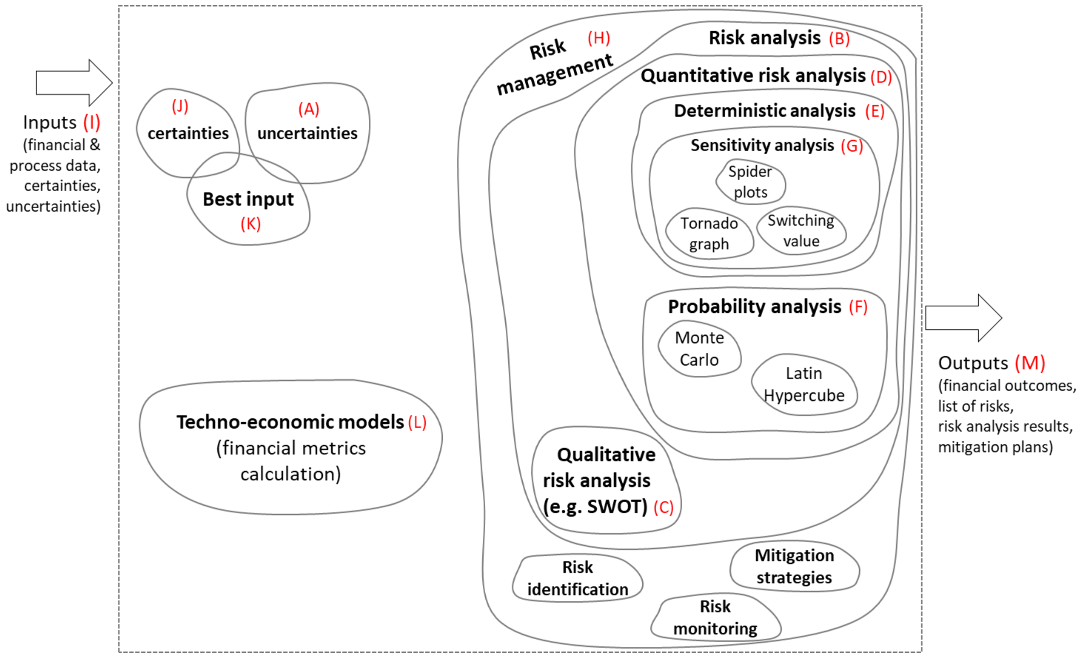


Figure 5-1: Risk concepts in the context of capital investment decisions.

Figure 5-2 shows the stepwise process for financial risk analysis of an investment using the components presented in Figure 5-1. The first step for profitability calculation is the input selection (A2), which consists of financial and process inputs. Examples of financial inputs are final product price, interest rates, subsidies, inflation, and costs related to raw material, equipment, labor, and capital. Process inputs are usually related to reaction yields, production rates, feedstock composition, catalyst consumption, final product specification, flowrates, utilities consumption and process conditions (temperature, pressure, reaction time, etc.). Traditional techno-economic analyses select the 'best' estimate of inputs (D2) among certain (B2) and uncertain (C2) values to run a deterministic model (E2) and estimate financial outcomes (F2) [279], [283], [292]. A single estimate from each input is used to generate a single value output [279]. Techno-economic models (G2) are commonly used for investment evaluation and are designed for each specific project. They are a combination of process models, which simulate the processes to convert raw materials into products with mass and energy balances, and financial models, which calculate financial outputs based on cash flow analysis.

As presented earlier, investment risk analysis can be carried out using qualitative and quantitative methods. Through qualitative methods (H2) the risks are identified (I2) based on subjective criteria. Sensitivity analysis (J2) is a quantitative pathway to assess the risks of a project. In this case, the financial outcome calculated (F2) is defined as the base value, and through sensitivity analysis it is recalculated for different input values (based on uncertainties in the input values (C2)).

As presented earlier, investment risk analysis can be carried out using qualitative and quantitative methods. Through qualitative methods (H2) the risks are identified (I2) based on subjective criteria. Sensitivity analysis (J2) is a quantitative pathway to assess the risks of a project. In this case, the financial outcome calculated (F2) is defined as the base value, and through sensitivity analysis it is recalculated for different input values (based on uncertainties in the input values (C2)).

Stochastic modelling (K2) is used to complement the deterministic model (E2). Similar to the deterministic model, the probability model is designed (G2) and the inputs are entered as the probability distributions of values (L2). As the number of inputs with probability distribution can be numerous in some situations, sensitivity analysis (J2) is used to select parameters with stronger impact in the output. In contrast to sensitivity analysis, the outcome of probabilistic models is the probability distribution of the financial outcome when all inputs (with their respective distributions) are iterating at the same time (M2). The probability analysis quantitatively exposes the venture’s risks.

It is not necessary to perform all methods for risk analysis. The selection of the most appropriate method will depend on the phase of the project and on the information available. It seems preferable to execute qualitative risk analysis in the early stages of design and the stochastic risk analysis in subsequent phases, when more reliable information is available. Nevertheless, there is no established rule when applying a methodology.

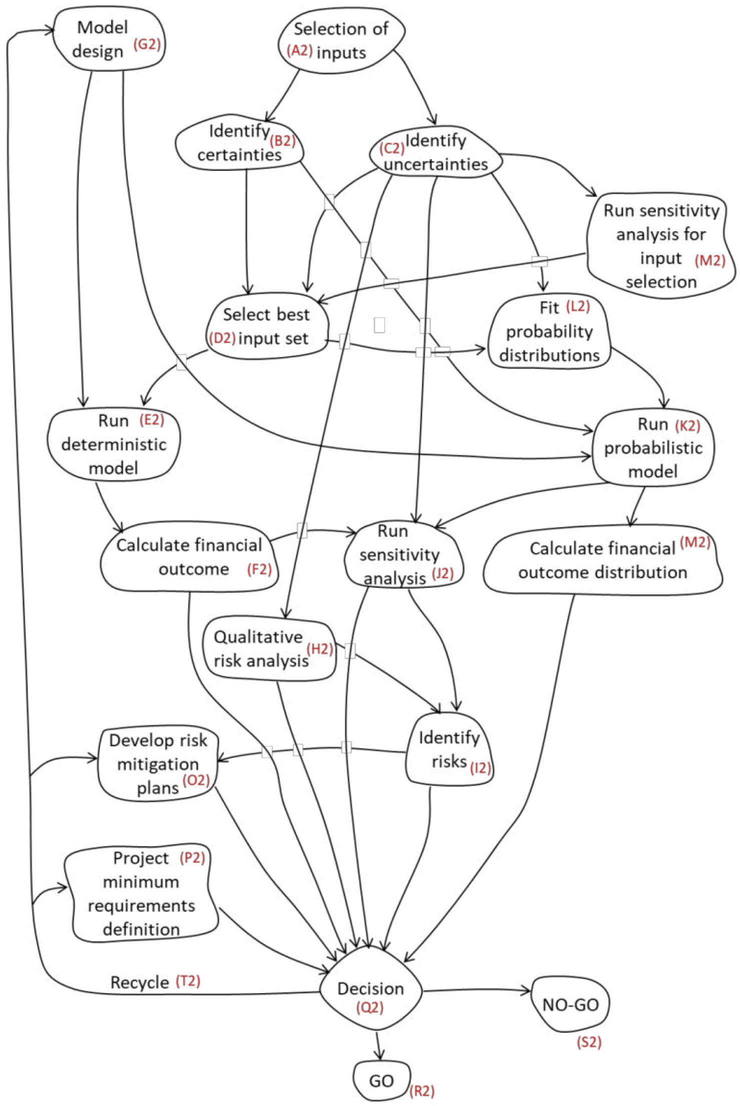


Figure 5-2: Stepwise process for investment analysis.

After the identification of specific risks (I2), mitigation strategies (O2) can be proposed to reduce their probability and severity. By having more information regarding the minimum financial and technical requirements for the project (P2), managers and investors can have a better understanding of the risks associated with the venture and the proposed mitigation strategies. With all this in hand, decision makers can decide (Q2) to initiate (R2) or reject (S2) the project or ask for additional details on the models and inputs (for example, defining the impact of new plant throughput or process conditions), adjust mitigation plans or even alter the minimum requirements for project approval (T2).

5.4 Risk assessment for investments in the bio-based industry

This analysis focuses on the application of quantitative risk assessment methodologies as well as commonly used tools and their respective advantages and disadvantages. There are a few dozen recently published articles (dating back to 2000) related to the application of financial quantitative risk assessment, with a greater share coming in the last 10 years. This is probably due to the relative novelty of bio-based technologies, recent policies to develop an economy less reliant on oil, and the development of easy-to-use computational tools such as Microsoft Excel® add-ins [273].

5.4.1 Final products and project scopes evaluated

As the United States and Europe have set ambitious targets for the use of renewable fuels [249], [293], [294], it is not surprising that most risk analyses have been concentrated on investments for liquid biofuels production using different renewable feedstocks [248], [249], [254], [256], [266], [271], [290], [293], [295]–[304]. Other works have assessed financial risks for biopower generation from woodchips and co-production of ethanol and power [253], [305], [306]. Few papers performed financial risk analysis for chemicals and biomaterials manufacture [255], [269], [307], [308].

Quantitative risk analysis has been most commonly used to estimate the probability of financial success for a single conversion pathway or to identify the most promising option among different project alternatives (e.g., use of different feedstocks and conversion routes to produce different final products) [248], [249], [253]–[256], [293], [296], [298]–[303], [306], [308], [309]. Other applications include (i) estimation of final product price [297] (ii) investigation of the uncertainties associated with the production process [255] and feedstock supply cost [295] (iii) evaluation on the impact of subsidies for an investment [266] (iv) guidance to optimize the conceptual design of a project or the operating conditions of a facility [290], [305] and (v) assessment of risk for different biomass supply contracts considering the farmer and facility standpoints [310], [311].

5.4.2 Main inputs and outputs assessed

Quantitative risk analysis has been commonly used for the assessment of specific risks, rather than for understanding those inherent to the entire supply chain. For instance, the risks of financial loss can be minimized (for both the farmer and the producing company) if raw material contracts consider two combined metrics: one based on dollar per cultivated acre and one on dollar per ton of biomass [310]. Similarly, the risks of feedstock cost based on cultivation location are lowered when sourcing from irrigated areas due to yield stability [295]. Finally, it has been shown that the impacts of feedstock composition variability on project profitability are profound, with small changes (around 3 %) altering the investment's NPV (Net Present Value) by tens of millions of dollars [249].

The consequences of key financial parameters' variations have been the most common focus of risk assessment [312], although in some situations the impact of reaction yield variability was also significant [302]. Final products and by-products prices, interest and inflation rates, and costs associated with raw materials, catalysts, utilities and capital investment, and contingency plans are the most common parameters analyzed [248], [249], [254], [256], [257], [266], [271], [293], [296], [300], [301], [304]–[306], [308]–[310]. The most common financial metrics used have been NPV, Return on Investment (ROI), and Internal Rate of Return (IRR) [248], [249], [254], [256], [257], [266], [271], [293], [296], [300], [301], [304]–[306], [308]–[310]. Other metrics include the minimum revenue price for the final product [249], [253], [266], [293], [297], [299], [302], and production costs [290]. While Zhao et al. (2015) [293] argue that breakeven price is a better measure than NPV in the decision-making process since it does not consider the uncertainties in the final product's price, we consider that the uncertainty in final product prices is highly important and should be taken into account in the evaluation of any investment, especially if the final product is a fuel or a commodity. In the literature review performed for this paper, we noticed that the variation in the final price of the product is among the most important parameters affecting the financial performance of a specific project.

Outputs from the sensitivity analysis have shown that feedstock cost and final product price are usually the financial parameters with greatest impact on a venture's profitability [248], [249], [255], [257], [266], [293], [296]–[301], [305], [306], followed by capital investment [253], [255], [257], [299]. For biochemical processes, enzyme price has also been found to be significant, depending on the final product obtained and the specific technology applied [249], [253], [257], [307]. For processes that use hydrogen as a raw material, it has been shown that its price variation, or the technology used to produce the hydrogen, significantly affects project profitability [293].

Variability in process inputs should be considered and can also have a major impact on investment risks. However, in many cases these parameters' impacts are not closely evaluated. Reasons for not including stochastic distributions on process inputs are related to data availability and the difficulty of performing several process simulations in parallel [297], [299]. Major non-financial risks evaluated include feedstock availability, composition, input flowrate, and reaction yields [249], [253], [290], [293], [296], [297], [299], [302], [305]. In an unusual evaluation, Morales-Rodriguez et al. focused solely on uncertainties in process parameters and found that changes in reaction yields and feedstock inhibition were the most important risk factors for financial return from production of lignocellulosic ethanol [290].

Another type of risk assessment includes the evaluation of the impact of subsidies and policies on project profitability. The probability of having a profitable investment is significantly lower when government subsidies are not taken into account [309], or when tax rates increase or tax credits are not available [254], [303]. Some studies have used probability analysis to estimate the value of the subsidy required to increase the probability of achieving the desired financial outcome [304]. Some risk assessment methodologies have been used to illustrate that inputs used in deterministic modelling may be too optimistic. For example, stochastic analysis results showed relatively low probability of having IRRs higher than the calculated deterministic value [255]. Likewise, it was found that deterministic analysis results can underestimate the manufacture cost of biofuels when compared to the estimation using probability analysis [302].

5.4.3 Risk assessment approaches

Quantitative risk assessments for bio-based industry investments have two main approaches: studies that employ only probability analysis, and studies that consider both sensitivity and probability analysis. The first approach has been less common in literature, where the desired output is solely the distribution curve of the financial output [266], [295],

[304]. The second approach provides a deeper understanding of the outputs, and sensitivity analysis was commonly used to (i) identify the parameters with high impact on the model output [249], [253], [255], [257], [290], [293], [296], [297], [299]–[302], [306], (ii) help select inputs to assign stochastic distribution [248], [290], [305] (iii) identify major input parameters to be modified for conceptual design optimization [305], and (iv) reach cost-effective operating conditions [290].

It is imperative to carefully define uncertainty limits when performing risk assessment. These limits can be sourced from historical records, forecasted trends, literature data, reference cases, and expert interviews [248], [249], [254], [256], [257], [266], [271], [290], [293], [296], [298]–[302], [304]–[306], [308], [309]. Usually, the probability distributions for raw material costs and final product prices have been obtained by adjusting a distribution curve on real historical data [249], [253], [254], [256], [296], [300], [301]. Common adjusted curves are triangular, pert, normal, and log normal shaped [248], [255], [266], [297], [299], [303], [308], [313]. Uniform distributions have been used when there is high uncertainty on a parameter value, lack of information on the input mean value or unavailability of data distribution. Some examples where uniform distributions have been used are capital investment,8 reaction yield and by-products prices [255], [296].

5.4.4 Main gaps identified

Main gaps identified in the execution of this review are related to the underestimation of different types of uncertainties during the risk assessment process. Most of the previous publications have considered only specific uncertainties when performing risk analysis, mainly related raw material costs and final product prices. To the best of our knowledge, consideration of uncertainty across the whole supply chain has not been documented in literature. In addition, there are few studies on the impact of the shape of the probability distribution curves, since in many cases there is little data available. Finally, previous research has failed to analyze the development and role of mitigation strategies, a crucial step when evaluating investments. The chances of an endeavor’s techno and financial success can only increase when risks are adequately addressed and feasible plans for risk minimization or contingency are available.

5.4.5 Tools used for quantitative risk analysis

This section provides a short description of the tools used in sensitivity and probability analysis, and shows how these tools can be effectively used for financial risk assessment. Following, a case study is presented to better illustrate how the tools are used and the major differences between them.

5.4.5.1 Sensitivity analysis tools

Sensitivity analysis, occasionally called what if analysis, evaluates impacts on a given outcome based on changes in the input variables. It is a fundamental concept for the decision making process and simple to implement [314]. The independent variables are modified, one at a time, and the outcomes are recorded. A Microsoft Excel® spreadsheet can be used to perform sensitivity analysis, and numerical results are easily evaluated in graphical presentations, such as tornado diagrams and spider plots [249], [253], [255], [293], [296], [299], [301], [302], [306], [307], although they can also be presented in a table format (switching value analysis). The main drawback of sensitivity analysis is that it does not consider interaction among variables [266]. In-depth information on sensitivity analysis can be found in literature [268], [279], [314].

Tornado diagrams provide a quick overview of the most influential input model parameters [279]. In Figure 5-3(a), the vertical axis of the diagram is the base-case output from the deterministic model. The model is then recalculated by changing each input, one at a time, to the upper and lower values and this is reflected in the length of the bars on the $\underline{x}$ axis: longer bar lengths show a greater impact of the respective input on the outcome [288]. More information on how to construct tornado diagrams using Microsoft Excel® spreadsheets can be found elsewhere [315]. Some authors developed an advanced configuration of the tornado diagram, named uncertainty tornado chart [299], in which the bars have a boxplot format, enabling the analyst to identify outputs for the input ranges that are more likely to occur. The add-ins that perform Monte Carlo sampling usually express the tornado diagram in the form of a correlation parameter graph (Figure 5-3(b)). The software uses each independent input distribution to construct the correlation diagrams, in which coefficient values vary between +1 / -1. The closer the correlation coefficient is to +1 or −1, the more the output is dependent on the input, whereas a value of zero indicates no influence of the input on the output [279].

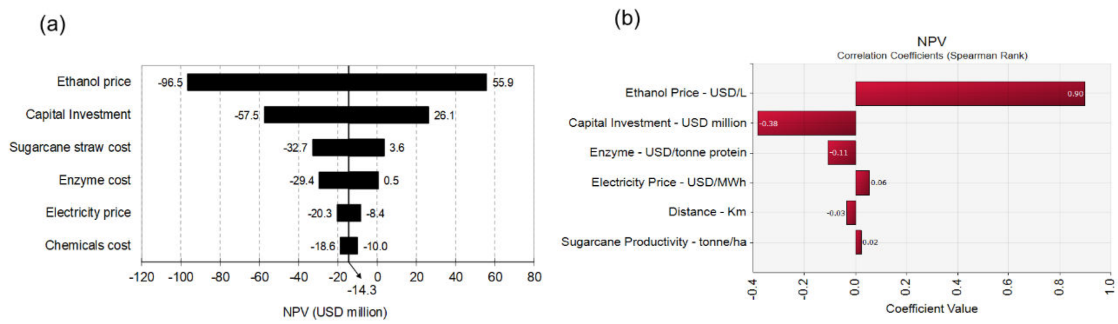


Figure 5-3: (a) Example of a tornado diagram. (b) Correlation parameter graph, based on Assis (2016) [317].

Spider plots (Figure 5-4), like tornado diagrams, illustrate the impact of changing one input at a time on the out-put results. The spider plot is constructed by plotting the output against different inputs for each independent variable on an x-y plot. Usually, the x-axis represents the percentage change from the defined base case scenario for each input [288]. The higher the absolute value of the curve slope, the greater the impact of input variability in the output value. The number of input variables should be restricted to four or five as visualization can easily become overcrowded [315].

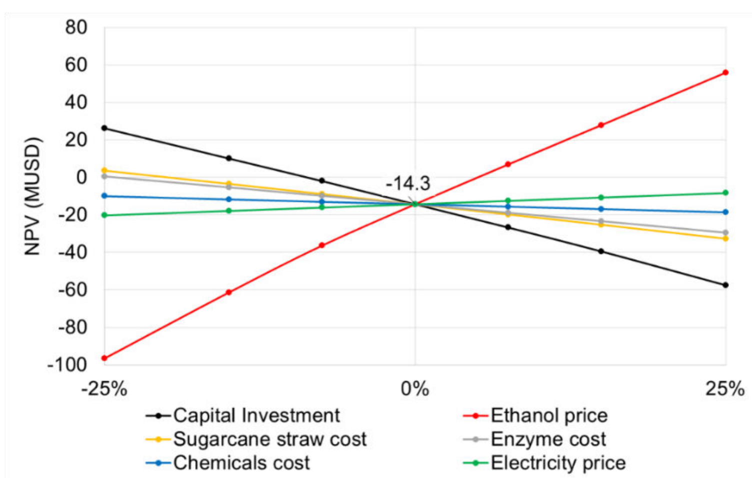


Figure 5-4: Example of spider plot (adapted from Assis, 2016) [317].

The switching value method (Table 5-1) expresses the percentage change of each variable, done one at a time, necessary to bring the project NPV to zero [316]. The smaller the switching value is relative to the others, the greater its impact [300]. The advantage of this methodology resides in displaying readily accessible numerical information to the analyst on how the inputs should be changed to achieve NPV zero.

Table 5-1: Switching value table.

Input variable	**Switching value (turns NPV to zero)**
Ethanol	+5.0%
Capital investment	– 8.7%
Sugarcane straw cost	–19.9%
Enzyme cost	–24.1%
Electricity price	+60.8%

5.4.5.2 Probabilistic analysis tools and computational add-ins

Computational add-ins are commonly used to perform risk assessment, mainly for probability analysis. The software package @Risk, from Palisade, has been extensively used for quantitative assessment of financial risks in bioprocess investments [248], [249], [253], [255], [266], [293], [295], [296], [300], [301], [306], [307]. Other software used are Crystal Ball [297], [313], and Simetar© [254], [256], [271], [304], [309], although some authors have developed their own routine models in Matlab® and Mathematica™ [290], [299]. Monte Carlo is a widely employed sampling method, in which the model normally runs between 1,000 and 5,000 iterations [318], with random selection of input values generating a representative range of output values [319]. The result is a clearly defined distribution curve for the outputs. While less commonly used, Latin Hypercube is another sampling method in which the stratified probability distribution is divided in equal intervals and a random value from each interval is sampled, thus faster converging the simulations [302], [310], [319]. Historically, Monte Carlo simulation methods were considered to be complex and time-consuming, requiring considerable amounts of information regarding input values and their expected ranges [305]. However, Monte Carlo simulation has become more popular due to reduced computing costs and the availability of computational software [271].

5.4.6 Case study: using quantitative risk analysis tools

In this section, results from a case study are illustrated to provide a better understanding of the risk analysis tools previously discussed. The techno-economic model is based on Assis (2016) [317]. In this analysis, the financial risk of producing second-generation ethanol and electricity from sugarcane bagasse and straw in a facility co-located with an autonomous distillery is assessed. The financial output is the NPV (calculated at a 12 % discount rate), and the inputs evaluated are ethanol price, electricity price, straw cost, enzyme cost, chemicals cost and capital investment.

Sensitivity analysis is performed to investigate how inputs' variation affects the NPV. The inputs are changed by ± 25 %. The base NPV value calculated by deterministic analysis is −14.3 MUSD. In Figure 5-3(a), the tornado diagram illustrates that ethanol price variation is the major cost driver (wider bar), followed by the capital investment. The diagram shows that a 25 % increase in ethanol prices increases NPV to 55.9 MUSD.

The same set of data is used to build the spider plot (Figure 5-4). All curves intersect in the base NPV value (−14.3 MUSD), and as anticipated by tornado graph, the ethanol price presents the higher curve slope, indicating that it is the major driver, followed by the capital investment.

It is worth mentioning that tornado diagrams show the major inputs in a clearer way when compared to spider plots. However, it can be challenging to identify if an increase in input increases or decreases the output in a tornado diagram. This information can be easily observed in the spider plot through the slope inclination. On the case study, the spider plot shows that the NPV increases for an increase in ethanol price while the increase in capital investment lowers the NPV. Additionally, spider plots illustrate how is the relation-ship between inputs and output (e.g., linear or non-linear) [288]. Nevertheless, when several inputs are evaluated in parallel, it is recommended to construct a tornado diagram, since the spider plot can be overcrowded. In summary, tornado diagrams and spider plots provide complementary information: the first summarize the impacts of each input variable in a clear and simple way, while the second give a more comprehensive view on the input–output relationship [283], [288].

Additional information can be explored using the switching value method (Table 5-1). For the case study presented, the table shows by how much each input should be changed independently to reach NPV zero. As previously mentioned, the estimated NPV is – 14.3 MUSD. Ethanol price, the input with major impact, need the smallest change (increase of 5 %), to turn NPV to zero. However, chemicals' cost – the input with less impact in the NPV — needs to decrease by 84.3 % to turn NPV into zero. As tornado diagrams and spider plots, the results of the switching value method consider the variation of one input at a time, so it is not possible to assess the impact of two or more inputs in parallel using this tool.

Probability analysis was performed for the same case study, using the software @Risk. In this case, distribution curves were adjusted for each input: ethanol price (based on historical data), electricity price (based on historical data), enzyme cost (from the literature), and capital investment (uniform distribution). Straw cost was calculated based in the sugarcane productivity (historical data) and the collection distance (information from the literature). The cost of chemicals was not considered in this analysis since it presented very low impact in the output.

The model was executed with the input distributions and the graph in Figure 5-5 was generated. The results of the probability analysis show that there is a chance of 47.5 % of NPV being positive. The mean NPV value, considering all the distributions, was calculated as 0.94 MUSD. Probability analysis provide additional information to the analyst, since the risk of a financial failure is assessed, based on the uncertainties provided. Nevertheless, the decision to proceed or not with the investment depends on the risk appetite of the decision maker. As mentioned earlier, @Risk software provides a correlation tornado diagram (Figure 5-3(b)). From this result, it can be inferred, as the tornado diagram and spider plot pointed out, that the NPV is highly dependent on ethanol price (correlation coefficient of 0.9), followed by the capital investment. From this tornado correlation diagram, it is possible to see if the correlation input–output is positive or negative, as it is in the spider plot. Assis (2016) [317] used probability risk analysis tools to calculate what would be the mini-mum ethanol price that guarantees 99.9 % probability of positive NPV, thus minimizing the investment financial risk. This information could be used to assess what would be the amount of subsidies needed to develop the second-generation biofuels industry, for example.

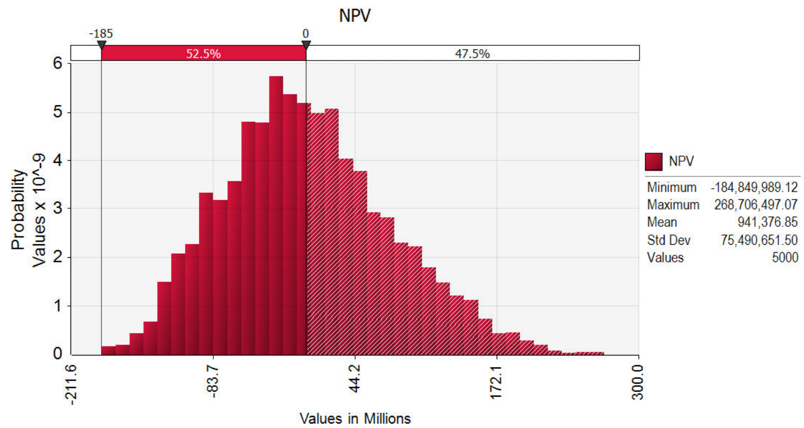


Figure 5-5: Distribution of NPV values for the case study (based on Assis, 2016) [317].

As was exemplified by the case study, sensitivity and probability analysis tools provide complementary information about the financial risks of the investment. The quality of the results is based in the quality of input information. These tools provide additional quantitative information for the decision maker and can point out where to devote eff orts in order to minimize the chances of project failure from a financial perspective.

5.5 What a complete financial risk analysis should include

In this section, we discuss how a complete financial risk analysis should be performed, considering the literature and tools reviewed. The following guidelines can be applied for any investment assessment. We believe that the use of quantitative financial risk analysis is especially beneficial for bioeconomy investments, due to the inherently uncertainties previously outlined.

Initially, one should identify the required amount of detail for the analysis considering the current project phase and level of information available. For example, when information about process conditions, equipment design and costs are not available, typically in the early stages of a project, a sensitivity analysis may be sufficient to determine whether to move forward on a project (often termed as GO/NO-GO).

A further step is to identify and define the inputs and their associated minimum and maximum values. The number of inputs included should be sufficient to cover the entire supply chain, and feasible minimum and maximum values for each input should be considered in order to have reasonable analysis results [288]. Sensitivity analysis is one available tool to select inputs for probability analysis. The probability analysis evaluates the effects of manipulating inputs simultaneously and is usually presented as the distribution of financial metric's values.

The outcome of the deterministic model (single out-put result) should be evaluated in conjunction with sensitivity and probability analyses to have a relatively complete picture of the risks. However, the combination of deterministic and stochastic models can be problematic (for instance, using a mean value calculated through the probabilistic analysis as an input for deterministic modelling can generate misleading results because the probabilities are not taken into account) [275]. Since the numerical precision of probability analysis results does not provide important information about their sensitivity to changes in the inputs [320], combining them with sensitivity analysis provides synergetic risk assessment results.

Figure 5-6 provides an effective way of selecting tools to use when performing quantitative risk analysis, which will depend largely on the information available. If there is no uncertainty in the input data, a deterministic model is sufficient to give a single-point output. However, a situation free of uncertainty is very unusual. When uncertainty exists, the tools used will depend on the requirements and on the approach defined by the project team. A qualitative risk assessment may be sufficient if there is no need to quantify the outputs and in the very early stages of a project when no quantitative inputs are accessible. If quantitative inputs are available, the use of tools will depend on the type of uncertainties present. For instance, if one has only the maximum and minimum values for the uncertain inputs, a sensitivity analysis can show how the model outputs vary with each individual input change, and probability analysis can be performed considering uniform distributions. In addition, consideration should be given to how results are presented when selecting specific tools. For example, as spider plots can become crowded, it would be more appropriate to use a tornado diagram for graphical outputs and a switching value for table outputs if there are more than five input variables.

Stochastic analysis is recommended when the distribution of uncertainty is available or it is possible to adjust distribution curves to historical records, forecast trends or literature data or even if there is a large uncertainty in the input values. The stochastic analysis results show the combined impact of including several uncertainties simultaneously and provides information on the probability of a successful investment, from the financial point of view.

There is no significant difference between Monte Carlo and Latin Hypercube models, and their use can be subjected to the software and models available.

The results of sensitivity and probability analysis provide meaningful information for investments in the bioeconomy sector. For example, stochastic analysis outputs show the probability of having a profitable investment (e.g., 30 % chances of positive NPV). Moreover, sensitivity analysis results elucidate which parameters should be investigated and changed to improve the probability of financial success (e.g., composition variation of a feedstock). The outcome from this analysis provides guidance on where to devote eff orts to improve efficiently the financial performance of the investment.

In addition to risk assessments, any comprehensive analysis should address risk management, including ranking and illustrating major risks according to their probability and severity in a numerical scale. For example, a scale from one to four can be used, where one represents low probability/severity and four high probability/severity. Risks with the highest impact and likelihood demand the most attention [321]. Risk severities, risk likelihoods and probability distributions can be inferred and/or estimated by sensitivity analysis, probability analysis, prior experience, or subjective evaluations by the project team. Major risks can be easily illustrated in a risk heat map [275], [321], [322], as shown in Figure 5-7. In this example, risks 3, 4, and 7 are the most impactful and should thus be the focus of mitigation strategies.

Mitigation plans are the final step in in the risk-management process. In many cases, mitigation plans require additional data, which may be resources and time consuming. Risks will always be a part of any investment, but risk awareness and mitigation strategies plans are essential for minimizing the chances of an investment failure.

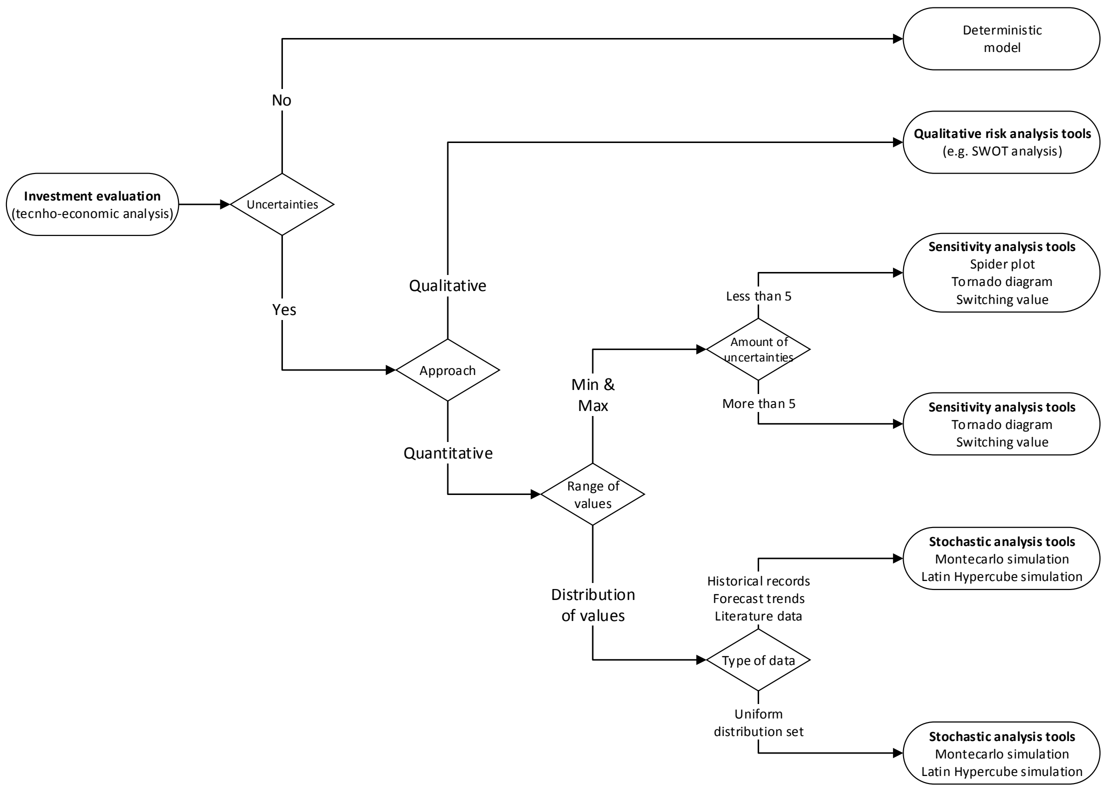


Figure 5-6: Decision tree for selection of qualitative and quantitative risk analysis tools.

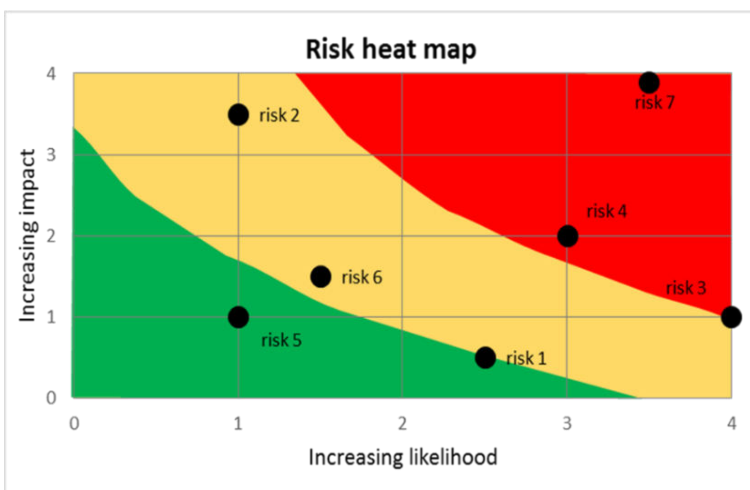


Figure 5-7: Example of a risk heat map (adapted from Branson, 2015) [321].

With a complete financial risk analysis and risk management, investors can have a more comprehensive view of a project and its uncertainties, making it possible to develop effective mitigation strategies and bring better technical information to support the decision-making process.

5.5.1 Major risks for the bio-based industry and proposed risk mitigations

Bio-based industries have unique risks, in addition to those found in any venture, which must be systematically identified and mitigated [323], [324].

Table 5-2, while not exhaustive, provides an overview of the major risks in the bio-based industry and possible mitigation strategies. This table illustrates the major risks identified from the literature review and from information related to recent bio-based industry project failures. Critical risks primarily relate to feedstocks, processes, products, market and technology [265], [267], [305], [324], in addition to operation, financial, legal, regulatory and environmental [305].

As previously mentioned, feedstock cost uncertainty can harm the development of the bioeconomy. While their prices will likely rise over the long run due to increased demand [324], it will be accompanied by significant volatility due to weather conditions, diseases, pests, and/or competition from alternative land uses. Feedstock supply and plant size trade-off s are another consideration. Although the increase in processing scale reduces operating costs per unit of product, larger collection areas can increase transportation costs of feedstocks [252]. Likewise, commodity processing plants scaled to typical forest biomass supplies can be too small to be economically viable whereas those at an economically-sensible size will face higher feedstock costs [252], [325]. Establishing mid- to long-term contracts and diversifying suppliers can help mitigate risks concerning raw material supply and cost volatility. Finally, contracts between farmers and companies can be modified to minimize risks of biomass supply and prices [310], [326].

Table 5-2: Main sources of risk and risk drivers for the bio-based economy.

Risk category	**Risks**	**References**	**Proposed mitigations**
1 – Market	1.1 Uncertainty on raw material cost	[249], [253], [255], [306], [324]	Identify feedstock cost variability based on past data. Establish mid to long-term contracts. Diversify suppliers to avoid one-to-one dependence. Consider cheaper feedstocks options (such as rejects and wastes).
	1.2 Volatility on final product price	[249], [255], [306]	Establish mid to long-term contracts.
	1.3 High enzyme cost and variability	[248], [307]	Develop R&D plans to minimize enzyme consumption. Consider mid to long-term contracts on enzyme supply.
	1.4 Competition with commodities / petrochemical industry	[252], [325]	Find products with unique characteristics to have less price competition. [252] Diversify production, [253] preferably with value-added products. [252], [324]
2 – Technology	2.1 Scale-up	[327]	Perform pilot trials, and, if possible, do scale-up in steps.
	2.2 Technology risk - general	[265], [267]	Perform pilot trials, especially for the reaction section. Identify risky process conditions.
	2.3 Use of genetically modified organisms (GMOs) for fermentation	[327]	Identify regulations and restrictions for GMOs in the region where facility will be constructed. Perform bench scale experiments to have enough data for yields.
	2.4 Technology use feedstock specific enzymes or microorganisms	[327]	Investigate restrictions of specific organisms and the impact on financials.
	2.5 Feedstocks flexibility	[267], [327]	Perform pilot trials with several feedstocks. Preview operational margins on equipment design.

Table 5-2 (continued).

Risk category	Risks	References	Proposed mitigations
2 – Technology	2.6 Level of sterility demanded by the equipment	[327]	Perform pilot trials, and, if possible, do scale-up in steps Investigate the trade-off between having several smaller scale equipment (cost implications) and difficulty to sterilize big equipment. Preview cleaning and sterilization conditions for equipment.
	2.7 Low or variable reaction yields	[249], [253], [307]	Develop R&D plans focusing on reaction yields optimization. [293]
3 – Financial	3.1 High capital costs	[13], [249], [253], [255], [307], [324]	Consider low complexity technologies, if available. Explore co-location options. [253], [309] Calculate the trade-off capacity vs. feedstock cost. Evaluate the impact of capital cost uncertainty. [313] Perform pilot and/or demonstration scale trials to provide design information for new technologies. [302]
	3.2 Low investment return	[324]	Improve margins through product diversification. [324] Mitigations for risks 1.2, 1.3, 1.4 and 3.1 also apply to this risk.
4 – Regulatory	4.1 Policies, subsidies	[254], [271], [309]	Carefully measure the impact of subsidies in project financials. Deep understanding on duration and values of subsidies.
5 – Supply chain	5.1 Feedstock growth yield and variability	[295], [326], [328]	Model the impacts of feedstock growth on delivered cost. Select the most suitable biomass species and varieties for the intended process.
	5.2 Feedstock distribution / biomass supply chains are on early stages of development	[295], [326]	Evaluate trade-offs between feedstock yield and transportation cost (related to density) to define plant location. [295]
	5.3 Final product distribution		Identify how final product distribution can limit project profitability.

Final price volatility is another major known market risk and is common when the final product is a commodity or a substitute for a product derived from petroleum. Prices for liquid biofuels are dependent on the price of gasoline, an inherently price volatile commodity [271]. This helps to justify policy support for biofuels, which are exposed to political and social changes. Bioproducts (such as biochemicals and biomaterials) that have unique characteristics com-pared to the petrochemical derived products, will be less challenged by oil prices [252], and can present fewer risks than commodity biofuels. A company can increase profitability and reduce risk by diversifying the final product portfolio as it would reduce exposure to price volatility in a single market [253]. However, this should be carefully evaluated from technological and financial perspectives as relevant studies vary their results. For example, Mariano et al. observed that the introduction of the butanol and acetone production via ABE fermentation in a first- and second-generation ethanol from sugarcane mill increased and diversified the revenue [257]. In another analysis, although a techno-economic evaluation of butanol and ethanol production showed higher revenues than a single ethanol facility, NPV and IRR were decreased due to higher capital and operating costs [255].

High production costs can lead to low project profitability. For example, bioethanol and bio-butanol production costs using sugarcane bagasse as feedstock are strongly impacted by the enzyme cost whose prices are inherently volatile [248], [307]. If enzymatic technologies become widely available, the risk of an increase in enzyme cost due to higher demand is real, but at the same time the overall production costs should decrease as manufacturers become more skilled. These trends will affect the financial return for a new venture, and both price scenarios should be considered during risk assessment.

High capital costs can limit the development of bio-industries. The shape of distribution curve of the capital cost values can highly affect the profitability calculation results, so the uncertainty of the values should be carefully assigned [313]. This risk can be minimized by evaluating the main components related to capital costs, such as investment scope and main equipment costs. Several strategies can be employed to reduce capital costs. For instance, co-locating with existing mills and pulp and paper industries utilizes existing infrastructure, such as roads, buildings, and processing equipment. Further, including higher ‘capital contingency’ (an amount of money to cover known-unknown costs) is common for these new ventures because unmitigated risks may need extra expenses; however, higher contingency plans also lead to higher financing costs.

Government policies such as excise tax credits or accelerated depreciation should help the bio-based industry development by increasing profitability and reducing risk [255], [302], [324]. However, most of the policies are temporary and subject to shifting social and political landscapes and, unless officially approved for the project, should not be considered as a permanent fact when conducting long-term financial projections and early stage scenario comparisons [248]. Policymakers generally echo this sentiment and argue that biorefineries should be feasible with-out subsidies or unique incentives [324].

Technological risks are among the greatest sources of concern in the bioeconomy because of its relative nascent state. Information on lignocellulosic-based technologies is usually scarce and being developed by small and medium enterprises who lack the capital needed for prolonged development and testing [323]. In addition, equipment and technology is often adapted from other industries and while they serve well as a cost saving measure, they cannot be used for certain bioproduct applications. Technological risk should be compensated by greater financial returns, or mitigated by using conservative start-up time and initial production volume estimates [255]. Running a large-scale pilot plant before commercial deployment of a specific technology is a crucial step for any venture in the bio-based business, since it helps to mitigate risk and direct future R&D strategy.

The information available in the risk mitigation strategy literature is generally descriptive rather than specific, but is still useful for bioeconomy investments. For example, ASTM provides a guide for developing cost-effective mitigation strategies for new and existing facilities, although it focuses on hazard prevention [292]. This guide provides a generic framework to assess risks and develop risk mitigation strategies, using financial performance to identify the most cost-effective combination of risk taking and risk mitigation. Kaplan and Mikes propose risk mitigation strategies based on their classification (preventable, strategic or external) [329]. Preventable risks should be avoided and the probability and impact of strategic and external (uncontrollable) risks reduced [329]. Partnering with other companies can be a good strategy to share risks, however this approach is not common in the forestry industry [324]. A midterm strategy needed to mitigate risks during the first few years of operation may be different than the longer term needed over the complete lifetime of the technology [324]. Finally, some industries are simply more risk averse than others and it is important to change risk perception and appetite in order to minimize and overcome the inherent risks for the bio-based industries [324], [330].

5.6 Concluding remarks

While there is no consensus on the concepts of uncertainty, risk, and risk analysis, this review paper suggests the following definitions in the context of capital investments: (i) uncertainty can relate to randomness or designate both the existence of more than one possibility for a input value, or the absence of information; (ii) risk is a random event that can negatively affect a company's goals; and (iii) risk analysis is a methodology used to estimate the likelihood and frequency of an event and the extent of its consequences. Financial risks can be quantitatively assessed via deterministic and probabilistic analysis, and the tools available for this purpose were presented. Risk management is a broader concept and incorporates the ranking of risks and the development of risk mitigation plans. Investors can have a more comprehensive understanding of a venture when the uncertainties are known and risk assessment and risk management are applied.

6 RISK ANALYSIS, PRACTICE, AND CONSIDERATIONS IN CAPITAL BUDGETING: A CASE STUDY IN THE BIO-BASED INDUSTRY

6.1 Abstract

Purpose. This study aims to examine how organizations in the bio-based industry perceive risks and perform risk analysis within the capital investment decision-making process. More specifically, we aim to assess sources of uncertainty commonly considered, identify tools and methods used for risk assessment, and understand how risk analysis is considered in capital budgeting.

Approach. Eighty-six respondents were electronically surveyed, including C-suite and upper management from different organization sizes and segments in the bio-based industry. IBM SPSS Statistics 25 software was used to conduct statistical analysis.

Findings. Some forms of risk analysis are utilized either in project assessment and/or for decision making by the majority of respondents; however, qualitative and deterministic assessment practices dominate over probabilistic methods. In addition, risk assessment is most commonly performed in the later stages of a project, with less than 50 % of adoption at the early stages. Overall, the main sources of uncertainties considered when performing risk assessment are financial, market and sales, and technology, with competition being considered mostly by upper management levels. Additionally, consistent with previous studies in other industry sectors, IRR, ROI, and NPV are the most common financial indicators used to evaluate capital investments.

Practical implications. The current study elucidates that businesses in the bio-based sector would benefit from implementing risk assessment at the early stages of project evaluations, along with quantitative methods (probabilistic methods) for a more comprehensive and efficient risk assessment.

Originality / value. The novelty of this assessment resides in i) the use of risk analyses in capital budgeting for the bio-based sector, ii) the broad variety of business segments selected within the bio-based industry, iii) the detailed investigation of risk assessment practices, and iv) the evaluation of important aspects currently practiced in the industry that were not covered in previous surveys, such as sources of uncertainty considered and the perceived benefits of using risk analysis in decision making.

6.2 Introduction

Previous studies have performed a comprehensive analysis of the unique and inherent risks found in the bio-based industry, as well as methodologies used to perform risk assessment [65]. The bio-based industry is defined as the collection of companies that use predominately renewable feedstocks, such as pulp and paper, biomaterials, and biochemical manufacturing, as well as the forest industry sector (timberland). Factors such as continuous development of new technologies [331], [332], variability in feedstock composition [249], feedstock availability [333], uncertain product prices [121], [192], [334], and geopolitical dynamics [335], [336] add more complexity to the already intricate investment decision-making environment [65]. In order to reduce chances of project failure and generate/maximize value, it is crucial to incorporate risk assessment into the decision-making process [270], [322]. In the present study, we aimed to investigate how risk analysis practices are used in organizations within the bio-based industry, and how risk analysis outcomes (outputs) are considered in the investment decision-making process. To fulfill these goals, we have conducted a survey with decision-makers from different organizations in the bio-based sector. In this study, *risk* is defined as a random event that negatively affects a company's goal. *Risk analysis* (or *risk assessment*) is a methodology used to estimate the sources and the consequences of a risk [65]. We hope that our findings help researchers and organizations from the public and private sectors to understand how risk analysis is perceived and used for decision making in the bio-based sector, opening space to evaluate and improve practices, aiming more comprehensive and efficient risk assessment and management.

Previous academic studies have investigated capital budgeting practices in organizations across different regions [337]–[340], levels of consolidation (multinationals) [341], [342], and over defined periods [343]. In said studies, the use of risk analysis and assessment techniques have been briefly explored since it was not the main emphasis. In contrast, other studies have focused on risk analysis in capital budgeting and corporate investments, and often investigated how organizations measure, handle, and incorporate risks associated with project returns [245]. Additionally, those studies investigated how the use of sophisticated techniques to handle risk have influenced the number of capital investment projects approved [344] and evaluated the influence of organizational culture in adopting risk analysis [345]. It is worth noting that these studies define risk as the impossibility of the decision-maker to estimate outcomes related to their investment decisions, and consider a financial perspective of risk (the sampled population was composed only by financial executives and directors). Outside academia, consulting organizations often release results from surveys on risk assessment practices for different industry sectors (e.g., manufacturing, banking) [346], [347], examine trends in enterprise risk management (ERM) application [348] and evaluate how organizations respond to external uncertainties [349]. Findings from previous works confirm that risk assessments practice and its perceived importance are increasing within organizations.

Studies collecting evidence from the field on methods, sources of risks, and the use of risk assessment in decision-making for the bio-based industry is fairly limited; indeed, relatively very few studies have focused on understanding risk assessments in the pulp and paper, forestry, lumber, and timberland sectors [350]–[353]. These studies, which were conducted at least fifteen years ago, have focused on capital budgeting practices, with a superficial assessment of risk analysis procedures. Topics analyzed and discussed comprised the perception of “risky” investment and the techniques used to adjust project risk from a financial perspective. The novelty of our assessment resides in i) the use of risks analysis in capital budgeting for the bio-based sector, ii) the broad variety of business segments selected within the bio-based industry (pulp and paper, personal care, consulting, chemicals, fuels, biomaterials, forest management, among others), iii) the detailed investigation of risk assessment practices (e.g., existence of a dedicated department within the organization, use of risk analysis in different project stages, the use of qualitative vs. deterministic assessment, and investigation of the tools used), and iv) the evaluation of important aspects currently practiced in the industry that were not covered in previous studies (such as sources of uncertainty considered and the perceived benefits of using risk analysis in decision making). In this paper, we aim to provide a more comprehensive view on the use of risk analysis in areas other than finance, contemplating additional sources of risk, such as those found in supply chain, technology, competition, raw materials, management, among others. Although environmental and social risks are not the focus of this study, we have investigated if these aspects are considered by firms when they perform risk analysis and how their importance is perceived in the decision-making process.

Three hypotheses have been defined for this study, and questions have been developed in order to validate these hypotheses.

Hypothesis 1 (H1): *Less complex risk assessment methods are more commonly used by the bio-based industry*. More specifically, qualitative risk assessment and deterministic risk assessment are preferred over probability analysis. Qualitative tools are usually less complex, needing less detailed information, and may provide information for further quantitative analysis [268]. Among quantitative assessments, sensitivity analysis dominates over other risk assessment methodologies (such as probability analysis) due to its simplicity and direct interpretation of outcomes [245], [289], [343].

Hypothesis 2 (H2): When performing financial risk assessment, price and cost-related uncertainties are primarily considered over other risk sources. Our previous review has shown that mainly price and cost-related uncertainties (e.g., variations in raw material costs and prices of final products) are considered during financial risk analysis for investments [65]. Other sources of uncertainty, such as technical feasibility, intellectual property, regulations, sales volumes, and market competition, are less commonly evaluated.

Hypothesis 3 (H3): Although risk analysis for investments is performed by organizations, its outcomes are not extensively considered in the decision-making process. Organizations rely on deterministic financial methods rather than probabilistic methods for decision-making. Before the access to computational tools became popular, researchers believed that more complex techniques, such as probabilistic analysis, would have difficulty gaining acceptance by managers and reducing their enthusiasm for investments [245]. Indeed, this behavior seems to be consistent. Previous studies indicate that a relatively small number of companies have been regularly using probabilistic risk assessment [343], and two-thirds of forest products industry respondents have not used risk simulation frequently [245], [345], [351].

6.3 Methodology

6.3.1 Questionnaire preparation

A survey questionnaire instrument was used to collect data for this study. The questionnaire was prepared using “Google Forms” application and consisted of two sets of questions, one aimed at respondents who do actually perform risk analysis for investment assessment and another set for respondents that do not perform risk analysis. The initial versions of the questionnaire were developed from risk analysis and management literature across various industries and included previous studies focused in the forest and bioproducts industry [245], [343], [344], [350], [351], [354]. The questionnaires were then modified based on comments from experts in the areas of risk and investment management, finance, organizational behavior, supply chain, forest products industry, and survey development, all of them from the Department of Forest Biomaterials and the Poole College of Management at North Carolina State University, and from the Department of Statistical Science at Duke University. The questionnaire was refined in order to minimize ambiguity in questions and ensure the evaluation of the hypotheses. The updated questionnaires were submitted for a second round of reviews to the same group of experts.

The final version of the questionnaires were organized as follows: the first question identifies if the respondent uses risk analysis for investment assessment. For those who responded affirmatively, they were then asked fifteen questions concerning risk analysis practices, analytical approaches used, sources of risk usually considered, and how risk assessment results were used in the investment decision-making process. For survey participants who responded negatively on the use of risk analysis for investment assessment, five questions were asked aiming to understand the reasons for not adopting risk assessment practices. Finally, all respondents were requested to provide individual and organizational demographic information and their contact email as an optional input. The entire questionnaire was designed in a multiple-choice setup, and additional space was provided for comments (see APPENDIX B: Risk assessment survey questionnaire).

6.3.2 Sample

As previously mentioned, the survey targeted organizations within the bioeconomy, which included firms primarily involved in forestry activities and affiliated organizations that used bio-based feedstock – the so-called *bio-based industries* [4], [13], [14].

A final sample of 2,040 participants was selected for the survey, representing over 220 organizations. This includes an email distribution list (1,927 contacts) from "The Technical Association of the Pulp and Paper Industry" (TAPPI) comprising managers and upper level employees in the pulp and paper and related industries. The email body to this group (available in APPENDIX B: Risk assessment survey questionnaire) included a brief explanation of the survey goals and the time estimated to complete the questionnaire, the link to the questionnaire, and assurance of confidentiality. The first electronic invitation to this group was sent in February 2018. Two reminders to non-respondents were sent, one in May and another in June 2018.

The remaining 113 respondents (from now on indicated as *direct contacts*) were individually contacted by email. These contacts hold decision-making positions, managerial or upper level employment in the pulp and paper, forest management, engineering, consulting, fuels, chemicals, biomaterials, personal care, wood products, and timberland organizations. The majority of contacts were put together with advice from the Department of Forest Biomaterials / NC State faculty and their networks. In addition, *direct contacts'* emails were gathered from publicly available online information (such as press releases, reports, or conference presentations). Emails were sent between March and June 2018, with one email reminder to non-respondents. Only one email reminder was sent because the people in this list are known by the authors and consequently are more likely to respond.

From the TAPPI mailing list, it was possible to identify the number of participants that actually opened the message. For this group of participants, the response rate was calculated based on the number of messages opened. For the *direct contact* list, the response rate was based on the number of messages delivered. Response rates varied between the two groups contacted, as shown in Table 6-1; response rates were considerably higher for the *direct contacts* group, as expected. The overall response rate was 22 %.

Table 6-1: Contacted participants and response rates.

TAPPI mail list		**Direct contact**		**Overall**	
Sent messages	1,927	Sent messages	119	Sent messages	2,046
Opened messages	341	Delivered messages	113	Opened / delivered	454
Responses	61	Responses	39	Overall responses	100
Response rate	**18%**	**Response rate**	**35%**	**Response rate**	**22%**
				Relevant responses	**86**
				Overall Adjusted response rate	**19%**

From the initial 100 responses collected, 14 were excluded for the following reasons: the organization was not directly related to the bio-based industry (e.g., equipment and chemicals suppliers for the bio-based industry), duplicate responses (same person responding twice – in this case the first response was recorded), responding organization was a research center or university, and incomplete responses. Thus, with a total of 86 selected responses, the overall response rate was 19 %, which is in accordance with previous voluntary surveys [245], [341], [342], [350], [351].

Differences between responses from the two groups (TAPPI and direct contacts), were verified by chi-square tests. IBM SPSS Statistics 25 software was used to conduct statistical analysis. Responses evaluated comprised risk assessment practices (existence of guidelines and dedicated department or employee, the frequency of use, the use of methodologies, software, and analytical approaches, and major sources of risk considered), financial metrics considered for investment assessment, and demographical information. It was confirmed that the TAPPI contacts group was mainly composed by pulp and paper segment, while direct contacts presented a more diverse group of people. Except for the question related to industry segment, no significant differences between the responses from the two groups were found; thus, results will be presented as a single group.

6.4 Results and discussion

6.4.1 Survey demographics

Demographic information provided by survey respondents were validated using information from Hoover's Company Profiles[6]. The 86 respondents belonged to at least 65 different organizations (10 % did not provide organization information). The majority of respondents were from the pulp and paper segment (Table 6-2).

Organizations' size varied broadly, with 26 % of the respondents representing companies with more than 10,000 employees, and 27 % of companies with less than 100 employees. Organizations' revenue was also widely distributed, varying from less than USD 1 million to more than USD 10 billion. Around 13 % of respondents did not provide revenue information (mostly startups or private firms). The number of employees and firm revenue was strongly correlated (R^2=0.83), so the organizations were grouped as small (< 100 employees, revenue < 10 million USD), medium (100 – 5,000 employees, revenue between10 – 1,000 million USD), and large (> 5,000 employees, revenue > 1,000 million USD). The categorization resulted in 23 small, 29 medium, and 34 large organizations.

Most of the respondents represented organizations headquartered in the U.S. and Canada. Overall, 56 % of the respondents were from local organizations and 44 % from multinationals. Approximately 80 % of the respondents hold management positions (21 % held C-suite or presidential positions; 18 % were vice-presidents or directors - *upper management*, and 41 % were managers or coordinators - *middle management*). The remaining were engineers, scientists, specialists, and analysts.

[6] https://search.proquest.com/marketresearch/advanced

Table 6-2: Demographics of survey respondents.

Industry segment	**N°**	**%**
Pulp and paper	48	56%
Chemicals / fuels / materials	11	13%
Consulting	10	11%
Consumer products / personal care	5	6%
Forest management	5	6%
Wood products	4	5%
Others	3	3%
Number of employees		
< 100	23	27%
100 – 1,000	21	24%
1,000 – 5,000	8	9%
5,000 – 10,000	12	14%
> 10,000	22	26%
Revenue (million USD)		
< 1	8	9%
1 – 10	12	14%
10 – 500	13	15%
500 – 1,000	7	8%
1,000 – 10,000	19	22%
> 10,000	16	19%
no revenue / no information	11	13%
Headquarters location		
U.S. or Canada	54	63%
Europe	11	14%
Latin America	12	13%
Asia Pacific	7	8%
Africa	2	2%
Respondent position		
C-suite / President	18	21%
Upper management	16	18%
Medium management	35	41%
Other positions	17	20%

6.4.2 Risk analysis practices and procedures

The use of risk analysis relative to organization's size is illustrated in Figure 6-1. Overall, 98 % of respondents indicated that risk analysis is considered for investment, with 76 % indicating it is always considered and 22 % indicating it is sometimes considered. Statistical analysis shows that larger organizations tend to perform risk analysis more often than smaller organizations. No significant statistical difference was found between pulp &

paper and other industry segments concerning the use of risk assessment practices (chi-square = 0.74).

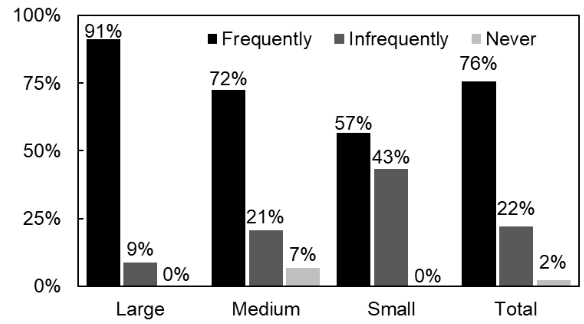
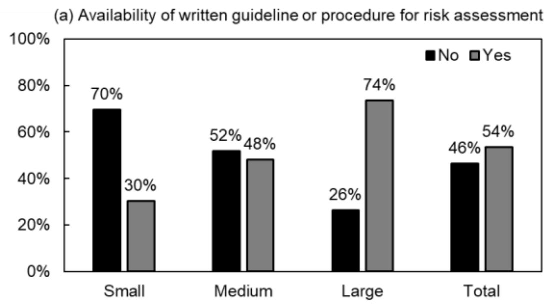


Figure 6-1: Use of risk analysis by organization size.

For respondents who performed risk assessment, it was investigated if risk analysis was formalized, which factors, if any, were mostly considered during risk analysis practice, and how risk assessment was considered in the investment decision-making process.

Among the organizations that used risk analysis, approximately half of them (54 %) had written guidelines or procedures, and only 42 % had a formally dedicated department or employee to conduct risk assessment (Figure 6-2(a) and (b)). It is worth noting that responses within an organization were not unanimous in recognizing the existence of a written procedure or a dedicated risk analysis department. There were 22 respondents representing 10 companies who provided contradictory feedback regarding the existence of these instruments. Therefore, it is evident that risk analysis definition and practice is still not widespread among decision-makers. Statistical analysis results show that it is more common to have formalized procedures of risk analysis in large companies (chi-square = 0.005), as well as a formally dedicated department (chi-square = 0.031). Risk analysis procedures were more prevalent in European-headquartered organizations (75 % of them indicated having a formalized risk assessment procedure, compared to approximately 50 % for organizations with headquarters in other locations). However, the existence of a dedicated department was less common: only 30 % of Asian-Pacific headquartered locations had a dedicated department, compared to an average of 43 % for other locations.



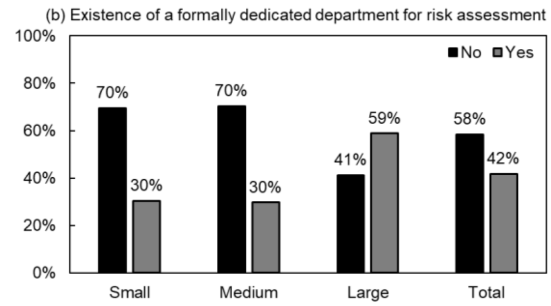


Figure 6-2: (a) Availability of written guidelines or procedures for risk assessment according to organization size. (b) Existence of a formally dedicated department for risk assessment according to organization size.

6.4.3 Use of risk assessment in capital budgeting

About one-third of respondents (30 %) have indicated that risk analysis is performed for every investment, and 40 % used it only for investments over a minimum value. One-fourth of the respondents did not have a defined criterion on the use of risk analysis. Remaining respondents (5 %) indicated that risk analysis was used according to customers' requirements or on a defined schedule (e.g., annually).

The use of risk analysis in different project phases was also examined. It was found that risk assessment is mainly performed during feasibility studies, with more than 80 % confirming risk assessment application (Table 6-3). Less than half of respondents confirmed the use of risk assessment practices during initiation and conception phases, the so-called early stages. It was expected that risk assessment would be used more frequently at these stages, as there are more uncertainties and unknowns at initial project phases [24]. The use of risk analysis at different project phases is not dependent on organization size or participant position (chi-square > 0.05).

Table 6-3: Frequency of risk assessment application by project stage.

Company size (N°)→	**Small (23)**		**Medium (27)**		**Large (34)**		**Total (84)**	
Project phase ↓	**N°**	**%**	**N°**	**%**	**N°**	**%**	**N°**	**%**
Initiation	10	43%	12	44%	11	32%	33	39%
Conception	11	48%	10	37%	18	53%	39	46%
Feasibility studies	19	83%	21	78%	30	88%	70	83%
Engineering design	12	52%	10	37%	23	68%	45	54%
Execution	12	52%	13	48%	17	50%	42	50%

We believe that there should be more emphasis on the use of risk analysis in investment assessment at early stages by academic and industrial organizations. Although the cumulative cost of an investment is not significant at the early stages [24], [39], [355], the decisions made at these steps highly impact project outcomes, such as investment cost and project revenues. The use of risk analysis during the early stages of a project is vital for a comprehensive project assessment and allows the formulation of mitigation strategies, thus reducing the risk of investment failures.

6.4.4 Tools and methodologies used for investment risk assessment

Analytical approaches commonly used for risk assessment were investigated (Table 6-4). The qualitative risk analysis tool to evaluate strengths, weaknesses, opportunities and threats (SWOT) was used by 64 % of respondents, prevailing over quantitative tools. Qualitative tools are usually less complex, use less detailed information, and may provide information for further quantitative analysis [268]. Worst-case analysis was the most used quantitative tool, followed by decision trees and what-if analysis (which can be qualitative or quantitative). Probability distribution tools were used by approximately one third of respondents. The use of decision-trees has been increasing (Hogaboam and Shook, 2004 found an adoption rate of 20 % for the Forest Products Industry, versus 37 % for the present study). About 10% of the respondents reported that no analytical approaches were used to assess risk, presumably due to their reliance on discussions. Tornado diagrams and risk heat maps were found to be more common for large organizations (chi-square < 0.05), although their adoption is lower than 40%. Cost-benefit analysis was an option in the questionnaire, but it was excluded since it is not a risk assessment tool. Overall, spider plots and risk heat maps were the less popular methods. Care should be taken when analyzing these results, since respondents may not be aware of all approaches available within their organizations.

Regarding the use of software, spreadsheets were the most popular tool to perform risk analysis (82 % of adoption), followed by software internally developed, although its adoption was significantly lower (23 %). Probability assessment software (@Risk and Crystal Ball) presented less than 10 % adoption rate, being used only by respondents from medium and large organizations. Some respondents performed only qualitative risk assessments, which explains why computational software was not used. One respondent emphasized that more time was spent on discussion than on software-assisted methodologies.

Figure 6-3 illustrates how different approaches are distributed. Qualitative and quantitative deterministic assessments were used by 70 % and 76 % of the respondents, respectively, while probabilistic assessments are used by 31 % of the participants. It is more common to combine qualitative and deterministic assessments (33 % of participants) than qualitative and probabilistic (2 %) or deterministic and probabilistic assessments (2 %). One-fourth of the respondents (25 %) used all three types of approaches.

Survey findings confirm *hypothesis 1*, which indicates that less complex risk assessment methods are preferred. SWOT analysis provides direct and simple risk assessment. The same applies for worst-case analysis and decision-trees. In addition, the use of Excel Spreadsheets rather than specific software confirm the preference for simpler methods. Probabilistic analysis is more complex; however, participants from previous surveys have agreed that it improves decision quality and confidence [344].

Table 6-4: Use of analytical approaches to assess risk by organization size.

Type of assessment	**Organization size (Nº)→ Analytical approach ↓**	**Small or Medium (50)**		**Large (34)**		**Total (84)**	
		Nº	**%**	**Nº**	**%**	**Nº**	**%**
Qual.	SWOT analysis	30	60%	24	71%	54	64%
Qual. / Quant-D	What-if analysis	18	36%	12	35%	30	36%
Semi-quantitative	Risk heat map	6	12%	12	35%	18	21%
Quant.-D	Worst-case analysis	20	40%	16	47%	36	43%
Quant.-D	Decision trees	15	30%	16	47%	31	37%
Quant.-D	Switching value table	11	22%	13	38%	24	29%
Quant.-D	Tornado diagrams	6	12%	11	32%	17	20%
Quant.-D	Spider plots	6	12%	9	26%	15	18%
Quant.-P	Probability distribution	12	24%	14	41%	26	31%
-	None	6	12%	2	6%	8	10%

Qual. = qualitative approach, Quant.–D = quantitative approach /deterministic analysis, Quant-D/P = quantitative approach with only deterministic or deterministic and probabilistic analysis / Quant–P = quantitative approach / probabilistic analysis. Some approaches may be performed through either a qualitative or a quantitative fashion.

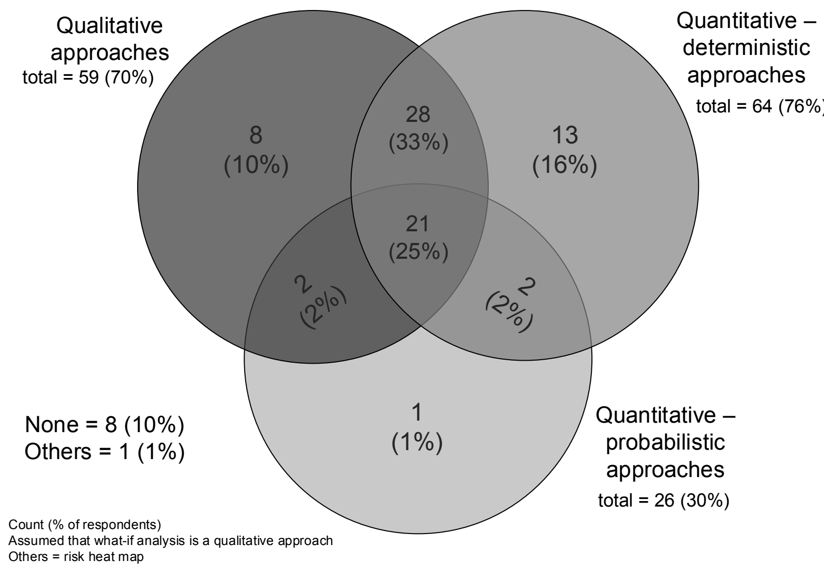


Figure 6-3: Use of different analytical approaches for risk assessment.

6.4.5 Major sources of uncertainty considered for risk analysis

We have examined which sources of risk were normally considered during investment assessment; in addition, participants were asked to indicate the three major sources of uncertainty that should be considered for risk assessment. With this analysis, our goal was to assess the perception of uncertainty factors, as well as to validate *hypothesis 2*.

When questioned about the main sources of risk considered during investment assessment, respondents indicated an average of seven different sources from the fourteen listed. Prices, costs, market and sales were the most selected, overall. Statistical results showed that there was no relevant divergence between major sources of risk by an organization's size, except for environmental regulations, which is considered more commonly by large organizations (chi-square=0.036). The less common sources of risk were management, social factors, and sustainability. Overall, the consideration of price and cost-related uncertainties was an important factor for most respondent positions surveyed, which confirms *hypothesis 2*.

Perceptions on the three most important sources of risks for decision-making showed similar patterns (Table 6-5). Financial sources of risk were the most selected by all respondent levels, followed by market and sales. Statistical analysis showed that competition was more important for the group composed of C-suite and presidents + upper management (chi-square = 0.016) than lower levels, while technology was considered to be more important for respondents at lower levels (middle management and others – chi-square = 0.027) within organizations. Only 9 % of the C-suite and upper management participants considered this source among the top three. It might be the case that lower management levels are more concerned about technology risks, since they are more involved in project details than upper management levels; the same is valid for upper managers, which are more concerned to competition than technology since it is part of their day-to-day work. The selection of other factors (resources, management, government policies, timing, supply chain, R&D, social, environmental regulations and others) is not dependent on participant position (statistical analysis indicated chi-square > 0.05).

Table 6-5: Perceptions on the top three sources of risk, by respondent position. [a]

Respondent level (N°) →	**C-suite / President / Upper management (33)**		**Middle management Other levels (51)**		**Total (84)**	
Sources of risk ↓	**N°**	**%**	**N°**	**%**	**N°**	**%**
Financial (e.g., price and cost variation)	23	70%	35	69%	58	69%
Market (e.g., product adoption)	21	64%	26	51%	47	56%
Technology	11	33%	21	41%	32	38%
Operational	9	27%	16	31%	25	30%
Engineering	3	9%	15	29%	18	21%
Competition	11	33%	6	12%	17	20%
Resources	4	12%	7	14%	11	13%
Timing	2	6%	8	16%	10	12%
Environmental regulations	3	9%	5	10%	8	10%
Supply chain	3	9%	4	8%	7	8%
R&D	2	6%	4	8%	6	7%
Management	3	9%	3	6%	6	7%
Social	2	6%	1	2%	3	4%
Government policies	2	6%	1	2%	3	4%
Others[b]	0	0%	1	2%	1	1%

[a] Respondents were asked to select the top three sources of risk that should be considered for investment assessment/ [b] One respondent indicated operational safety and health impact as "others".

6.4.6 Perceptions on the benefits of performing risk analysis

Next, we assessed whether organizations and respondents were aware of risk assessment benefits. Most of the respondents indicated *better understanding of risks for decision-making* (58 %), *reduction of project failures* (54 %), and *development of risk mitigation strategies* (49 %) as benefits of performing risk assessment. On the other hand, *compliance with regulatory requirements* was seen as a benefit by only 6 % of the respondents, which confirms the growing importance of performing risk assessment rather than a compliance issue. The perception of the benefits did not vary significantly by company size or respondent position.

When asked if the organizations' management was aware of the benefits of performing a risk assessment, 87 % of the respondents confirmed it, 12 % were not sure, and only 1 % believe their management was not aware. Although the perceptions on risk analysis practices and tools may differ, the bio-based industry is conscious of the innumerous benefits of performing risk assessment, as well as other business sectors [344], [346]–[348].

6.4.7 Use of risk analysis in investment decision-making

Finally, we investigated how risk analysis was used for investment decision-making, in order to validate *hypothesis 3*. We asked respondents how often results from qualitative, deterministic and probabilistic analysis were used for investment decision-making. Qualitative risk analysis is always considered for decision-making by 65 % of the respondents and 58 % always consider deterministic risk analysis (Table 6-6). Probabilistic analysis is the least used type of risk assessment for decision-making (25 % of respondents always used it and 21 % never considered this type of assessment).

The use of qualitative and deterministic assessment for decision-making was not impacted by organization size. However, larger organizations tend to use probabilistic risk analysis for decision-making more often than small and medium organizations (chi-square=0.035). No significant difference for pulp and paper versus other industry segments was found (chi-square>0.05). These results validate *hypothesis 3*, indicating that risk analysis is not extensively considered for decision-making.

Table 6-6: Use of risk analysis for decision-making, by organization size.

Industry size ↓	Qualitative assessments			Deterministic assessments			Probabilistic assessments		
	Always	**Some-times**	**Never**	**Always**	**Some-times**	**Never**	**Always**	**Some-times**	**Never**
Large	68%	32%	0%	68%	32%	0%	35%	56%	9%
Small and medium	64%	36%	0%	52%	42%	6%	18%	52%	30%
Total	65%	35%	0%	58%	38%	4%	25%	54%	21%

6.4.8 Financial metrics used for investment evaluation

The financial metrics used by the forest products industry to evaluate investments has been changing over the years. Bailes *et* al. (1979) found that organizations in the forest products industry rely on payback and internal rate of return (IRR) as metrics for investment assessment; payback used primarily in small revenue organizations and IRR most commonly used by larger organizations. Similarly, Cubbage and Redmond (1985) observed that the forest products industry uses IRR, followed by ARR (accounting rate of return), and discounted payback as criteria for investment assessment. A survey conducted in 2001 confirmed that IRR is still among the preferred criteria for investment assessment, although net present value (NPV) has been gaining space [351]. Likewise, studies conducted with the 200 largest UK companies have showed increased adoption of IRR and NPV between 1975 and 1992, due to the increased use of computational tools; however, payback led preference, with 94 % of adoption against 81 % for IRR and 74 % for NPV in 1992 [343].

To investigate current practices in the bio-based industry, we have inquired on the financial metrics used to assess investment attractiveness and the ones considered for financial risk assessment. Similar to early findings, IRR and NPV were among the most common metrics used to assess investment attractiveness, in addition to return on investment (ROI) (Table 6-7). [343], [350], [351], [356] IRR was more common in large organizations, with 94% of adoption rate (chi-square = 0.001). Payback (discounted or non-discounted) was less popular, used by only 21 % of the respondents. Other methods listed by respondents include Economic Value Added (EVA), profitability index, price-to-earnings ratio, Adjusted Present Value (APV), breakeven point, social value, project cost, and productivity ratios (this last specifically for forest management organizations). Similar to early studies [343], there was a tendency to combine several metrics for financial assessment; 17 % of respondents relied on only one financial metric while 60 % of respondents used between two and four financial criteria for investment attractiveness.

Financial metrics commonly used when performing risk assessment are slightly different from the metrics used for investment attractiveness. ROI, IRR, and NPV are among the most used metrics for risk analysis; however, payback has been more extensively considered when assessing risk than for investment assessment.

Table 6-7: Financial metrics used to assess investment attractiveness and to perform risk assessment, by organization size. [b]

	Used to assess investment attractiveness						**Used for risk assessment**	
Company size → Financial metric used ↓	**Small and medium**		**Large**		**Total**		**Total**	
	N°	**%**	**N°**	**%**	**N°**	**%**	**N°**	**%**
IRR	30	58%	31	94%	61	72%	54	65%
ROI	37	71%	22	67%	59	69%	57	69%
NPV	27	52%	24	73%	51	60%	48	58%
ROCE	15	29%	16	48%	31	36%	25	30%
Payback (discounted and non-discounted)	7	7%	11	17%	18	21%	21	25%
Hurdle rate	8	15%	7	21%	15	18%	12	14%
Other	25	10%	20	12%	45	53%	39	47%

[b] 85 responses were considered for this analysis since one was not valid (the name of the financial metric used was not provided). “Other” metrics include Economic Value Added (EVA), profitability index, price-to-earnings ratio, Adjusted Present Value (APV), breakeven point, social value, project cost, and productivity ratios.

6.5 Concluding remarks

The present survey aimed to identify risk analysis practices for capital budgeting in the bio-based industry, with a major footprint in America and Europe. The novelty of this study resides in investigating a broad variety of segments within the bio-based industry, and overcoming limitations from previous studies by investigating in detail risk assessment practices, the sources of risk considered, and the perceived benefits of using risk analysis.

Eighty-six respondents from at least 67 organizations worldwide were surveyed. The vast majority (98 %) used some type of risk analysis for investment assessment; however, the use of qualitative and quantitative deterministic methods dominated over probabilistic approaches. Results have shown that larger organizations tend to perform risk assessment more frequently and have formalized procedures and dedicated departments more often. Although previous studies have shown the increase of importance and development of risk analysis capabilities, it was evident from our findings that risk analysis definitions and practices are still not widespread among decision-makers in the bio-based industry. Overall, one-fourth of the participants that perform risk assessment do not have defined criteria on the use of risk analysis, in addition, we have found disagreements in the perception of risk assessment application and practices even within the same company.

Less complex analysis tools, such as SWOT and worst-case analysis, were among the most used approaches by the bio-based industry, as well as Microsoft Excel spreadsheets that were used by more than 80 % of participants.

In addition, more than 80% of respondents performed risk assessment in later project stages (feasibility studies), while less than 50% of respondents used risk analysis in earlier phases. We believe that there should be more emphasis on the use of risk analysis in the early stages of investment by academic and industrial organizations, since the use of risk analysis may uncover project risks and aid in the proposition of adequate and efficient risk mitigation strategies.

Regarding the sources of risk considered for risk assessment, price and cost related risks (financial risks) were primarily considered, across different organization sizes and management levels. Other common sources of risk considered are market and sales, competition, and technology. An additional assessment on capital budget practices revealed that IRR, ROI, and NPV were the most used criteria for investment assessment and for risk analysis.

Although the industrial community is aware the benefits of risk assessment practices in decision-making, its use in initial project phases is not well established. Further, the bio-based industry shows limited application of more sophisticated risk assessment methods (e.g., probabilistic analysis). We believe that there is room to use adequate risk assessment tools from the initial steps of an investment, and this is vital for a sustainable growth of the bio-based industry.

7 METHODOLOGY FOR THE ASSESSMENT OF INVESTMENTS IN THE BIO-BASED INDUSTRY AT EARLY STAGES

7.1 Abstract

This chapter consolidates the concepts previously studied and proposes a simple and applicable methodology for investment assessment at the early stages. It consists of a preliminary technical, market, and financial assessments, followed by a cash-flow analysis including probabilistic risk assessment. Tools to estimate the most relevant inputs are also part of the methodology, such as the product price based on market size, early-stage capital investment, and major operating costs. The proposed methodology was applied to three case studies previously discussed in this work: cellulose nanocrystals (CNC), cellulose micro- and nanofibrils (CMNF), and lignin micro- and nanoparticles (LMNP) in addition to the manufacturing of wood pellets. The execution and outcomes of the methodology were compared to the detailed analyses previously performed. Significant time and resources were saved by applying the proposed methodology, and the results of the analyses led to conclusions similar to those generated from the detailed assessment, although higher uncertainty for the early stage analysis was observed, as expected. In addition, the methodology includes a questionnaire covering common risks for the bio-based industry, which add value to the analysis and provide additional guidance on where to devote efforts on subsequent project stages.

7.2 Introduction

As previously discussed in the introductory chapter, to the best of our knowledge, there is a lack of methodologies for the assessment of projects at early stages, addressing multiple aspects that affect project feasibility in addition to quantitative risk analysis. A systematic and relatively simple methodology to evaluate project alternatives at early stages helps to establish a reliable and robust decision-making process, saving time and resources, and provides information for the design of mitigation plans.

Following, a literature review on previous efforts toward early stage assessments for the bio-based industry is provided, discussing main accomplishments and gaps. It is divided into two sections: the first part contemplates current approaches, and the second part is a discussion on the factors and uncertainties considered in previous public assessments.

7.2.1 Methods for early stage assessment of bio-based projects

Previous research efforts on tools and methods for project assessment at early stages can be divided into three main categories, based on the goals of the assessment: i) product screening, ii) technology and/or configuration selection, and iii) investment evaluation considering multiple criteria. By early stage we mean the initial phases of a project lifecycle when project conceptualization and initial planning are performed [23]. Product screening methodologies aim to identify and select the most promising products for further research and development efforts. Technology and/or configuration selection methods assess manufacturing pathways for different products and feedstocks alternatives. The last type of methods aim to evaluate multiple aspects of project, and are usually applicable after product and technology selection has been completed.

7.2.1.1 Bio-based product screening

A significant challenge for new investments, as well as research and development (R&D) activities in the bio-based business, is the selection of which product(s) to pursue. There is a vast range of products that can be manufactured from bio-based sources, using different types of feedstock and processing routes. In general terms, the products obtained can be classified as *drop-ins*, which directly substitute existing products (such as chemicals and fuels from fossil sources), or as *new materials*, which are new products that replace existing products functionalities [25], [28]. Studies have attempted to systematize the product screening process by using different methodologies and selection criteria. A pre-selection can point out the most promising options, directing research efforts for efficient development of the bio-based industry [29].

A summary of the publications analyzed is presented in Table 7-1, illustrating the goals of the analyses, input information used, products assessed, and screening criteria defined. Also, it identifies if uncertainty analysis was performed.

The majority of the studies have been focused on the selection of chemicals, especially *drop-ins*. Only one study has included new materials (e.g., bacterial cellulose) in the initial list of alternatives [27]. Some screenings have been mostly based on technical assessments, i.e., the selection was performed considering product properties and the potential as building block [28], [29]. Others have relied on economic aspects, such as the difference in price between the bio-based product and the fossil-based alternative [25], or the maximum potential revenue from a bio-based product [30]. The Technology Readiness Level (TRL), an index to classify the maturity of a given technology [357], is commonly used as one of the selection criteria for the methodologies assessed [12], [29], as well as market information, such as market size and expected market growth. It is worth noting that uncertainty and risks were rarely included in these assessments.

Most of the studies have not provided information on how the inputs and the selection criteria have been considered for the decision-making process, hindering the possibility to apply these methods. More specifically, several studies have employed multiple criteria during the screening process, although it is not clear if all of them were considered equally relevant or if some were more important than others. We believe that systematization of the screening process and the inclusion of uncertainty is beneficial for an efficient and reliable selection of promising products.

Table 7-1: Summary of bio-based product screening methods.

Reference	Assessment goals	Products evaluated	Input information	Criteria for decision-making	Inclusion of uncertainty	Comments
Leeper and Andrews (1991) [20]	Identify promising candidates for economical production via bioconversion	Organic chemicals	**Technical:** reaction yield **Market:** market volume, number of producers, product price **Financial:** feedstock cost	- high potential return (PR) - high return ratio (RR) - high market volume	No	
Landucci *et* al. (1994) [27]	Identify near-, mid-, or long-term opportunity candidates produced from bioconversion of renewable materials	Chemicals and materials	**Technical:** reaction yield, technical feasibility, mass and energy balances **Market:** volume, product price **Financial:** feedstock cost, petrochemical raw material cost, capital investment, operating costs	- high yield - high market interest - high production volume - non-food application - ability to be synthesized from common sugars - low feedstock cost to product price ratio (Fraction of Revenue for Feedstock - FRF) - low raw material cost for bio-based route - low bio-based predicted selling price	Sensitivity analysis of FRF to feedstock costs, product prices, and reaction yields	- Novel products are in the initial list, such as bacterial cellulose. - No detailed information on how to weight factors and criteria for decision-making. Qualitative analysis results were considered peripherally
Werpy and Petersen (2004) [28]	Identify the "top ten" building blocks that can be produced from sugars	Building block chemicals (molecules with potential to be transformed into new families of useful molecules)	**Technical:** number of potential derivatives, complexity of pathways **Market:** volume, product price, expected growth	- high functionality - feasible production from lignocellulosic or starch - not aromatics derived from lignin - not co-products from petrochemical refining - high market potential - high product price - low technical complexity - high potential to produce derivatives	No	No detailed information on how to weight factors and criteria for decision-making.

Table 7-1 (continued).

Reference	Assessment goals	Products evaluated	Input information	Criteria for decision-making	Inclusion of uncertainty	Comments
Bozell and Petersen (2010) [29]	Update the analysis performed by Werpy and Petersen (2004), considering new information available	Building block chemicals (potential to be transformed into new families of molecules)	**Technical:** intensity of research activity, flexibility to generate other materials, TRL (technology readiness level) **Market:** market volume	- amount of research reported - technology applicable to multiple products - generates direct substitutes for existing petrochemicals - generates high volume products - strong potential as a platform - scale-up is underway - established commercial production	No	Cost evaluations were not included in the assessment, justified by low reliability at development stages. A qualitative score was provided for each criterion assessed.
Biddy *et* al. (2016) [12]	Identify bio-based products that can be deployed in the near term	Chemicals (finished products or intermediates)	**Technical:** TRL (technology readiness level), process pathway **Market:** volume, product price, expected growth, saturation **Financial:** manufacturing cost	- high market volume - value greater than fuel - mature market, not saturated - feedstock flexibility, low biomass cost - potential to integrate with DOE research - no natural gas competition - high TRL (technology readiness level) - current research efforts for production	No	No detailed information on how to weight factors and criteria for decision-making
Culbertson (2017) [30]	Screen and evaluate the commercialization potential of a bio-chemical	Chemicals	**Technical:** reaction yield, process pathway **Market:** volume, product price, expected growth **Financial:** feedstock costs	- preference for direct conversion pathways - high market size and expected growth for downstream products - high maximum potential revenue	No	
Straathof and Bampouli (2017) [25]	Rank existing commodity petrochemicals based on economic potential of bio-based production	Commodity chemicals	**Technical:** reaction yield, Gibbs energy of formation **Market:** product price **Financial:** feedstock cost, energy cost	- price of bio-based route lower than fossil route price	No	Practical feasibility of bio-based routes was not assessed

7.2.1.2 Technology and process configuration selection

Methods to select conversion pathways and process configuration have been proposed for bio-based products manufacturing. These assessments aimed the selection of technology pathways, definition of process steps for a given process and facility characteristics (e.g., capacity), as well as the identification of promising final products for a defined technology. A non-extensive summary of these methods is shown in Table 7-2.

In contrast to methods aiming bio-based product screening, studies focusing on bio-based technology and/or configuration selection usually identify the most promising alternative(s) or a combination of them from a limited number of options. This limitation is due to the extensive effort to develop complex computational models tailored to a set of alternatives, and the amount of time needed to collect input information. Some of the methods integrate computational tools that perform process and economical modeling [34].

A common feature of the studies assessed is the use of financial metrics as criterion, such as NPV (net present value) and EBITDA (earnings before interests, taxes, depreciation, and amortization). Sustainability criteria were also included in some studies by selecting processes with reduced greenhouse gas emissions and energy usage [358]. Uncertainty has been commonly included on these assessments, usually through variations in raw material costs and final product prices.

Although these methods claim to be used at project early stages, they focus on optimization procedures, which may be cumbersome to perform at initial phases, since detailed input information, complex calculations, and specific software are necessary. In order to be applicable, an early stage assessment tool should be simple and straightforward in its execution.

Table 7-2: Summary of methodologies for bio-based topology selection.

Reference	Methodology goal	Technologies assessed	Input information	Criteria for decision-making	Uncertainty analysis	Comments
Cheali, *et* al. (2014a, b) [31], [32]	Identify the optimal processing route for the production of biofuels (gasoline, diesel, and bioethanol) from lignocellulosic feedstocks (corn stover and wood)	Thermochemical and biochemical conversions	**Technical:** mass and energy balances, **Financial:** raw material costs, final product prices, capital investment, operating costs	- maximize production - maximize EBITDA	Probability analysis, considering uncertainties in raw material costs and product prices	Superstructure modeling Technical uncertainties were left out
Cheali *et* al. (2015) [358]	Identify the optimal biorefinery configuration to produce biofuels (bioethanol and FT-products) and value-added chemicals from bioethanol	Biofuels production: via thermochemical and biochemical route Chemicals from bioethanol: chemical routes (oxidation, esterification, etc.) and biological routes (fermentation)	**Technical:** mass and energy balances **Financial:** raw material costs, final product prices, capital investment, operating costs	- maximize EBITDA - minimize green house gases emissions and energy usage	Probability analysis, considering uncertainties in product price	Superstructure modeling Inclusion of sustainability aspects as a criterion for decision-making
Geraili *et* al. (2016) [34]	Design and optimize the production of succinic acid, cellulosic ethanol, and electricity from switchgrass	Pretreatment, enzymatic hydrolysis, and fermentation	**Technical:** mass and energy balances, capacity constraints **Financial:** final product prices, capital investment, operating costs **Market:** product demand	- maximize NPV	- Sensitivity analysis to identify the most critical parameters - Probability analysis, considering financial and operational uncertainties	- Integration of different computational tools (Aspen and Matlab) - Process route is fixed, capacity and operating conditions are optimized - Land availability assumed as a constraint

7.2.1.3 Multi-criteria investment screening

A comprehensive project assessment should be performed beyond financial aspects. Competition, market, availability of resources, management, ability to manufacture, among others, are aspects also considered when assessing an investment. Methodologies for project assessment aiming to help in the decision-making for new investments using multiple criteria have been proposed. Although we could not find specific tools for the bio-based industry, several studies have been performed for chemical and petrochemical industries and will be described next. These tools may be suitable for bio-based investments due to similarities in unit operations and processes. To assess investment alternatives, more information is necessary when compared to bio-based product screening, for example. Nevertheless, the challenge resides in performing a reliable screening, using as minimal information as possible, eliminating less-promising alternatives early, and thus focusing time and resources on options with higher chances of success. Moreover, the application of investment screening tools may help in identifying which aspects of the project require additional information for the decision-making [359].

Most of the tools proposed for project screening were published between the 70s and 90s. Harris (1961) proposed a tool to screen investments for the chemical company Monsanto that is still being used for product development [359], [360]. The author suggests using the tool before any major research expenditure is made. In the proposed methodology, projects are assessed according to 26 aspects and scored from a low (-2) to a high (+2) level of suitability to the investor. Projects with more aspects ranked closer to +2 have higher chances to succeed. Scores are placed in the form of a chart, and the charts for each alternative are visually compared. Figure 7-1 illustrates the charts for two projects analyzed that later resulted in success and failure. Aspects assessed are related to financial metrics (e.g., return on investment, payback value), industrialization ability (raw material and equipment availability), R&D (*know-how*, patent status, and research payback time), and finally, marketing (market impact, competition, and product life). The list of aspects assessed was later updated by Odioso (1987), by the inclusion of additional marketing criteria (such as product uniqueness and advertising advantage), as well as consumer safety and environmental aspects [36].

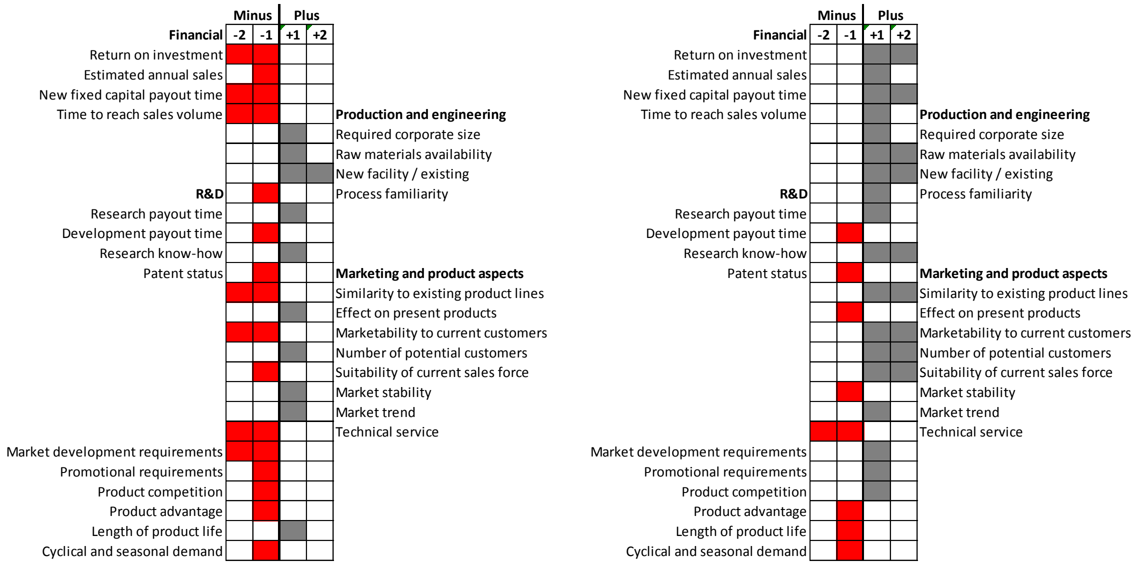


Figure 7-1: Example of product profile charts for a project failure (left) and success (right). Based on Harris (1961) [359].

Udell and Baker (1982) proposed a systematic approach to screen project ideas, named PIES (Preliminary Innovation Evaluation System) [361]. The approach is based on 33 questions involving project aspects considered relevant by product managers, such as project safety, technical feasibility, profitability, market acceptance, and competitiveness. Each answer provides a score, and weights can be applied to indicate the relative importance of one criterion to others. Finally, an overall score is calculated for each project, which may be used as a screening tool.

A semi-quantitative methodology has been developed by Merrifield (1994) to assess investment opportunities in different manufacturing industries [37]. The assessment is based on 12 factors related to business attractiveness and fit to an organization, which were identified as the most critical parameters for project success. If these factors are satisfied, the project success can be predicted 80 % to 90 % of the time. The proposed methodology was successfully applied to Japanese corporate projects [362] with 80 % accuracy.

Table 7-3 illustrates and compares the aspects considered by each method. Financial, R&D, production and engineering, and market aspects were taken into account for all methods assessed. Only one methodology (Harris, 1961) did not consider environmental impacts in the analysis, and uncertainty was not included in any assessment. For all approaches, a significant amount of aspects were evaluated, and no information on how to obtain the inputs was provided, making its application more difficult at project early stages. Nevertheless, these methodologies provide relevant insights on what factors to consider for general project evaluation, which may need to be adapted to include the unique aspects of the bio-based industry.

Table 7-3: Aspects considered for multiple criteria investment screening methodologies.

Reference → **Aspects considered ↓**	**Harris, J. (1961) [359]**	**Udell and Baker (1982) [361]**	**Odioso, R. (1987) [36]**	**Merrifield, B. D. (1994) [37]**
Financial	✓	✓	✓	✓
R&D	✓	✓	✓	✓
Production and Engineering	✓	✓	✓	✓
Marketing & product	✓	✓	✓	✓
Safety / Environmental		✓	✓	✓
Uncertainties				

Although not completely related to early stage investment assessment, worth to mentioning are methodologies that aimed to structure the evaluation process for new product development. Undoubtedly, the development of the bio-based industry is associated with the development of new products and processes.

Perhaps one of the most known approaches to managing the new product innovation process, from idea generation to market commercialization, is the "Stage Gate systems," proposed by Robert G. Cooper during earlier 90s [38]. The approach was based on product development methods designed by NASA in the 60s [363]; the innovation process is divided into a defined set of stages comprising mandatory and voluntary activities. To move from one stage to another, the project should pass through a gate, where main outcomes of the previous stage are examined, and a decision to go to next stage, abandon the project, or review the stage is made [38], [363]. Five stages are typically considered: i) preliminary assessment, ii) detailed investigation/business case preparation, iii) development, iv) testing and validation, and v) full production and market launch. Main characteristics of a stage-gate system are its systematic structure with defined decision points and the involvement of different functions within an organization during product development activities [363]. Lately, efforts for a more fluid and flexible stage-gate system are being performed [363]; however, details on the activities of each stage and gate are not provided. Indeed, the absence of well-defined activities is intentional, allowing it to be tailored to different projects and industrial segments.

Organizations have frequently been using the principles of stage-gate systems for capital project management. Benchmark data has confirmed that using a project process improves project performance regarding schedule, cost, operability, and safety [24]. The most common stage-gate procedure for capital project management has five stages and gates at the end of each phase: business assessment, feasibility, front-end engineering design (FEED), execution, and operations [24].

7.2.2 Factors and uncertainty consideration in early-stage assessments

The methodologies previously discussed have utilized different input factors to perform the assessments. Most of the bio-based product screening approaches, for example, have relied on technical, market, and financial information to aid the decision-making process. Some methodologies have used technical information as a criterion to select most promising bio-based products to invest (e.g., bioconversion yields and technology readiness level); others have added market information (such as market size and product price) for product selection. Methodologies to evaluate project configuration have typically required more information, such as detailed mass and energy balances and capital and operating costs. Since the collection of detailed process and financial information at the early stages may be time and resources consuming, simplifications and assumptions should be applied when estimating these values. On the other hand, multi-criteria project screening methodologies have usually relied on several aspects, ensuring that factors that may lead to project failures have been evaluated. Table 7-4 illustrates the several causes of project failure, based on published studies on new product development and recent bio-based projects that failed. Six main categories were identified: market, competition, financial, sales, technical, resources and management, and others, which are similar to the categories assessed in multi-criteria project screening methodologies. Previous studies have shown that organizations that rely only on financial assessment for new product selection tend to have unsuccessful project outcomes [364]–[366], and that most of project failures can be related to poor assessments at initial steps of a project [367]–[370], which corroborates to the need of an early-stage assessment that goes beyond the simple techno-economic analysis.

Table 7-4: Common causes of project failure.

Category	Examples
Market	Number of customers was overestimated [367], [368] Customer requirements were not understood [367] Market need was nonexistent or optimistically forecasted [367], [369] Product price was overestimated [263], [367]
Competition	Competitors were better established in the market than expected [367] Product was the same as competing products [367] A similar competitive product was introduced [367] Competitors lowered the prices [367]
Financial	Investment costs exceeded expectations [368] Profit margins were below expectations [371]
Sales	Selling and distribution efforts were misdirected [367], [368] Inadequate selling, distribution and promotional efforts [367] Government action hindered the sale of the product [367]
Technical	Technical difficulties to produce, manufacturing deficiencies [258]–[260], [263] Inability to produce the product as desired [367] Low reliability of manufacturing equipment [263] Poor preliminary technical assessment [372]
Resources and management	Poor initial product screening [369] Lack of skills (e.g., in market research, management, R&D) [368] Lack of resources (e.g., financial, production, personnel) [368] Company internal conflicts [371] Lack of product fit with corporate goals [369] Poor marketing research [368]
Others	Timing was too late [367] Timing was premature [367] Lack of regulations [370] Changes in government policies [370]

Finally, it is worth noting that uncertainty has not been extensively considered at early-stage assessments, although the vast majority of inputs considered are uncertain. Only one of the bio-based product screening methodologies evaluated has included uncertainty, by investigating the impact of feedstock costs, product prices, and reaction yields in product revenues [27]. For technology and process configuration assessments, uncertainty on financial, market and technical parameters has been more commonly incorporated, usually as an input for optimization and selection of robust configurations. Uncertainty assessment has not been contemplated during multiple criteria project screening.

7.3 Proposed work

Given the importance of early stage analysis and the multitude of project alternatives for the development of the new bio-based industry, a methodology is proposed for the assessment of projects at early stages including uncertainty. The proposed method uses, adapts, and integrates elements from existing studies in a unique way. The execution of the methodology consumes significant less time and resources than traditional approaches, and the methodology outcomes provide relevant information for decision-making. It is worth noting that the proposed methodology is targeted for projects aiming industrialization.

The methodology is intended to be used at project early stages when no detailed information is available. Outcomes from different projects may be compared to identify the most promising project alternatives.

The methodology is composed by several assessments organized in three steps (Figure 7-2). The first step comprises market, technical, and financial assessments. Outcomes from the first stage include a market score, the technology readiness level, and the economic potential of the project, respectively. If more than one project is being evaluated, the three outcomes can be compared to select the most promising alternatives. The second step consists of a cash flow analysis including risk assessment. Financial metrics such as NPV (net present value), IRR (internal rates of return), and payback are estimated. Quantitative risk analysis is performed to investigate the impact of market, process, and financial uncertainties on project financials. The financial metric outcome is used for decision-making, and the project can be abandoned, revised, or advance to the third step. Additional aspects of the project are then evaluated in the form of a check-list, ensuring that other significant aspects that can harm the project are addressed early (e.g., safety, environmental, regulations, and supply-chain issues). If the project is still promising with no major drawbacks it is selected for further assessment at the organization discretion.

Supporting tools to estimate product price, capital investment, and operational costs at early stages are part of the methodology. By using these tools, the analyst saves significant time and resources when compared to common project appraisal practices. Overall, the application of the methodology provides a digest of relevant quantitative and qualitative information to aid the decision-making process. It is not our intention to use the proposed methodology in later project stages (e.g., detailed capital investment estimation), but rather to provide sufficient information for project screening and decision making before advancing to more time and resource-consuming project phases.

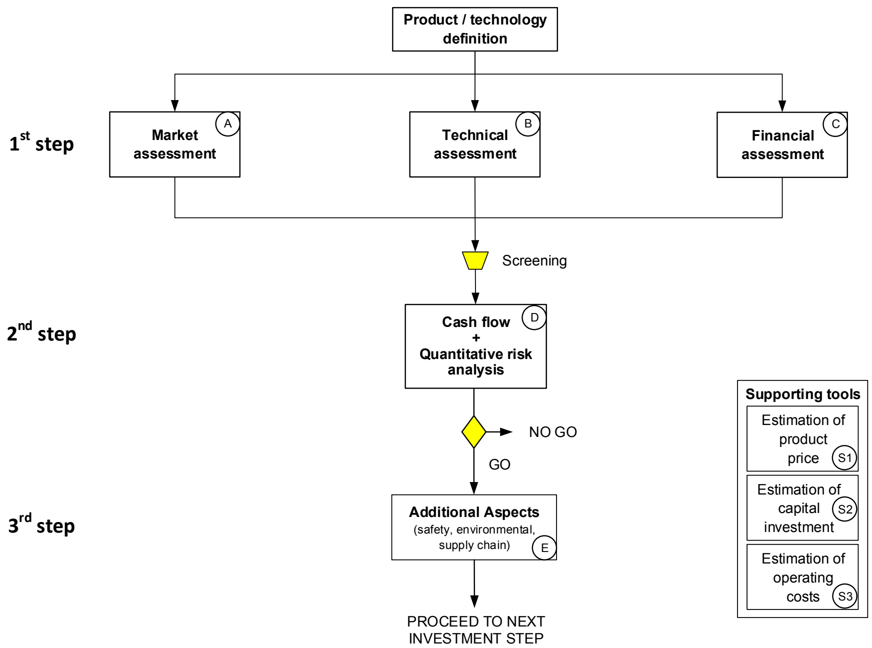


Figure 7-2: Preliminary proposed guideline structure.

A brief description of each step of the method is following provided.

1) Product/technology definition: A product/technology to be evaluated is defined. The product can be identified as a *drop-in* (when there is an existing product from non-bio-based sources) or a novel product that can displace existing products in the market. Since the method is intended for projects aiming for industrialization, it is recommended to identify applications and/or current products that can be displaced. This information is used for subsequent assessments.

2) Market assessment (A): The main purpose of this assessment is to evaluate the attractiveness of a project from a market perspective. A scoreboard is proposed to evaluate relevant market aspects, such as market size and growth, competition, market development, and product uniqueness. If the product is a *drop-in*, market

information can be easily found through market research. For novel products, market information for possible substitutes or potential markets should be used. For all scenarios, literature research and voice of the customer are encouraged. Outcomes of this analysis are a score of the market assessment.

3) Technical assessment (B): The technical assessment is based on the technology readiness level (TRL) of a project. A description of the different TRLs is provided in the method, as well as the activities involved in each TRL and how to consider process and cost uncertainties. Although the TRL classification does not lead to a decision to advance or stop the project, it may provide important information for screening project alternatives. The decision might be to avoid projects with higher technological risks (lower TRL), depending on the analyst/organization goals. Outcomes of the technical assessment point out further technical research and development activities, as well as indicate the uncertainties to be considered in subsequent steps of the method.
4) Financial assessment (C): In this step, the economic potential of the project is calculated based on the estimated revenue from product sales and the cost of raw materials. Reaction yields, raw materials costs, and final product prices are used as inputs. If available, information on other operational costs can be used (energy, labor, catalysts). In addition, sensitivity analysis is performed to evaluate how uncertainties in inputs (e.g., variation in raw materials costs and final product prices, lower reaction yields) influence the economic potential. If the economic potential of a project is negative, it is recommended to not move to the next step of the method, and revisit the inputs used for the assessment. Revision of technologies, raw materials, or even final products selected may be necessary. As for the market and technical assessments, the outcomes of the initial financial assessment may be used to select the most promising option from a financial perspective.
5) Cash flow and quantitative risk analysis (D): After the market, technical, and financial assessments are performed, a cash flow analysis is proposed. Minimum product selling price and financial metrics such as NPV, IRR, and payback values are estimated. Input information for this step are raw materials consumption, production rates, financial assumptions, operating costs, and capital investment values. A

quantitative risk analysis including market, technical, and financial uncertainties is following performed. Market risks are accounted by including variations in sales and final product prices. Technical risks are accounted by uncertainties in estimated capital investment, operating costs, and process inputs. Financial risks are accounted by variation in feedstock and raw materials costs. Outcomes of the risk analysis are the probability distribution of the financial metric and manufacturing costs.

6) Evaluation of additional aspects (E): Marketing, supply-chain, ability to produce, safety, and environmental aspects are evaluated through a questionnaire. If there is an issue that can significantly prevent the project to succeed (e.g., unavailability of raw material in the selected location for the facility), it is recommended to not move forward until this issue is solved.
7) Supporting tools: A relevant part of the methodology is the selection, evaluation and adaptation of existing tools that estimate necessary inputs, such as product prices, capital investment, and manufacturing costs.
   - Estimation of product price (S1): To cope with the difficulty of estimating raw material costs and product prices during early assessments, a tool to estimate prices based on market size and product classification is proposed. As for the feedstock cost, this information can be used as an input for the *Financial Assessment* (C) or *Cash Flow Analysis* (D).
   - Estimation of capital investment (S2): Tools to estimate capital investment at early stages of design are proposed, based on existing methods available in literature.
   - Estimation of operating costs (S3): Estimated operating costs include raw material, labor, energy, and expenses related to the fixed investment [373]. Tools to estimate these values, as well as the uncertainty associated when comparing to case studies, are provided as part of the methodology.

As previously discussed, it is expected that the execution of the methodology will save significant time and resources for project assessment. In addition, uncertainties are accounted for from the early stages of project assessment, which can provide more comprehensive information for the decision maker. Following, the elaboration of each step is exposed in detail; then the complete method is applied for case studies and the results are discussed.

7.3.1 Market assessment

Carrying out a market assessment at early stages of a project provide substantial information to guide product and process development when commercialization is envisaged. Information on the market landscape of a product can aid in screening out less promising alternatives when several ideas are being evaluated. For the proposed methodology the goal of the market assessment is to provide essential market information to understand investment circumstances and potential market risks. Outcomes of a market assessment should support the investment decision-making process. In addition, the impacts of market uncertainties on project profitability should be evaluated in order to provide a comprehensive understanding of project scenarios. Furthermore, performing market assessment at early stages will stimulate the discussion between different areas across an organization (e.g., technical and sales departments) in specific topics identified as essential for the success of the project; this might trigger additional market assessment work resulting in better information at later steps for better screening.

A literature review was performed to identify factors to be evaluated in market assessment and is following presented.

7.3.1.1 Literature review

Assessment of market-related factors is a common activity of projects aiming product commercialization. Understanding market conditions helps to identify market scenarios, risks, and to plan upcoming project activities.

Table 7-5 illustrates common market aspects considered in the literature when bio-based product screening was performed, in addition to aspects evaluated for overall investment assessment. The aspects were divided in five categories: market size, market status and trends, status of the product in the market, competition, and market strategy. It is worth noting that market information is collected considering a product rather than a technology.

Table 7-5: Market aspects evaluated by different studies available in literature.

Category	Aspect	Comments	References
Size	Market volume (t/yr)	One study defined a minimum market size (200 kt/yr) [374]; other studies do not propose a cut-off	[12], [15], [26], [37], [374]–[376]
	Market value (USD/yr)		[15]
	Product market share	Share of a product in an application category	[12]
Status and Trends	Market growth		[12], [36], [37], [375], [376]
	Market stability		[36]
	Market saturation		[12]
	Market attractiveness, opportunities to develop the market	Aspects to be considered as market attractiveness are not defined [12]	[12], [376]
Status of product in market	Uniqueness of product to market		[36]
	Product novelty	Introduction of new products can be riskier than existing products	[15], [376]
	Product demand - cyclical or seasonal	Cyclical or seasonal demands are riskier than stable demands	[36]
	Product class (e.g., commodity, specialty)		[376]
	Product value compared to other product categories	e.g., bio-based chemicals with values higher than fuels are preferred	[12]
Competition	Competitive entries		[36]
	Direct competition with other products	e.g., products directly competing with natural gas were eliminated	[12]
	Market share	Of a specific organization for a product	[37], [376]
Organization strategy	Market pull / technology push		[371]
	Need of market development		[36]
	Capacity to fulfill product demand		[376]

Market volume is the most common aspect evaluated, followed by market growth. Market attractiveness, product novelty, and market share were also considered by some studies. It is clear that the most promising products are the ones that present larger market size, growing market trends, unsaturated markets, less competition, and enduring customer need. In addition, it was observed that overestimation of market size, overestimation of product price, and underestimation of competition are common causes for project failure (Table 7-4), so estimates and forecasts should be made with caution. Most of the studies do not define a clear criteria on how each market aspect is used to exclude or retain an alternative. It is not our intention to propose cut-off values for each aspect, since they may vary according to the organization and the products being studied. Nevertheless, it is not suggested to invest in products that have a decreasing or saturated markets when aiming for commercialization.

In addition to the factors commonly considered during market assessments, an investigation of tools available for market analyses was performed. Worksheets used for the Technology Entrepreneurship and Commercialization (TEC) coursework at NCSU[7] [377] (portfolio score, product attribute and market matrix (PAMM), market technology readiness, evaluation of market size, and functional assessment) as well as the new product profile chart proposed by Harris [35] and the constraint analysis proposed by Merrifield [37] were tested for case studies on CNC [121], CMNF[192], and ethanol from corn stover [99]. These tools are usually used by startups to evaluate the attractiveness of product attributes for different market segments, to define the commercial readiness of an opportunity, and to investigate market potential and market development needs. Ultimately, these are guides to understand and document the market landscape of a project. Although the tools evaluated provide significant information for market assessment, they can be cumbersome to execute at the early stages of a project. For this work, the most relevant market aspects were selected based on the literature review and causes of project failure, and a method is proposed to evaluate them.

7.3.1.2 Description of the proposed tool

A market assessment tool to be used at project early stages was developed. It contemplates five relevant aspects evaluated in previous assessments, which have also been

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[7] MBA 576 - Technology Evaluation and Commercialization Concepts and MBA 577 – High Technology Entrepreneurship.

identified as major sources for project failure. The format was inspired in the functional assessment tool from Markham's and the visual analysis proposed by Harris [359], [377]. The aspects comprise market size or volume, market growth, the need of market development, product competition, and the advantage of the product in the market or its uniqueness.

Each aspect is rated from one to five (Figure 7-3, left). The lower the rate, the lower is the classification of the aspect evaluated. A total market score is calculated by adding the rates for each aspect and dividing by the maximum rate (25). The closer the score is to one, the more promising is the project from a market perspective. A visualization of each rate is also available (Figure 7-3, right). The tool can be modified according to project particularities, by adding or removing the aspects to be evaluated.

7.3.1.3 Additional market assessment tools suggested

It is common to start an academic research for a given product without knowing the applications or the possible markets the product or technology can be applied. We suggest the analyst to use the Product Market Attribute Matrix (PAMM) when assessing possible markets for a product. This tool, proposed by Markham and Mugge (2015) [377], identifies the need of product attributes to different market segments. In the example provided in Figure 7-4, attribute 4 of the product is attractive to segment 2 of market A, segment 2 of market B, and segment 1 of market C, while attribute 1 is only attractive to segment 1 of market A. If one wants to minimize risks of market adoption, it would be recommended to select products which attributes are attractive to multiple markets and segments. This tool can be used to support the rating of aspect *E. Product advantage/uniqueness to the market*.

Market evaluation | XXX | Input values

#	Market aspects	Rating	Comments
A.	Market size ($/yr or ton/yr)	1	Less than 100 MUSD/yr, 13.8kt/yr for nanocellulose
B.	Market growth	4	Expected 22.1% CAGR (2015-2020) for nanocellulose
C.	Need of market development	3	Few applications available - customer education needed
D.	Product competition	2	CNC may displace existing products
E.	Product advantage / uniqueness	4	Renewable, nanoscale, high strength, etc.
Total score (0 - worst / 1 - best)		0.56	= sum of ratings / 25

Suggested rates

#A - Market size ($/yr or ton/yr)
1 Very small / Inexistent
2 Small
3 Medium
4 Large
5 Very large

#B - Market growth
1 Decreasing
2 Low growth
3 Average growth
4 High growth
5 Very high growth

#C - Need of market development
1 Extensive customer educational program
2 Significant customer education
3 Moderate customer resistance
4 Low customer resistance
5 Ready customer acceptance

#D - Competition with other products
1 Very high - pulverized market, several alternatives available
2 High - alternatives available
3 Moderate - some alternatives available
4 Low - very few competitors
5 Inexistent

#E - Product advantage / uniqueness
1 Very inferior
2 Inferior
3 Similar
4 Superior
5 Very supperior

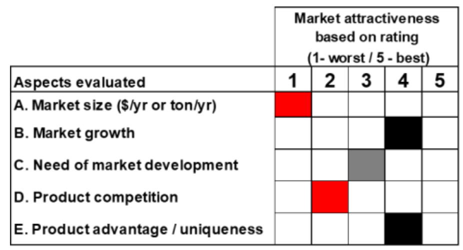

Figure 7-3: Proposed preliminary market assessment tool.

PAMM: Product Attribute and Market Matrix Worksheet						
	Market A		Market B		Market C	
	Seg 1	Seg 2	Seg 1	Seg 2	Seg 1	Seg 2
Attribute ✖						
Attribute 2		✖				
Attribute 3		✖				
Attribute 4	✖		✖	✖		
Attribute 5					✖	

Figure 7-4: Product Attribute Market Matrix (adapted from [377]).

7.3.2 Technical assessment

The proposed technical assessment is based on the Technology Readiness Level (TRL) assessment, which provides information on the technology status of the project and may serve as a screening factor in the initial stages of an investment.

Following, a brief explanation of the TRL concept is provided as well as the classification proposed for bio-based projects, and how the results of the initial assessment can be used for screening and/or evaluation purposes.

7.3.2.1 Technology Readiness Level (TRL) concept

The TRL concept was developed by the National Aeronautics and Space Administration (NASA) in the mid-70s. It aimed to support planning of space technologies, classifying the innovation stages according to the level of maturity, providing clear documentation and communication of different projects [378]–[380].

The definitions proposed by NASA were adapted for several purposes, such as drug development [381], research on geoscience and mineral resources [382], and chemical technology developments [379]. Institutions including the U.S. Department of Energy (DoE), the U.S. Department of Defense (DoD), and the European Association of Research and Technology Organization (EARTO), have adapted the TRL scale to fit their particular projects [357], [380], [383]. Usually, the technology readiness level is divided into nine stages, starting from basic principles observed (TRL 1) and ending at proven technology with successful operations (TRL 9). Differences among the adapted scales are related to the activities involved and the documentation needed for each step.

7.3.2.2 Description of the proposed tool

The proposed technical assessment consists of defining the TRL of the technology being profiled. This information can be used to identify the maturity level of a technology, as well as research and development needs in future steps. In addition, tools for profitability assessment and uncertainty on process information, capital investment, and operational cost estimates are provided according to the maturity level of the project. For instance, the lower the TRL of a given technology, the less information is available, and the higher is the uncertainty for estimated capital investment.

The proposed classification of TRL is based on the scale defined by Buchner *et* al. [379] (Table 7-6). Small modifications on the “description” and “tangible work results” were made in order to facilitate understanding, and common project activities were added to the framework.

The TRL is defined based on the *description* and *common project activities* exhibited in Table 7-6. If several projects are being evaluated at the same time and the resources to perform cash flow analysis for all of them are limited, the analyst may use the results from

TRL, market, and financial assessments to screen alternatives. Projects that are more risky on the technical side (TRL 1 or 2) may be discarded, as well as technologies that have already been proven and commercialized (e.g., TRL 8 and 9), which may suffer more competition and be riskier on the market side. The final criteria for decision-making is at the discretion of the analyst, considering the circumstances of each project.

Table 7-6: Technology readiness level (TRL) for bio-based projects, approaches and uncertainties (using information from [379]).

TRL classification	TRL 1	TRL 2	TRL 3	TRL 4	TRL 5	TRL 6	TRL 7	TRL 8	TRL 9
Subdivision	**Idea**	**Concept formulated**	**Proof of concept**	**Preliminary process development**	**Detail process development**	**Pilot trials**	**Final engineering**	**Commissioning**	**Production**
Description	Opportunities identified, basic research translated into possible applications (e.g., brainstorming, literature review)	Technology concept and/or application formulated, patent research conducted	Applied lab research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)	Concept validated in laboratory, scale-up, preparation started, conceptual process design (simulation based)	Shortcut process models found, simple property data analyzed, detailed simulation of process and pilot plant using bench scale information	Pilot plant constructed and operated with low rate production, products tested in application	Parameter and performance of pilot plant optimized, demo plant constructed and operating, equipment specification including components that are conferrable o full-scale production	Products and processes integrated in organizational structure (hardware and software), full scale plant constructed, startup initiated	Full-scale plant audited, turn-key plant, production operated over the full range of expected conditions in industrial scale, performance guarantee enforceable
Common project activities	- Preliminary research on technology (lit. review, discussion with experts) - Opportunities identified	- Formulation of technology concept - Formulation of R&D activities	- Initial laboratory research - "Black-box" mass balance	- Validation of concepts in laboratory - Scale up studies initiated - Block diagram - Mass balance	- Design of pilot facility - Preliminary process flowsheet - Mass balance - Advance in scale-up studies	- Pilot facility running - Process flowsheet - Mass balance based on pilot - Design of demonstration plant (if needed)	- Pilot facility optimized - Demonstration plant running - Design of industrial scale facility	- Start up and stable production	- Process optimization with existing asset - Strategy for market expansion
Tangible work result	- Idea - Rough concept - Vision - Strategy paper	- Technology concept formulated - List of solutions - Future R&D activities planned	Proof of concept (in laboratory)	Documentation of reproducible and predictable experiment results, first process ideas	Simple parameter and property data, process concept alternatives evaluated	Working pilot plant	Optimized pilot plant, working demo plant, sample production, finalized and qualified system and building plan	Finalized and qualified system and building plan	Full-scale plant tested and working
Workplace	Sheets of paper, whiteboard or similar	Sheets of paper, whiteboard or similar	Laboratory	Laboratory / miniplant	Laboratory / miniplant	Pilot plant, technical center	Pilot plant, technical center, demo plant (optional, potentially incorporated in production site)	Production site	Production site

7.3.3 Financial assessment

The financial assessment aims to investigate project feasibility from a financial standpoint considering little technical and economic information. This assessment is recommended before more time-consuming activities are performed, such as a detailed cash-flow analysis.

The financial assessment is based on the hierarchical decision procedure for chemical processes proposed by Douglas [384], [385]. The principle of the hierarchical decision procedure is to decompose the process synthesis problem into a hierarchy of process decisions including economic analysis in each hierarchy level.

The financial assessment hereby proposed considers that the manufacturing process is defined and major input and output flows are defined. Following, the Economic Potential at level 1 (EP1) is estimated as the difference between revenues and costs (Eq. 7-1). The economic potential can be estimated as dollars per year or dollars per quantity produced.

$$\text{EP1 (USD/yr or USD/t)} = \text{Product Value} + \text{Byproduct Value} - \text{Raw Material Costs} \qquad \text{(Eq. 7-1)}$$

It is known that product price estimation can be challenging, especially for new materials that do not have a defined market yet. In the *Supporting Tools* section (7.3.5), a tool to estimate product prices based on market size or type of material is proposed. These estimated prices can be used in the absence of more accurate information.

If the revenues are higher than raw materials costs, then the project is still promising. Utilities and labor costs are included to estimate the second level of the Economic Potential (EP2) (Eq. 7-2). Tools to estimate utilities and labor costs at early stage are provided in the *Supporting Tools* section (7.3.5).

$$EP2 = EP1 - labor\ costs - utility\ costs \qquad \text{(Eq. 7-2)}$$

If the EP2 is positive, annualized capital investment and maintenance costs are added to estimate EP3 (Eq. 7-3). Tools to estimate capital investment at early stages are also provided in the Supporting Tools section (7.3.5). The annualized capital investment is estimated using (Eq. 7-4).

$$EP3 = EP2 - \text{maintenance costs} - \text{annualized capital investment} \quad \text{(Eq. 7-3)}$$

$$Annualized\ capital\ investment = \frac{(Investment\ value * Discount\ rate)}{(1-(1+Discount\ rate)^{-\ Number\ of\ periods})} \quad \text{(Eq. 7-4)}$$

The suggested *discount rate* can be based on the cost of capital for a given industry. For instance, for the cellulose nanocrystals case study a discount rate of 16 % was considered, which is about twice the cost of capital for specialty chemicals (8.1 %) and paper/forest products (8.5 %) in 2019 [102]. The suggested *number of periods* is 10 years, value commonly used for straight-line depreciation schedules.

Sensitivity analysis is performed to verify the impact of changing process conditions, uncertainty in product prices, operating costs (raw materials, energy, and labor), and investment value in the EP. The suggested variation is ±25 % on each input. These analyses provide the decision-maker with information on the most important factors for the financials of a project before a significant amount of time is invested in cash flow and quantitative risk analysis.

7.3.4 Cash flow and quantitative risk analysis

The second step of the methodology consists of a cash-flow analysis followed by quantitative risk assessment.

To perform the cash-flow analysis the following information is needed:

- Production rate
- Raw material consumptions and respective costs (estimated in the financial analysis)
- Labor and energy costs (estimated in the financial analysis)
- Capital investment value (estimated in the financial analysis)
- Maintenance and property taxes costs (calculated as a percentage of the investment)
- Financial assumptions: inflation, discount rate, taxes on EBIT, depreciation schedule, working capital, terminal value, and financial evaluation horizon. Suggested values are in Table 7-7.

- Sales ramp up: it is assumed that, in the first three years of operation, 80 % of the production is sold. This can be changed, according to the project conditions and expectations in product adoption; this assumption will be further evaluated in the quantitative risk analysis.

Table 7-7: Suggested financial assumptions.

Financial assumption	Value	Reference
Inflation	1.2 % / yr	Average for U.S. between 2012 and 2015 [94]
Discount rate	16 %	Twice the cost of capital for specialty chemicals [102]
Taxes on EBIT	35 %	Considered for NREL reports; values for different sectors can be found at [100].
Depreciation schedule	10 years	Assumed
Working capital	10% of sales for next year	Assumed
Terminal value	4 – 5times EBIT in year 10	Assumed
Project evaluation horizon	10 years	Assumed

The cash flow analysis is used to estimate the manufacturing costs and the minimum product selling price. The minimum product selling price is the calculated price of the product to satisfy a project financial condition (e.g., NPV = 0 at a given discount rate). In addition, project financial metrics are estimated (NPV, IRR, and payback). Estimated product minimum selling prices are compared to product market prices, if available, or to possible product substitutes.

7.3.4.1 Quantitative risk analysis

Although the use of risk analysis does not reduce project risks, it allows the analyst to balance risks and opportunities effectively [375]. Execution of quantitative risk analysis is a relevant part of the proposed methodology. It consists in evaluate cash flow analysis outcomes (manufacturing costs and financial metrics) considering uncertainties in process, market, and financial inputs. Probabilistic analysis is performed to estimate the probability distribution of the outcomes and the chances of unwanted project outcomes (e.g., chances of NPV<0).

Uncertainties on process, financial, and market inputs are considered for the assessment. Inputs that most affect the project outcomes are selected to simplify the analysis. The sensitivity analysis performed in previous financial assessment provides information on the importance of each input. A brief explanation of common uncertainties considered for quantitative risk analysis is provided.

7.3.4.1.1 Process uncertainties

Process uncertainties are uncertainties related to the manufacturing process. They comprise mainly variations in reaction yields and efficiency in processing steps (e.g., separation, heating, cooling). These variations commonly impact the consumption of raw materials and utilities. Table 7-8 indicates the basis of process information and uncertainty estimation for different technology readiness levels. A decrease on process uncertainties is expected when projects advance to more mature technology levels.

Table 7-8: Basis of uncertainty estimation for different technology readiness levels.

TRL classification	**TRL 1**	**TRL 2**	**TRL 3**	**TRL 4**	**TRL 5**	**TRL 6**	**TRL 7**	**TRL 8**	**TRL 9**
Subdivision	**Idea**	**Concept formulated**	**Proof of concept**	**Preliminary process development**	**Detail process development**	**Pilot trials**	**Final engineering**	**Commissioning**	**Production**
Uncertainty on process information	N/A	Based on literature information (theorectical yields)	Based on laboratory data	Based on laboratory data	Based on pilot facility data	Based on pilot facility data	Based on demonstration facility data	Based on demonstration facility data / existing facility data	Based on existing facility data

7.3.4.1.2 Financial uncertainties

Financial uncertainties are related to the estimation of operating costs (labor and energy) and investment values. There are uncertainties associated with the accuracy of estimation methods and uncertainties associated with the project maturity. Uncertainties related to operating costs are related to the accuracy of the approaches selected for this methodology; values are detailed on section *7.3.5.3 - Estimation of operating costs at project early stages (S3)*. The uncertainty in capital investment values depends on the method used for the estimation and the technology maturity as well. Higher uncertainty in capital investment is expected for projects at lower maturity levels, due to unknown process details. Table 7-9 illustrates suggested capital investment estimation methods and the uncertainties to be considered according to the technology maturity level. The proposed table was constructed based on capital cost estimation practices and information on early-stage estimation methods [386]–[389]. More details on the methods and accuracies are found on section 7.3.5 - *Supporting tools*.

Table 7-9: Suggested capital investment estimation methods and uncertainty based on TRL.

TRL classification	**TRL 1**	**TRL 2**	**TRL 3**	**TRL 4**	**TRL 5**	**TRL 6**	**TRL 7**	**TRL 8**	**TRL 9**
Subdivision	**Idea**	**Concept formulated**	**Proof of concept**	**Preliminary process development**	**Detail process development**	**Pilot trials**	**Final engineering**	**Commissioning**	**Production**
Suggested CAPEX estimation methods and uncertainty	N/A	N/A	- Power law methods using literature information - Step-count equations (e.g. Bridgwater) - Uncertainty= ±100% - 70%	- Step-count methods (e.g., Taylor, Klumpar) - Uncertainty= ±70% - 60%	- Step-count methods (e.g., Taylor, Klumpar) - Uncertainty= ±60% - 50%	- Step-count methods (e.g., Taylor, Klumpar) - Uncertainty= ±50% - 40%	- Step-count methods, uncertainty (e.g., Taylor, Klumpar) = ±50% - 40% - Detailed CAPEX estimation using equipment costs if available, uncertainty < 30%	- Power law using information from existing plants, uncertainty= ±30% - 40% - Step-count methods, uncertainty= ±50% - 40% - Detailed CAPEX estimation using equipment costs if available, uncertainty < 30%	- Power law using information from existing plants, uncertainty= ±30% - 40% - Step-count methods, uncertainty= ±50% - 40% - Detailed CAPEX estimation using equipment costs if available, uncertainty < 30%

7.3.4.1.3 Market uncertainties

Market uncertainties are related to market circumstances that may influence the profitability of the project evaluated. Common market uncertainties include variations in prices paid for raw materials, utilities, and final products. Uncertainties related to prices are typically centered on historical values, assuming that past behavior is an indicative of the future [65], [390]. Sophisticated approaches to forecast prices use mathematical models to account for the expansion and decline of technologies in addition to supply and demand circumstances [390]; however, these are not in the scope of current work.

To identify additional uncertainties to be considered in the analysis an investigation on causes of project failure was performed (Table 7-4). Project failures that involve market and competition factors were evaluated. If i) customer requirements were not understood, ii) competitors were better established than expected, iii) product was similar to competitors, or iv) competitors lowered their prices, then it may be necessary to lower product prices to stay in the market. If the number of customers was overestimated, the market need was inexistent, or new competitors were introduced in the market, then sales volume might be reduced. In summary, market uncertainties can be translated into variation of product prices and product sales volume. The extent of these uncertainties varies from project to project and may be challenging to estimate even by market specialists. Nevertheless, their impact should be evaluated since the early stages of a project. For instance, estimating the chances of negative NPV for scenarios with reduced product price or reduced sales volume provide relevant information of market uncertainties impact. If no historical information on prices is available, variations of ±10 % to ±20 % can be used. The impact of selling 50 %, to 100 % of production in the first three years of operation can be also evaluated.

7.3.5 Additional assessment

The third and final step of the methodology consists in the qualitative evaluation of project aspects that were not included in previous assessments. The aspects evaluated were selected from previous studies on risk for the bio-based industry (chapters 5 and 6): subsidies, availability of feedstock, existence of distribution channels for feedstock and final products, safety concerns, and regulations impacts. The assessment is proposed in the form of a checklist so the analyst can acknowledge and evaluate if there are any significant risks before moving to the next project step.

The checklist template is presented in Figure 7-5 and can be modified according to project needs. It is known that more detailed investigation might be necessary to answer the checklist, and in some cases the questions are only valid if the facility location has been defined. Nevertheless, the checklist aims to point out to the analyst significant aspects for the investment that should be considered since the early stages of design.

Checklist - additional aspects to be evaluated	
A. Existence of subsidies and their impact in project profitability	
B. Availability of feedstock in facility location	
C. Availability of feedstock distribution channels	
D. Availability of final product distribution channels	
E. Specific regulations to be considered (e.g., use of genetic modified organisms - GMO)	
F. Safety concerns (related to product and/or process)	
G. Need of compliance to regulations for final product (e.g., pharmaceutical use)	

Figure 7-5: Additional assessment - checklist template.

7.3.6 Supporting tools

Perhaps the most complex and time-consuming tasks when evaluating a project is the collection of data to perform the assessment. Following a description of the proposed supporting tools to estimate product prices, operating costs and capital investment is provided.

7.3.6.1 Estimation of product prices (S1)

It is known that product pricing is essential information for assessing capital investment economics. Incorrect product pricing might result in approval of unprofitable projects or rejection of promising alternatives.

However, product prices are not always available. In the case of large volume bulk chemicals, usually identified by a specification [391], prices can be found on databases such as ICIS Chemical Business (www.icis.com), SRI Consulting (www.sriconsulting.com) and Chemical Market Associates Inc. (www.cmaiglobal.com) [392]. On the other hand, prices of specialty chemicals or novel materials are not commonly presented in databanks. Obtaining information from suppliers can take weeks and price information might not be shared if the inquiry is considered speculative [392].

Considering the accelerated market demand for new products and the challenges to obtain information, it is useful to have tools to easily estimate product prices at project early stages. Studies for developing new tools have been conducted since the 1950s and aimed at bulk chemicals given the expansion of the chemical and petrochemical industries in that time.

One of the first documented methods to estimate the price of a product was the *Exclusion charts*, developed by Zabel in 1956 [393]. Selling prices were estimated based on production volumes for each class of chemical product [394]. Later, Massey & Black (1969) proposed an empirical equation to predict future prices of materials, based on the historical cumulative market volume (= production volume x price) of a product [395]. Another study associated product price with its free energy of formation in addition to the production volume [396]. Although these methods are applied, an update considering current prices and volumes is necessary.

Hart & Sommerfeld (1997) developed a tool to estimate prices for chemicals produced in developmental or specialty quantities based on laboratory supply quotations, [397] using information of 24 chemicals. Likewise, Qi *et* al. (2015) estimated discount values for buying chemicals in bulk quantities. Lab and bulk-scale quotations for metal salts, organic compounds, and solvents were used as reference values [398]. However, low reliability on the results is observed for these two later studies, since little information was used to build the models.

With increased interest on bio-based products in late 2010s, information of prices and market volumes for several organic chemicals was collected by different authors [12], [26], [399], [400]. For the current methodology, we grouped and updated information on materials prices as a function of market size (Figure 7-6) using market reports[8] and literature information. Detailed information to build the graph is available on APPENDIX A: . Although not strong (R^2 = 44%), a relationship between market prices and market volumes is observed and can be used in the absence of more accurate data. A guidance according to the type of product according to market size and product prices is also provided through the colored circles. For example, commodity products have usually market volume higher than 1 million metric tons per year and prices varying between \$300 and \$1,300 / metric ton.

7.3.6.2 Estimation of capital investment at early stages (S2)

Invariably, most decisions to invest in a venture or to launch a new product involve capital investment. Capital investment is necessary to build a new facility or remodel an existing one. Capital investment is a relevant input for investment decision-making, given the significant sum of money that should be invested in a short period [401]. From our previous assessments, capital investment, together with raw material costs and final product price, is among the major cost drivers for projects in the bio-based industry [65].

Capital investment estimates can be classified in different ways, depending on the amount of information and resources available, as well as the accuracy on the estimate. Typical classifications are illustrated in Table 7-10. There is a trade-off between the level of accuracy required and the effort invested in the project. The higher the effort to prepare the

[8] https://www.ibisworld.com/industry-trends/

estimate, the more accurate it is expected to be. As the project advances toward later steps, more information is available for the design, and consequently the estimates are more detailed and accurate.

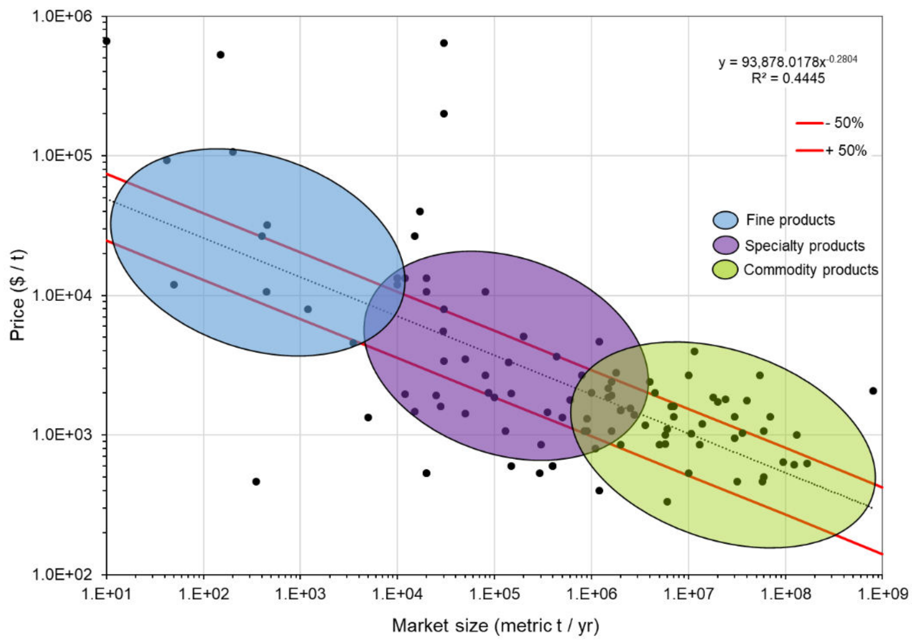

Figure 7-6: Estimation of existing product prices as a function of market size.

Traditional methods for capital investment estimation involve several tasks, such as flowsheeting, mass and energy balances, equipment sizing, and cost estimation [386]. Project activities are typically executed by a team involving engineers from different areas (such as process, mechanical, electrical, automation, and civil), and cost estimators, led by a project manager; the execution time can vary from one to several months, depending on the project complexity and the accuracy required for the estimate.

Estimations for screening or feasibility purposes (Class 5 / order of magnitude), herein called early-stage estimates, are of extreme importance. At the early stages, several ideas are available; however, time and monetary resources are scarce and those should be used for the most promising projects. The decision to proceed or not with a project should be performed as fast as possible, with reasonable and traceable information. Several methods have been proposed for estimating capital investment at early stages, and they can be divided into four main categories: i) the power law method, ii) factorial estimates, iii) estimations based on thermodynamics, and iv) step-counting methods [402], which are summarized in Table 7-11.

Table 7-10: Classification of cost estimates, accuracy and preparation effort necessary (based on Turton et al. (2018) [386], Christensen and Dysert (2011) [387], and Peters and Timmerhaus (2003) [145].

Purpose of the estimate [145], [386], [387]	**Design engineer-ing step**	**Accuracy of the estimate**		**Project maturity (as % of definition) [387]**	**Preparation effort [387] (as % of the TIC) [c]**
		AACE [387] [a,b]	**Peters and Timmerhaus [145]**		
Screening or feasibility	FEL 1	Class 5 L: -16 % to +24 % H: -80 % to +120 %	Order of magnitude over -30 % to +30 %	0 % - 2 %	0.015 % - 0.3 %
Concept study or feasibility	FEL 2	Class 4 L: -12% to +18 % H: -48 % to +72 %	Study -30 % to +30 %	1 % - 15 %	0.03 % - 1.2 %
Budget, authorizatio n or control	FEL 3	Class 3 L: -8 % to +12 % H: -24 % to +36 %	Preliminary -20 % to +20 %	10 % - 40 %	0.045 % - 3.0 %
Control or bid / tender		Class 2 L: -4 % to +6 % H: -12 % to +18 %	Definitive -10 % to +10 %	30 % - 75 %	0.075 % - 6.0 %
Check estimate or bid / tender		Class 1 -4 % to +6 %	Detailed -5% to + 5 %	65 % - 100 %	0.15 % - 30 %

[a] American Association of Cost Engineers International, recommended practices.
[b] L = low, H=high. Assuming that a class 1 estimate has an accuracy range between -4 % and +6 % (typical accuracy for a chemical plant detailed estimate) [386].
[c] Assuming that the effort to prepare a Class 5 estimate is between 0.015 % - 0.3 % of the total installed cost (TIC) of the facility – a typical value for chemical processing. [386]
[d] FEL stands for Front End Loading

In power law methodology, the capital investment for a facility is extrapolated from one scale to another [403]. To estimate the capital investment for a facility at a given capacity (facility A), the analyst needs an estimation for a similar facility at another capacity (facility B). The relation between the costs and capacities is given by an exponent, *e*, which is usually 0.6 (the well-known *six-tenths factor* rule). Exponent values are available for ordinary process facilities, such as commodity chemicals [404]–[406]. Nevertheless, applying the power law methodology may be restricted if existing capital investment information is not available, as it is the case for novel bio-based processes [402]. The power law is also applied to estimate the cost of a single equipment, based on quotations of similar equipment at different scale. Exponent values suggested for different equipment estimation, including common biorefinery equipment, are available on literature [402], [407].

Table 7-11: Summary of existing early stage capital investment estimation methods.

Method	Main characteristics	Advantages	Limitations
Power law	Relates the capital investment of facilities A and B [403]. $\frac{Investment\ A}{Investment\ B} = \left(\frac{Capacity\ A}{Capacity\ B}\right)^e$ e = exponent (generally = 0.6) $\frac{Capacity\ A}{Capacity\ B}$ (recommended ≤ 2)	Simple calculation Exponent values available in literature (for chemical facilities) [402], [407]	Relies on existing capital investment information Plants A and B must have similar processes and products
Factorial methods	Total investment cost (TIC) is a function of purchased equipment $TIC = Equipment\ cost\ * EF$ EF = equipment factor (also called Lang factor) [408]	Information on equipment cost is available in literature	Need preliminary equipment design and detailed process information Time-consuming
Thermodynamic methods	Correlates capital investment with the *energy lost in process* and the *free energy of formation*	Simple calculation No detailed flowsheet and equipment design needed	Not recommended for small-scale, heat neutral or batch processes
Step-counting methods	Correlates capital investment with *major process steps* and *process parameters*	No detailed flowsheet and equipment design needed Few process information necessary Simple calculation	Definition of process steps is not unanimous among the methods proposed

The factorial estimate considers that the total investment cost is proportional to the cost of purchased equipment. Typically, estimated accuracies range from - 30 % to + 50 % [408]. The relation between total cost and equipment cost is given by a multiplier, named *equipment factor*. One of the most common equipment factors is the so-called *Lang factor*, which varies from 3.1 for solid processing facilities to 4.7 for fluid processing facilities [408]. More detailed factorial estimates, common in concept or feasibility studies (or Class 4 estimates), use specific multipliers for each portion of the investment, such as equipment installation, piping, electrical, buildings, engineering, and contingency. The analyst selects the appropriate multiplier based on a range provided in literature and according to the level of complexity of the process [145], [406]. The total investment cost is the sum of the bare equipment cost multiplied by each one of the multipliers. Drawbacks of this methodology are the need for detailed process information for equipment design, in addition to cost estimates or quotations for the main equipment.

Thermodynamic-based models to estimate capital investment have also been proposed. These methods correlate capital investment with the free energy of formation of a chemical, the energy losses[9] in a process, or the heat duty of process steps [409], [410]. Good correlations (R^2 = 94 %) were found between facility investment and energy losses for fuels, power, and chemicals facilities; although they are not recommended for small-scale facilities, heat neutral, or batch processes [410].

Finally, step counting methods correlate capital investment with the number of process steps (also named functional units), production capacity, and main operating conditions (e.g., temperature, pressure, material of construction, residence times). Some methods claim reasonable levels of accuracy (± 25 % to ± 30 %) [404], [409]–[416], possibly due to the narrow ranges of capacities and limited segment of the process industry considered [417]; however, usual accuracies are between – 40 % to + 60 % [401]. An advantage of step count methods is that traditional flowsheeting and equipment design activities are not necessary [412]–[415]. A recent review of existing methods can be found elsewhere [402], and some examples are following discussed.

One of the first step-count methodologies was proposed by Zevnik & Buchanan (1963); correlating capital investment with plant capacity, number of functional units, material of construction, and maximum temperature and pressure for the process [412]. Taylor (1977) proposed a similar methodology, but aimed at more accuracy by using input information from each process step independently (throughput, residence time, temperature, pressure, and materials of construction) [413], [414]. The regression between the input information and capital investment estimate is based on data from 45 chemical facilities, with

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[9] Energy losses are defined as difference between the low heating values (LHV) of the streams entering a facility (including feed and fuel), and the product stream leaving the plant.

claimed precision of - 26 % / + 36 %. Bridgwater (1978) suggested equations for capital investment estimation for gas, liquids and/or solid processing facilities [415], [418]. The equations were derived from different processes, using as inputs the number of functional units and facility capacity; some equations include reactor conversion and maximum temperatures and pressures. Klumpar *et* al. (1983) defined a new equation for capital investment based on 20 plants, applicable to a broader range of capacities and including solid-processing facilities [417].

Similarly, the inputs considered are average throughput, number of process steps, maximum temperature and pressure in the facility. Also, an attempt to clarify the definition of *process steps* was performed. More recently, Petley developed a new set of equations for estimating capital investment [419]; using the same regression methods of previous studies; although based on a new set of data from 79 different chemical processing plants. An effort to include additional inputs such as workforce and reaction steps was not successful, resulting in approximately 30 % lower accuracy. Buchner *et* al. related early stage cost estimation methods with the Technology Readiness Level (TRL) of a given project [379].

Most of the existing methods were developed for process industries, including chemical, fuel, petrochemical, paper, sugar, food, metal refining, and power generation [402], [409], [410]. Bio-based processes have similarities with chemical and petrochemical industries; however, there is no methodology directed to these type of processes. The use of step count and thermodynamic estimation methods allow savings in time and resources, provide capital investment information using fewer inputs, can be easily updated when the project is modified, and consequently provide sufficient information to aid the decision-making process at early stages. Evidently, a lower accuracy for step-counting estimations is expected when compared to more traditional methods (power law and factorial estimate). However, the fewer process inputs that are used, the faster investment estimation can be performed, compared to traditional engineering design. I also contend that a trained process engineer can execute the methods in a matter of days to a few weeks.

Independently of the method selected, estimation of capital investment at early stages is challenging, due to lack of project definition and information available in such stages of a project. In many situations, the only information available is a simplified block diagram, with scarce process data, and few information on equipment configuration. The estimation accuracy will depend on the methodology used as well as the quality of input information available.

Considering specificities of bio-based processes and the need for early stage estimation methodologies for this segment, recent research has investigated existing early-stage methods for biorefinery processes. Step-counting and thermodynamic estimations were compared with more detailed methodologies (concept or budget estimations) for three liquid fuel facilities: ethanol from dry corn, biodiesel from soy oil, and ethanol from biomass gasification [388], [402]. Results showed that the accuracy of the estimation varies according to the process and capital cost estimation method. Overall, the methods proposed by Taylor [413] and Lange [410] have shown relatively accurate results, although the need for biorefinery-tailored methods aiming to improve accuracy is discussed [307], [402]. Few studies have used step-counting methods for early-stage capital estimation of the bio-based process. For instance, Torres (2016) used Taylor's methodology to estimate capital investment for bio-butanol and muconic acid facilities [307], although no comparison with detailed capital cost estimation was performed; similarly, Hermann *et* al. (2007) used a functional unit method to estimate capital investment for sugar to chemicals processes, but no detailed information on the methodology applied was provided [374].

For the proposed work, we believe the most suitable methodologies for early stage capital investment are the step-count and thermodynamic methods. The application of these methodologies is simple, does not need detailed flowsheets, and is relatively easy and less time-consuming than traditional capital investment methods. Although previous research showed some inaccuracy on estimations by existing methods, they provide relevant information for the screening process, can be executed relatively fast, and exempt the participation of an engineering team at this stage. In addition, the uncertainty of input values at the early stages of design may be substantial, relaxing the need for highly accurate estimations at this phase.

In the following parts of this chapter, we aim to elect few capital investment methods to be used as early stage capital estimation of bio-based projects. Existing step-count methodologies were applied for different bio-based processes including solid and liquid fuels, bio-nanomaterials, and chemicals. The results obtained were compared to more detailed capital investment estimates, such as factorial methods. It is worth noting that this study does not aim to propose a new method for capital investment estimation. We evaluate and discuss the alternatives available in literature, selecting the most suitable methods for the processes evaluated and making suggestions for further assessments. A limitation of the current analysis is that the reference investment values are estimates and not actual investment values, and there is uncertainty in those values too.

7.3.6.2.1 Processes selected

The following case studies were selected: i) cellulose nanocrystals (CNC) [121], cellulose micro-and nanofibrils (CMNFs) [192], wood pellets [420], and ethanol from corn stover [99]. The studies selected cover a variety of processes, technologies, and final products. All processes selected have detailed capital investment estimates, which was used as a reference value.

7.3.6.2.2 Early-stage capital estimates methods

The following step-count methods were tested: i) Taylor [413], ii) Bridgwater (different equations) [401], [421], iii) Klumpar [417], and iv) Petley [419]. The application of Zevnik and Buchanan (1963) method was ruled out since more updated methods were available and previous studies claimed high inaccuracy of the correlation [421]. The thermodynamic method was not evaluated due to the significant low thermal energy requirements of some bio-based processes selected (such as cellulose nanocrystals and cellulose micro- and nanofibrils). A summary of the equations selected, updated to 2016, is presented in Table 7-12. Details on the equation updates are found in APPENDIX C: Supplementary information - capital investment assessment tools.

Table 7-12: Summary of step-count and thermodynamic methodologies for early-stage cost estimation.

Method [Reference]	Total investment (USD, 2016)	Comments	Variables
Taylor [413]	$216.1\sum_{1}^{N}(1.3)^{CS}Q^{0.39}$	based on data from 45 chemical facilities	***N*** = # of functional units ***CS*** = complexity score
Bridgwater A [421]	$538.1N\left(\frac{Q}{s^{0.5}}\right)^{0.85}\left(\frac{T_{max}n}{N}\right)^{-0.17}\left(\frac{P_{max}n'}{N}\right)^{0.14}$	valid for liquid and solid-liquid processes, T and P above ambient based on 24 hydrometallurgical processes ISBL = 75% of investment	***Q*** = capacity ***s*** = process conversion $\boldsymbol{T_{max}}$ = maximum temperature
Bridgwater B [401]	$1092N\left(\frac{Q}{s}\right)^{0.675}$, Q/s > 60000 t/yr $95687N\left(\frac{Q}{s}\right)^{0.3}$, Q/s < 60000 t/yr	liquid and solid-liquid processes	$\boldsymbol{P_{max}}$ = maximum pressure
Bridgwater C [401]	$\left[2774547 + 9.01\left(\frac{Q}{s}\right)\right]N$	same set of data as equation B, but linear equation	***n*** = # of functional units operating at T greater than $T_{max}/2$
Bridgwater D [401]	$1333N\left(\frac{Q}{s}\right)^{0.665}e^{2.58\cdot10^{-7}Q}T_{max}{}^{-0.022}P_{max}{}^{-0.064}$	valid for Q/s> 60,000t/yr, using the same set of data as B ISBL = 75% of investment	***n'*** = # of functional units operating at P greater than $P_{max}/2$
Klumpar [417]	$ISBL = 3{,}283 * F_m * N * G^v$	based in 20 plants involving solids, liquids, and gases emphasis on extraction of natural resources (metal, minerals) ISBL = 75% of total investment	$\boldsymbol{F_m}$ = material of construction factor ***G*** = average throughput
Petley [419]	$85809Q^{0.44}N^{0.486}T_{max}^{0.038}P_{max}^{-0.02}F_m^{0.341}$	based on data from 79 chemical facilities	***v*** = exponent for Klumpar equation, can be 0.57 or calculated based on the number of process steps

7.3.6.2.3 Application of selected methods

To run the assessment, a block diagram and simplified mass balance were constructed for each process. Main flowrates, operating temperatures and pressures, residence times and materials of construction were also gathered from reference case studies. In a few circumstances, some process information was not available for the case studies, and typical process operating conditions were retrieved from literature. It is worth nothing that operating conditions can affect in the capital estimation only when they are significantly different from ambient circumstances.

Although the selected methodologies are relatively simple to apply, the challenge resides in the definition of N (number of significant process steps, functional units, or process modules, generally named as *functional unit* in this dissertation). The number of functional units contributes considerably to the capital investment calculation, and the selected step-counting methods have different approaches to account for them.

The concept of functional unit was initially defined by Wessel (1952), in his correlations to estimate operating labor hours [421], [422]. For capital investment estimation, Zevnik and Buchanan (1963) were among the first to use functional units [412]; they describe it as *all equipment necessary to carry out a single significant process function*. Some examples of functional units are provided, such as a reaction system and a distillation column with its peripherals. Bridgwater (1976) defines a functional unit as *any operation (unit operation or unit process) acting on the main process stream or any substantial side stream, including recycle streams*. Pumping, heat exchangers, storage, and multistage operations are ignored, with few exceptions listed [421]. For Taylor (1977), a functional unit *refers to the operation that is performed on the material flow and not to the equipment*; and a list of operations that should be considered as process steps is provided (e.g., reactions, storage, distillation, and drying) [413]. Klumpar *et* al. (1983) discusses the uncertainty that relies on the definition of process steps among different methods [417], and proposes eleven types of process steps based on the change of a major process parameter. Finally, Petley (1997) uses the Institution of Chemical Engineers (ICheme) and the Association of Cost Engineers (ACostE) definitions of functional unit: *a functional unit is a significant step in the process and includes all equipment and ancillaries necessary for operation of that unit*, which is very similar to the definition used by Zevnik and Bridgwater.

The application of the selected methods carefully considered specific definitions of functional units. Table 7-13 illustrates the number of process steps defined for each case study and method used. Flowsheets and details on the application of the methods are available in APPENDIX C: Supplementary information - capital investment assessment tools.

Following, the results and discussion on the application of each method are presented.

Table 7-13: Number of process steps defined for each case study, for the different methodologies used.

Case study → **Method ↓**	**Cellulose nanocrystals (CNC)**	**Cellulose micro- and nanofibrils**	**Wood pellets**	**Ethanol from corn stover**
Taylor [413]	29	6	9	42
Bridgwater A-D [401], [421]	17	2	7	26
Klumpar [417]	24	5	8	20
Petley [419]	17	2	7	26

7.3.6.2.4 Results and discussion

Table 7-14 illustrates the estimated capital investment for the selected processes, in 2016 dollars. For CNC and CMNF processes, it can be noticed that the estimates by Taylor [413] method have resulted in values very similar to the detailed estimates. The same is valid for ethanol from corn stover, although Bridgwater methods (B, C, and D) have shown deviations at the same order of magnitude. For the wood pellets facility, Taylor estimate was among the ones with lowest deviation from the detailed estimation values, even though the difference was considerably high (+ 91 %).

Overall, Taylor's estimates presented the most reliable results. The application of Bridgwater method [401], [421] yielded reasonable deviations from the reference values; estimates from equations B, C, and D have consistently shown smaller deviations than estimates using equation A, although they usually underestimate the capital investment value. Equation A was based on a set of 24 hydrometallurgical processes, while equations B-D were based on several liquid and solid-liquid processes (not specified by the author). Differently on what was experienced by Bridgwater [401], the use of a linear equation (equation C instead of B) did not significantly improve the accuracy of the estimate. Similarly, the addition of process information on the method (equation D - Bridgwater) resulted in accuracy improvement only for CMNF and wood pellets facilities. It was noticed that estimated investment values were typically lower when temperature and pressure information was considered (equation D vs. equations B and C). Capital investments calculated using Klumpar [417] equations have presented more pronounced deviations from reference estimates, especially for the case of non-fixed exponent (Klumpar B). It was noticed that the estimate by Klumpar equation is extremely dependent on the calculated exponent, which in turn relies on the definition of functional units'. Klumpar *et* al. (1983) is the only author that lists the 20 processes used for the development of step-counting equations; at least 15 processes selected involved mineral and metal extractions and handling, which may explain the low adaptability to bio-based processing. The application of equations proposed by Petley [419] resulted in deviations at the same order of magnitude of Bridgwater's estimates, except for ethanol from corn stover.

Table 7-14: Comparison between detailed estimate and step-counting estimates for selected case studies. Values are in 2016 million USD; the number between parentheses is the deviation between the step count and the reference estimate.

Process → **Method ↓**	**Cellulose nanocrystals (CNC)**	**Cellulose micro- and nanofibrils (CMNF)**	**Wood pellets**	**Ethanol from corn stover**
Reference	188 (ref. [121])	37.7 (ref. [192])	12.0 (ref. [420])	372.2 (ref.[99])
Taylor [413]	185.0 (-2%)	35.7 (- 5%)	23.0 (+ 92%)	409.8 (+10%)
Bridgwater (A) [421]	358.2 (+ 91%)	90.3 (+ 140%)	111.2 (+ 826%)	631.3 (+70%)
Brigwater (B) [401]	152.1 (- 19%)	21.7 (- 42%)	35.9 (+ 199%)	393.9 (+6%)
Bridgwater (C) [401]	146.6 (- 22%)	20.6 (- 45%)	41.0 (+ 242%)	375.6 (+ 1%)
Bridgwater (D) [401]	120.7 (- 36%)	33.7 (- 11%)	21.2 (+ 77%)	334.2 (- 10%)
Klumpar (A) [417]	287.4 (+ 53%)	44.1 (+ 17%)	36.1 (+ 201%)	632.5 (+ 70%)
Klumpar (B) [417]	913.8 (+ 386%)	455.0 (+ 1,107%)	12.6 (+ 5%)	6,546 (+ 1,659%)
Petley [419]	134.4 (- 29%)	73.3 (+ 94%)	44.1 (+ 268%)	159.9 (- 57%)

Special attention is given to deviations found for the wood pellets facility. Differently from other case studies, the estimate using Klumpar-B method have presented the lowest deviation from the detailed estimate. This might be due to the somehow similar processing of pellets when compared to mineral extraction, such as grinding, furnace operation, and solids handling. However, Klumpar estimations are not suitable for the majority of bio-based processes.

The methodology proposed by Taylor [413] has shown the most reliable estimates when compared to the other methods investigated. We would recommend the use of this methodology for early stage investment estimation. However, as noted by Buchner *et* al. (2018), the selection of a methodology depends on the information available, which is closely related to the progress of a technology [379], [389]. It is acknowledged that the method proposed by Taylor can be cumbersome to use depending on the information available (such as projects at TRL 3 or lower). In such cases, it is recommended to use equation Bridgwater-B; which has shown relatively satisfactory results for the case studies evaluated, based only on number of process steps, capacity and conversion rate. Obviously, if information on capital investment for similar facilities is available (such as the ones presented by several NREL reports[10]), the use of power law method with an exponent of 0.6 is recommended.

It is worth noting that independently of the method selected for capital investment estimation, uncertainty should be accounted. Based on the results previously presented, it is suggested to consider uncertainties between ± 50 % to ± 100 % on the estimated capital investment, and were detailed in Table 7-9. These uncertainties account for inaccuracies of the inputs, capital investment estimation methods, and potential process steps and information not taken into account during early stages of design.

7.3.6.3 Estimation of operating costs at project early stages (S3)

Similarly to capital investment estimation, different strategies to estimate operating costs at early stages have been proposed [418]. Methods for estimating operating costs follow a pattern similar to capital estimation, using simplified process information. Operating costs guidelines available in literature can be derived to equations dependent on four factors: raw material costs (R), operating labor costs (L), energy costs (E), and fixed investment values (I) (Eq. 7-5). Proposed values for the coefficients a, b, c, and d are presented in Table 7-15. Information on how to calculate each portion of the equation, and the application of existing equations to case studies will be detailed next.

$$Operating\ costs\ \left({}^{USD}/_{yr}\right)^{11} = a * \boldsymbol{R} + b * \boldsymbol{L} + c * \boldsymbol{E} + d * \boldsymbol{I} \qquad \text{(Eq. 7-5)}$$

[10] Available at https://www.nrel.gov/bioenergy/biochemical-conversion-techno-economic-analysis.html
[11] Depreciation and interest are excluded from the equations

Table 7-15 :Equations for operating costs estimation (adapted from Bridgwater, 1975 [418]).

Coefficient value → **Reference ↓**	**a (raw material)**	**b (operating labor)**	**c (energy)**	**d (fixed investment)**
Aries et al (A), 1955 [423]	1.03	2.33	1.03	0.103
Aries et al (B), 1955 [423]	1.00	3.55	1.00	0.21/ra §
Bridgwater, 1975 [418]	1.10	2.50	1.10	0.140
Clarke, 1951 [424]	1.00	2.30	1.00	0.100
Holland et al (A), 1974 [425]	1.03	2.59	1.03	0.093
Holland et al (B), 1974 [425]	1.00	2.25	1.00	0.090
Jellen, 1991 [406]	1.08	2.72	1.08	0.140
Wells, 1973 [426]	1.00	1.25	1.00	0.130
Peters & Timmerhaus, 2003 [145]	1.14	2.50	1.14	0.157

§ ra stands for annual production rate
R = raw materials costs, L = operating labor costs, E = energy costs, I = fixed investment value.
Depreciation and interest are excluded in all estimations

7.3.6.3.1 Estimation of raw materials costs (R)

It is known that raw materials are among the major components of manufacturing costs, accounting for 10 % to 80 % of costs for chemicals production [145], [427], [428]. Although no specific information on bio-based products was found in literature, previous assessments have shown that raw materials represent between 20 % and 80 % of operating costs [30], [121], [192], [429], which are similar to the ratios found for the chemical industry.

Estimation of costs associated with raw materials is performed through direct calculation, based on materials consumption and their respective individual cost (Eq. 7-6). Consumption of raw materials can be estimated from simplified mass balances or information on reaction yields. Information on the cost for each raw material may be more complex and challenging to obtain. Cost of commodities can be easily found on literature, although some materials and specialty chemical costs may not be readily available. This aspect has been reviewed in section 7.3.5.1. It is worth noting that at early stages of design, the information on major raw materials consumption should be known; however, the consumption of raw materials not related to the main production route (e.g., additives or chemicals consumed in small quantities) can be neglected without hurting the result significantly. However, if the information is known and available, its use is recommended for better accuracy.

$$Raw\ material\ costs\ (R) = \sum_0^i Mi * Ci \qquad \text{(Eq. 7-6)}$$

Where: R = total raw material cost (USD/yr)

Mi = consumption of raw material i (t/yr)

Ci = cost of raw material i (USD/t)

It can be noticed that the coefficients used for raw materials costs may be higher than unitary values (e.g., Peters and Timmerhaus' and Jellen's values for coefficient *a* in Table 7-15). These coefficients account for costs that are dependent on raw materials or total product costs, such as distribution and marketing, royalties, patents, and R&D.

7.3.6.3.2 Estimation of operating labor (L) and total labor costs

Operating labor cost is a direct expense consisting on the wages paid to employees whose efforts are related to product manufacturing [423]. Operating labor cost is a portion of the total labor cost, which includes labor expenses of management and administrative personnel. Maintenance labor is included in the operating costs related to the investment value (I), and will be further discussed. The contribution of operating labor cost to manufacturing cost may vary between 5 % to 25 %, depending on the automation level of a facility, as well as the process characteristics [145], [423]. Some references define that operating labor cost for liquid or gaseous processing at large-scale can account for 5 % to10 % of the manufacturing expense, increasing to 15 % to 25 % when considerable solid handling is involved [423]. Published techno-economic assessments of new bio-based facilities have estimated the contribution of total labor cost to manufacturing cost from as low as 1 % to about 28 % (Table 7-16).

Valuation of operating costs starts with the estimate of operating hours needed in a facility, then multiplying this value by hourly employee rates. Total labor cost is calculated by multiplying the operating labor costs by a factor that accounts for other employees not directly involved in production, such as engineers and managers, and will be further detailed.

Estimation of operating hours

There are very few sources in literature concerning the estimation of operating costs. Most of published data rely on the equation proposed by Wessel (1952, 1953), which correlates the number of operating labor hours with number of process steps, plant capacity, and automation level (Eq. 7-7) [145], [373], [422]. The correlation proposed in the 1950s is still used and referenced by relevant publications in the chemical engineering field [103], [105], [145], [391]. Similar sources also propose an estimation of number of personnel per processing step, depending on processing type (batch *vs.* continuous, fluids *vs.* solids processing) [430]

It is worth noting that the estimated number of hours is highly dependent on the number of process steps [422], which are defined differently from the capital estimation procedures. A processing step for operating cost estimation purposes is defined as a process zone that can be controlled by an operator. As an example from Wessel's work, the process to produce ethanol from molasses requires five process steps: yeast preparation, fermentation, beer distillation, aldehyde distillation, and final rectification [422]. Indeed, the number of process steps for estimating operating hours is commonly lower than the number defined for capital investment estimation.

Table 7-16: Labor cost estimation as a percentage of total manufacturing costs.

Product	Total manufacturing cost	Total labor cost	Total labor cost / total manufacturing cost	Ref.
Butanol	137 MUSD/yr	1.9 MUSD/yr	1.4%	[307]
Cellulose nanocrystals (CNC)	51.5 MUSD/yr	3.2 MUSD/yr*	6.2%	[121]
Cellulose micro- and nanofibrils (CMNF)	28.6 MUSD/yr	1.4 MUSD/yr*	4.9%	[192]
Ethanol (from corn stover)	83.5 MUSD/yr	4.2 MUSD/yr	5.0%	[99]
Ethanol (from wood biomass)	N/A	N/A	2.0%	[249]
Ethanol (from mixed hardwoods)	N/A	N/A	23.2%	[332]
Gasoline (from DME)	331.8 M€/yr	3.3 M€/yr	1.0%	[431]
Levulinic acid / pellets	N/A	N/A	5.0%	[432]
Liquid biofuel (gasification)	355.8 M€/yr	3.2 M€/yr	0.9%	[433]
Wood pellets	13.6 MUSD/yr	3.8 MUSD/yr	27.9%	[420]

DME stands for dimethyl ether / N/A = not available
*Overhead costs not included

$$L = K * N * Q^{-0.76} \qquad \text{(Eq. 7-7)}$$

Where: L = operating labor, (man-hours/ton of product)

N = number of processing steps

Q = plant capacity (ton/day)

K = constant = 23, for batch operations

= 17, for operations with average labor requirements

= 10 for well-instrumented continuous process operations

For the purpose of present work, Wessel's correlation was crosschecked with actual facility data and detailed estimates for bio-based facilities. Information from actual facilities was gathered using Fisher*Solve*™ database (plant capacity, number of operators, and flowsheets, which allowed estimation of the number of process steps). Evidence from nine facilities, including pulp, pulp & paper, linerboard, tissue, and newsprint processes located in

North and South America was collected. A benchmarking assessment using Fisher*Solve*™ was performed to ensure that the selected facilities represent an average production cost among similar plants. Unfortunately, no public information on actual production costs was found for other bio-based facilities.

Also, data from detailed case studies published in literature was collected. Care was taken to make sure the case studies were not using Wessel's correlation to estimate operating labor hours, which would invalidate the analysis. Most of the case studies estimated the number of operators needed in each process area. The remaining studies used recommended number of operators per process area from sources different than Wessel [430].

The comparison presented in Figure 7-7 shows that, except for newsprint and one pulp facility evaluated, data from actual plants fit within the range of operating hours recommended by Wessel (1952, 1953). The average discrepancy from the curves is 25 %. It was expected that facilities producing only pulp would present reduced number of operating hours per process step when compared to more labor-intensive plants, such as tissue and linerboard. A possible reason for the divergence may be related to the geographic location of the mills. Plants that produce only pulp are located in South America while other facilities evaluated are in North America; higher labor costs in North America may lead to leaner organizations in this location. Another reason might be the age and technology of the facility, which can also affect the number of hours required.

The case studies evaluated presented consistent lower operating hours per processing steps than actual facilities. In some cases, including reports elaborated by U.S. National Laboratories, the number of estimated operating hours can be 2 to 3 times lower than the minimum values suggested by Wessel (1952). The discrepancy between information from actual pulp and paper mills and bio-based case studies might be due to more optimistic estimations of labor costs before operations, or even conscious consideration that a lower amount of labor is necessary for some of these facilities. Unfortunately, no actual information on other bio-based facilities was found to confirm the estimated values.

Limitations of the analysis previously described include the subjective estimation of process steps based on information provided on Fisher*Solve*™ database and the unavailability of actual data of other bio-based plants for a more comprehensive comparison. Ultimately, considering the information available for actual operating facilities and the limitations exposed, the use of Wessel's equation is recommended for early-stage operating labor estimation. It is foreseen that most of the facilities will fit into the curve C – large equipment, highly automated, or fluids processing only.

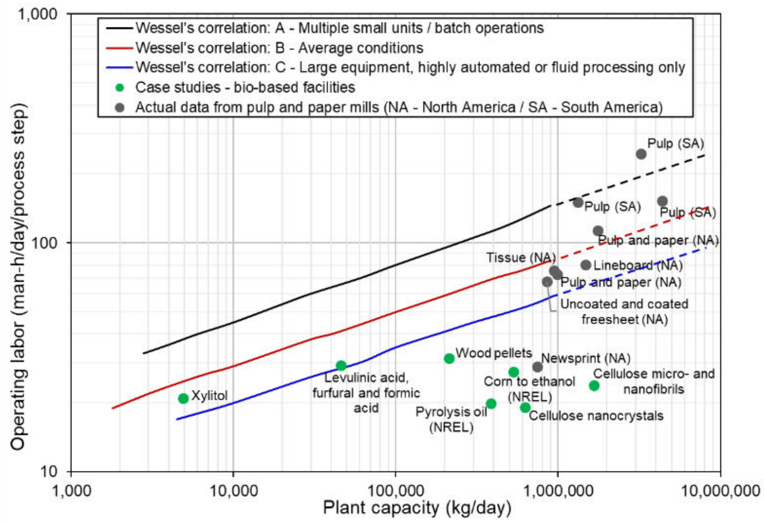

Figure 7-7: Comparison of estimated operating costs between Wessel's correlation, real pulp and paper data, and case studies for bio-based facilities.

Estimation of total labor costs

Cost estimation models previously presented (Table 7-15) have shown that the total labor cost (L_T) is on average 2.4 times the operational labor cost, with values varying between 1.25 and 3.55. In order to verify this ratio, information from actual pulp and paper mills was used (annual spend with operators and total labor retrieved from Fisher*Solve*™ database, for the 4th quartile of 2017, excluding maintenance labor). Data from 311 pulp and paper mills in North America, representing 99 different organizations, showed that the total labor cost is between 1.5 and 2.9 times the operational labor cost, with an average value of 2.0 and a standard deviation of 13% (Figure 7-8). About three-fourths of the mills have an average factor between 1.7 and 2.3. Although estimated coefficients from existing pulp and paper mills are around 20 % lower than recommended coefficients in literature, they are still reasonable for an early stage labor cost estimation. The recommended multiplier to estimate total labor from operating labor is 2.0, with uncertainty on total labor cost of ± 25 %.

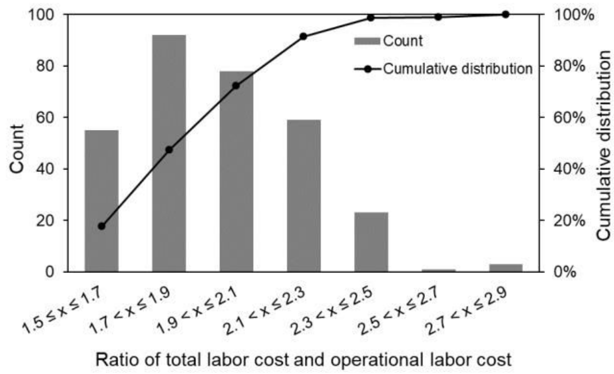

Figure 7-8: Distribution of ratio between total labor cost and operating labor cost for pulp and paper mills in U.S.

7.3.6.3.3 Estimation of energy costs (E)

Energy costs, also named utility costs, comprise materials necessary to maintain the conditions of a manufacturing unit. Steam, electricity, refrigeration, natural gas, fuel oil, and compressed air are examples of energy cost components. Energy costs can vary widely depending on energy source, type of process, and facility location [145], [373]. For general chemical processing, utility costs account for 10 % to 20 % of total product cost [145].

The energy consumption of a process can be calculated from material and energy balances. However, in the early stages of a project, when less detailed information is available, the estimation of energy consumption may not be straightforward. Previous studies have proposed a correlation to estimate energy costs based on investment, plant capacity, and number of functional units based on data from 39 processes [373]. This correlation was tested for four case studies (CNC, CMNF, corn-to-ethanol, and wood pellets); the results highly overestimated the energy requirement for all the facilities by more than two times; which makes this method unlikely to be used.

Considering that, a literature search on the shares of energy costs over total operating costs was done for different types of industry. Data from the US Census Bureau and reports from the European Union were used as sources of information [434], [435], and the data is presented in Figure 7-9. It can be noticed that the energy shares vary between 0 % and 27.3 % of the costs, depending on the process studied. On average, the energy consumption is around 5.4 %. Industries similar bio-based facilities, such as pulp and paper, have their energy shares between 2.5 % and 14.3 %; basic chemicals and sugar manufacturing presented similar ranges. The industries that present higher energy shares are cement and concrete, and fertilizers and pesticides, which usually deal with inorganic materials. The following recommendations are given for estimating energy costs, based on the information collected.

- If the energy balance is available, calculate energy costs using energy cost information from recognized institutions (such as the U.S. Energy Information Administration - www.eia.gov).
- If the energy balance is not available, estimate the energy cost as a percentage of the raw materials and labor cost. Based on the previous discussion, values of 5 % to 10 % are recommended for low energy consumption processes, and values between 10 % and 15 % of raw materials and labor cost are recommended for medium to high-energy consumption processes.

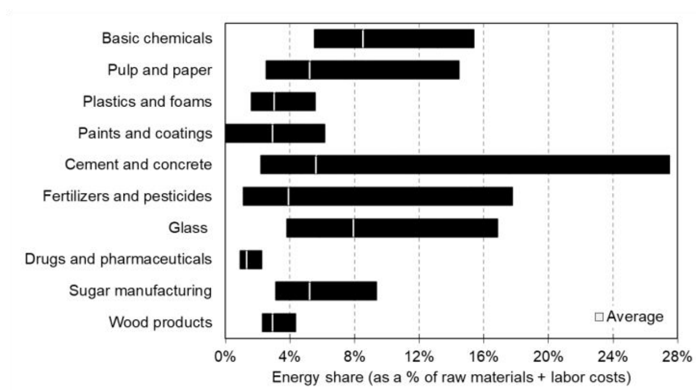

Figure 7-9: Share of energy cost in total production costs for different industry segments. (Based on [434], [435]).

7.3.6.3.4 Estimation of costs related to fixed investment value (I)

The estimation of the fixed investment at projects early stages has been discussed on section 7.3.5.2. Some operational costs depend on the investment value, such as maintenance, property taxes, and insurance. Maintenance costs involve materials and labor are usually between 2 % and 10 % of the investment value [145], [425], [426]. Property taxes and insurance vary between 2 % and 5 % of the investment value [145], [406], [423]–[425]. Suggested values are 6 % to account for maintenance costs and 4 % to account for property taxes and insurance with respect to investment value.

7.4 Application of the proposed guideline to case studies

7.4.1 Selected case studies

The selected case studies to validate the methodology are: cellulose nanocrystals (CNC), cellulose micro- and nanofibrils (CMNF), lignin micro- and nanoparticles (LMNP), and wood pellets [121], [192], [420], [429]. These case studies were previously studied in detail and can be easily compared to the proposed method in terms of time for execution and results obtained. A brief description of each process and the information used to run the proposed method is following presented.

7.4.1.1 Case study 1: Cellulose nanocrystals (CNC)

CNC manufacturing in a greenfield facility including acid recovery was selected as case study (Chapter 2) [121]. The facility capacity was defined as 50 t/day of CNC (dry equivalent), and the final product is sold at 8 % solids concentration (in weight). Process information was collected from the pilot plant facility from USDA, Forest Products Laboratory, in Madison, WI. The simplified block diagram with process conditions needed to perform the proposed methodology is illustrated in Figure 7-10. Dissolving pulp is shredded and fed to the reactor where it reacts with sulfuric acid at 64 % concentration (in weight). The sulfuric acid dissolves the amorphous regions of cellulose, forming sugars and exposing the crystalline part. The reaction is stopped by a quench of water, followed by washing and decantation to separate the acid and sugars from the final product. The washed product is decanted to increase solids concentration and filtered to remove unwanted particles (chars formed in the reaction). Finally, the product passes through a diafiltration step to remove remaining salts and then is concentrated to 8 % solids (in weight). The acid solution from the decanters is sent to an acid-sugar separation step. The acid is then concentrated to 64 % (in weight) and recycled to the reaction phase. The remaining acids in the sugar solution are neutralized with lime, forming gypsum. The effluents generated have their pH adjusted before sent to the waste water treatment (WWT) and a reverse osmosis system is used to polish the water from concentration step.

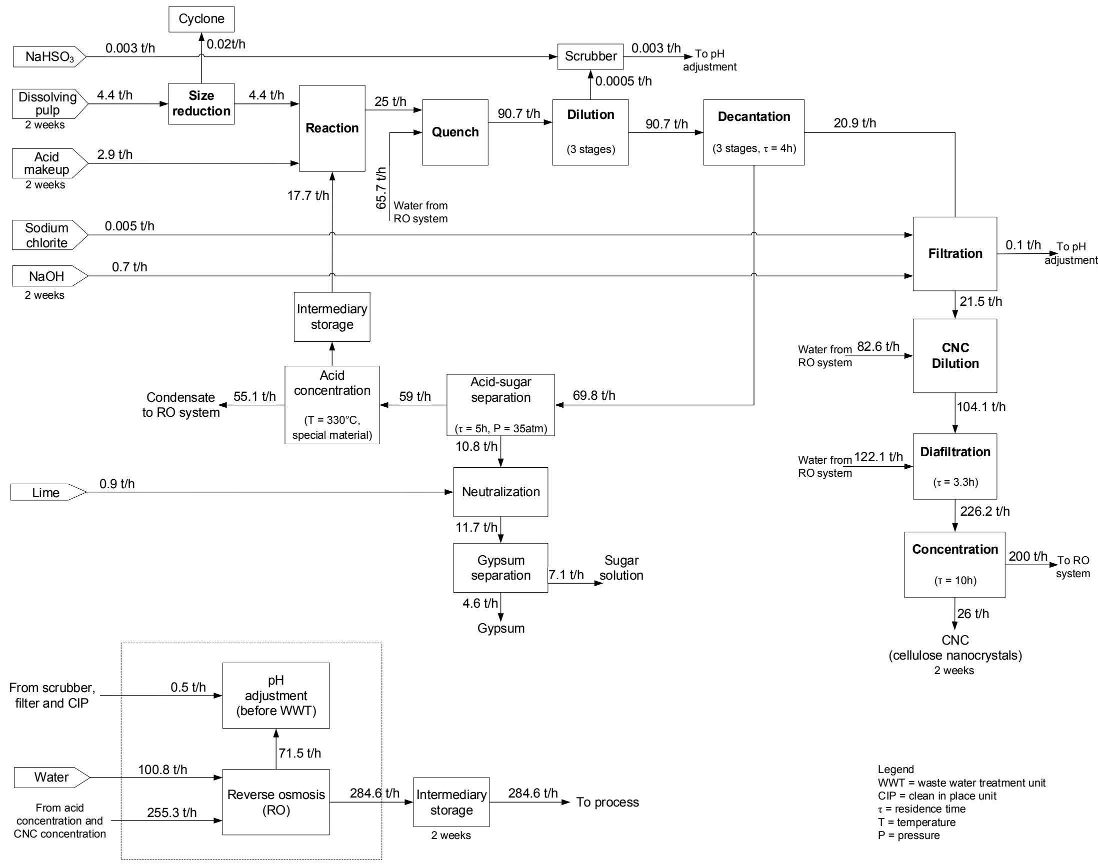

Figure 7-10: Cellulose nanocrystals production process. (If no process information is available, it means that: residence time (τ) ≤ 3h, temperature (T) is between 20°C and 500°C, Pressure (P) is between 1 and 10 atm, and storage time ≤ 1 week).

7.4.1.2 Case study 2: Cellulose micro- and nanofibrils (CMNF)

The greenfield scenario for producing cellulose micro- and nanofibrils, discussed in Chapter 3, is used for the analysis [192]. The facility capacity was defined as 50 t CMNF/d (dry equivalent), and process information from the pilot facility at the University of Maine is used as reference. A simplified block diagram of the process is presented in Figure 7-11. Market pulp is mixed with water to form a 3 % solids suspension (in weight). This suspension is refined until cellulose micro- and nanofibrils are obtained. The final product is the cellulose micro- and nanofibrils at 3 % solids concentration.

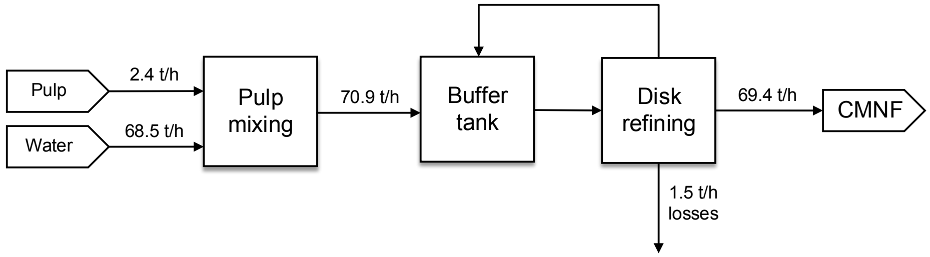

Figure 7-11: Cellulose micro- and nanofibrils (CMNF) production process (If no process information is available, it means that: residence time (τ) ≤ 3h, temperature (T) is between 20°C and 500°C, Pressure (P) is between 1 and 10 atm, and storage time ≤ 1 week).

7.4.1.3 Case study 3: Lignin micro- and nanoparticles (LMNP)

The scenario using kraft lignin and dimethylformamide (DMF) discussed in Chapter 4 is was selected to apply the proposed method [429]. Information from laboratory studies in Aalto University, Finland, is used as reference. The facility capacity is defined as 150 t LMNP/d. Kraft lignin is dissolved in DMF and then send to an atomizer to be dried with air, generating the micro- and nanoparticles. The solid material is separated from the gas phase, which contains air and the evaporated solvent. The solvent is recovered by condensation and recycled to the dissolution step. The dried particles are the final product.

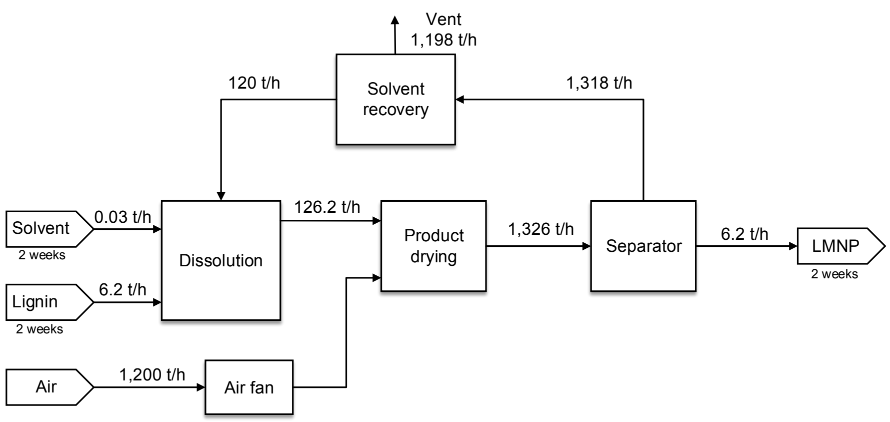

Figure 7-12: Lignin micro- and nanoparticles production process (If no process information is available, it means that: residence time (τ) ≤ 3h, temperature (T) is between 20°C and 500°C, Pressure (P) is between 1 and 10 atm, and storage time ≤ 1 week).

7.4.1.4 Case study 4: Wood pellets

Figure 7-13 illustrates the process and mass balance for wood pellets production. The case study selected is based on the techno-economic assessment of a 75,000 t of pellets / yr facility, performed by Pirraglia *et* al. (2010) [420]. The process consists of handling the initial biomass (at 55 % moisture content) by transporting it to the dryer. Water is removed in dryers until biomass reaches 4 % moisture content to facilitate grinding. The grinded biomass is conditioned by adding a controlled amount of steam, which softens the feed and partially gelatinizes the starch to create more durable pellets [436]. The conditioned biomass is pelletized, cooled down, and screened to remove fines before the final product is packaged. According to the literature [436], [437], the maximum operating temperature in the system was defined as 150°C for drying, conditioning and pelletizing process steps; the pressure in the pelletizing system can be as high as 3,000 atm [436], [437].

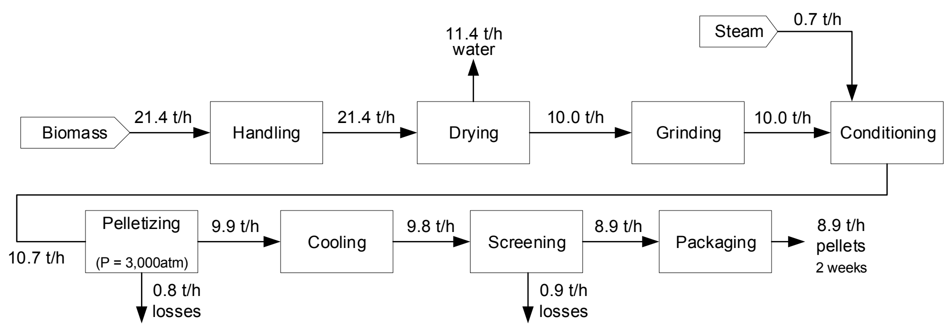

Figure 7-13: Process to manufacture wood pellets, based on Pirraglia *et* al. (2010) [420]. (If no process information is available, it means that: residence time (τ) $\leq$ 3h, temperature (T) is between 20°C and 500°C, Pressure (P) is between 1 and 10 atm, and storage time $\leq$ 1 week).

7.5 Proposed method application

The proposed method detailed in section 7.3 was applied to the four case studies. Figure 7-14 summarizes the steps performed, the inputs used, and the outputs obtained from the method application.

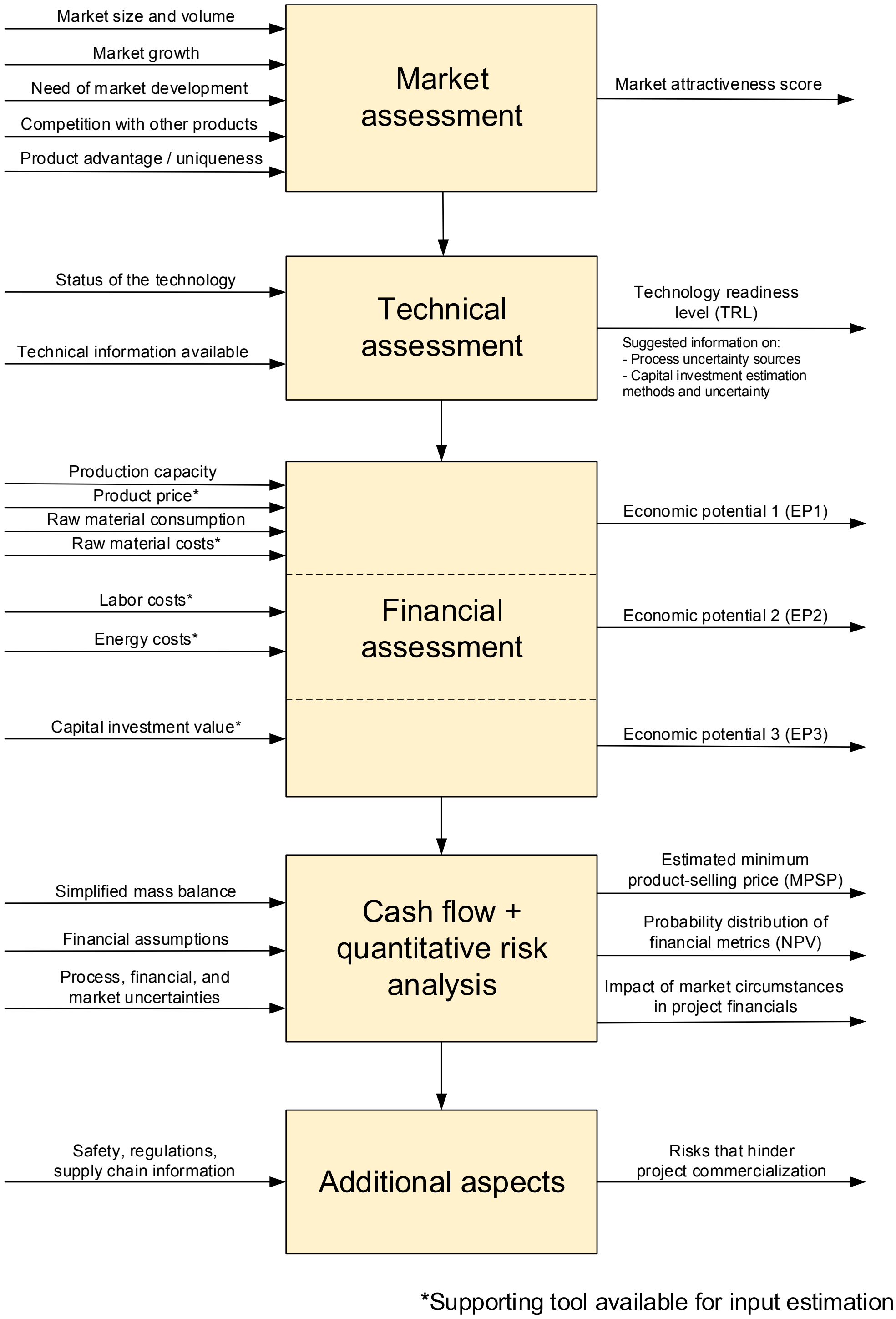

Figure 7-14: Summary of proposed method steps, inputs necessary, and outputs obtained.

7.6 Results and discussion

7.6.1 Market assessment

Market assessment was performed for all four case studies, using information from literature and from market reports [16], [53], [58], [438], [439]. It is worth noting that when multiple projects are evaluated in parallel the scores conferred should relative to one another in order to facilitate the assessment. Results from market assessment are presented on Figure 7-15. Detailed information on the assessment execution is available in APPENDIX D: Detailed information on proposed method application to case studies.

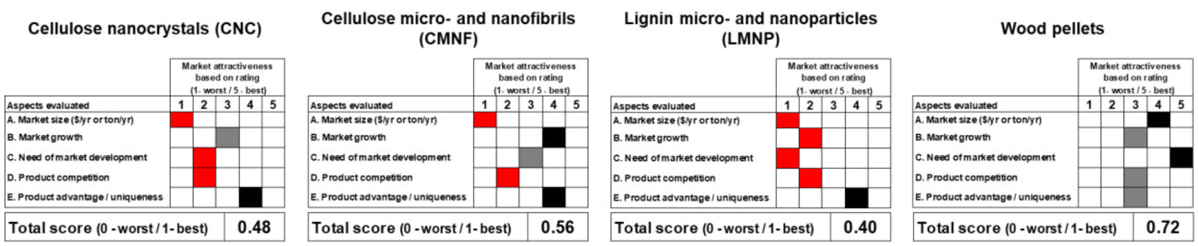

Figure 7-15: Market assessment results for the four case studies.

Market attractiveness scores are higher for wood pellets than other case studies. Wood pellets have an established market that is expected to growth and consequently need less market development efforts. Among the bio-based nanomaterials, CMNF presents better market perspectives due to expected market growth and lower need of market development (there are reported cases of industrial applications). The three bio-based nanomaterials have very small or inexistent market sizes and superior product advantages when compared to the wood pellets project; nevertheless, considering all the aspects evaluated the wood pellets are still more promising from a market standpoint.

7.6.2 Technical assessment

Results of technical assessment are presented in Figure 7-16. CNC and CMNF processes are classified as TRL 6 – *Pilot trials*. For both technologies, pilot plant facilities are available, along with simplified process diagrams and mass balances [53]. The LMNP technology was classified as TRL 4 – *Preliminary process development*, given that the production concepts were validated in laboratory and the scaling up studies were initiated [168], [172]. The wood pellets technology was defined as TRL 9 - *Production*, since the technology is validated and several commercial scale facilities are already in operation [16], [420].

				LMNP		CNC CMNF			Wood pellets
TRL classification	**TRL 1**	**TRL 2**	**TRL 3**	**TRL 4**	**TRL 5**	**TRL 6**	**TRL 7**	**TRL 8**	**TRL 9**
Subdivision	**Idea**	**Concept formulated**	**Proof of concept**	**Preliminary process development**	**Detail process development**	**Pilot trials**	**Final engineering**	**Commissioning**	**Production**
Description	Opportunities identified, basic research translated into possible applications (e.g., brainstorming, literature review)	Technology concept and/or application formulated, patent research conducted	Applied lab research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)	Concept validated in laboratory, scale-up, preparation started, conceptual process design (simulation based)	Shortcut process models found, simple property data analyzed, detailed simulation of process and pilot plant using bench scale information	Pilot plant constructed and operated with low rate production, products tested in application	Parameter and performance of pilot plant optimized, demo plant constructed and operating, equipment specification including components that are conferrable o full-scale production	Products and processes integrated in organizational structure (hardware and software), full scale plant constructed, startup initiated	Full-scale plant audited, turn-key plant, production operated over the full range of expected conditions in industrial scale, performance guarantee enforceable
Common project activities	- Preliminary research on technology (lit. review, discussion with experts) - Opportunities identified	- Formulation of technology concept - Formulation of R&D activities	- Initial laboratory research - "Black-box" mass balance	- Validation of concepts in laboratory - Scale up studies initiated - Block diagram - Mass balance	- Design of pilot facility - Preliminary process flowsheet - Mass balance - Advance in scale-up studies	- Pilot facility running - Process flowsheet - Mass balance based on pilot - Design of demonstration plant (if needed)	- Pilot facility optimized - Demonstration plant running - Design of industrial scale facility	- Start up and stable production	- Process optimization with existing asset - Strategy for market expansion
Tangible work result	- Idea - Rough concept - Vision - Strategy paper	- Technology concept formulated - List of solutions - Future R&D activities planned	Proof of concept (in laboratory)	Documentation of reproducible and predictable experiment results, first process ideas	Simple parameter and property data, process concept alternatives evaluated	Working pilot plant	Optimized pilot plant, working demo plant, sample production, finalized and qualified system and building plan	Finalized and qualified system and building plan	Full-scale plant tested and working
Workplace	Sheets of paper, whiteboard or similar	Sheets of paper, whiteboard or similar	Laboratory	Laboratory / miniplant	Laboratory / miniplant	Pilot plant, technical center	Pilot plant, technical center, demo plant (optional, potentially incorporated in production site)	Production site	Production site

Figure 7-16: Technical assessment results for the four case studies.

7.6.3 Financial assessment

The proposed financial assessment was conducted for the four case studies selected. For the three bio-based nanomaterials no information on market price is available. Using the supporting tool described in section 7.3.5.1 and Figure 7-6, product price values between USD 2,000/t to USD 9,000/t were defined for the assessment. These ranges of values consider that these materials will be used as specialty products. For the wood pellets, the values found in the reference for internal U.S. market were used (USD 276 / metric ton) [420]. The economic potential (EP) values in USD/yr and USD/t of product are illustrated in Table 7-17.

Table 7-17: Financial assessment results for the four case studies.

Case study		CNC [a]	CMNF [a]	LMNP [a]	Wood pellets
EP1	MUSD/yr	1.3 – 116	14.4 – 133	91.1 – 457	15.6
	USD/t	81 – 7,081	845 – 7,586	1,743 – 8,743	208
EP2	MUSD/yr	-8.2 – 107	10.0 – 129	87 – 453	9.7
	USD/t	-501 – 6,499	586 – 7,586	1,668 – 8,668	130
EP3	MUSD/yr	-57 – 57	0.4 – 119	49 – 415	9.5
	USD/t	-3,508 – 3,492	25.9 – 7,026	945 – 7,945	47

[a] The EP values are presented as ranges because product prices of USD 2,000 / t and USD 9,000 / t were considered for the assessment.

The values of EP decreased as the level of detail increases (from EP1 to EP3), as expected. Estimated EP for the three bio-based nanomaterials varied widely due to the broad range of prices considered. EP values for CMNF, LMNP, and wood pellets are always positive independent of the product price considered, while EP2 and EP3 are negative if CNC is priced at USD 2,000 / t, indicating no financial feasibility for CNC production if lower prices are practiced. EP3 values for LMNP are usually higher than CMNF for a similar price level, and are higher than the wood pellets case study.

Sensitivity analysis of EP values was performed considering variation of ± 25 % in inputs (Figure 7-17, Figure 7-18, Figure 7-19, and Figure 7-20). LMNP case study is the most robust project in financial aspects, followed by wood pellets and CMNF. For most case studies, variations in revenue values presented the highest impact on EP values, indicating the relevance of price variation when assessing project financial feasibility.

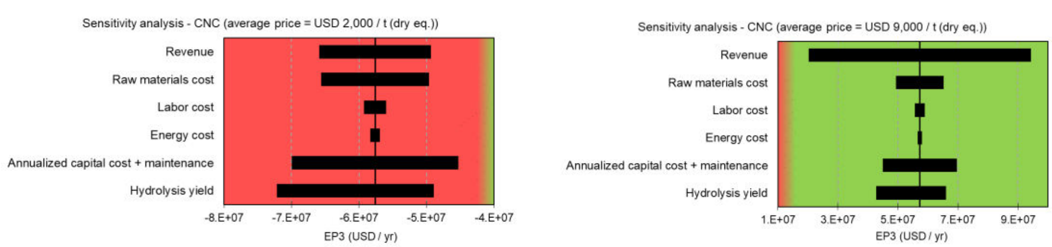

Figure 7-17: Sensitivity analysis results for the CNC case study.

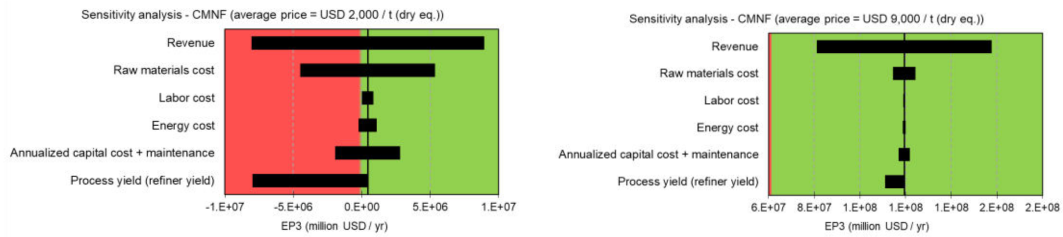

Figure 7-18: Sensitivity analysis results for the CMNF case study.

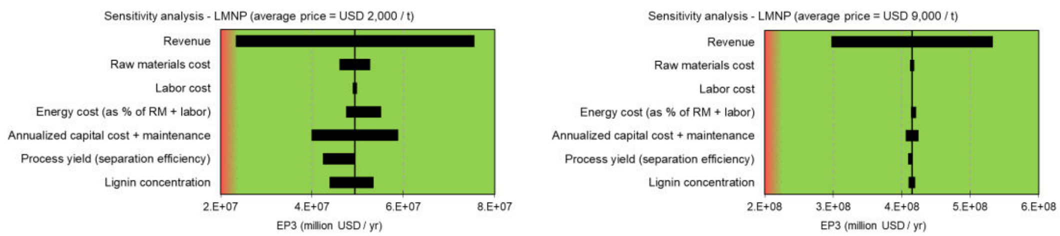

Figure 7-19: Sensitivity analysis results for the LMNP case study.

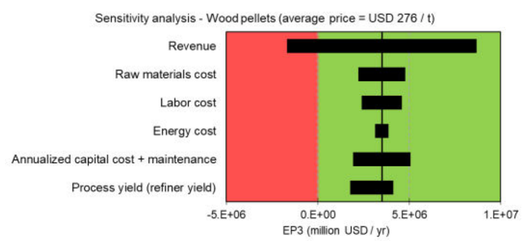

Figure 7-20: Sensitivity analysis results for the wood pellets case study.

7.6.4 Project screening after the first step of assessments

The first step assessments (market, technical, and financial) provide relevant information to screen out less promising projects if an alternative need to be selected to advance to subsequent steps. Results from the assessment of the four case studies showed that the wood pellets project is more attractive from a market perspective since the market is already established and reasonable growth is expected in the coming years. In addition, the pelletizing technology is mature, with several facilities operating at an industrial scale. The estimated economic potential for the wood pellets project is promising, although it can be potentially lower than the values found for LMNP and CMNF depending on their market price. For an investor aiming to build a new facility, we would recommend to advance with the wood pellets studies since the risks associated are smaller. A research institute would rather prefer to focus their efforts in the CMNF project, which is promising from the financial perspective, has a technology that is still under development toward industrialization, and has a somewhat promising market assessment. The LMNP is recommended as a second option for a research institute given the lower market attractiveness of the material; nevertheless, the final decision is at the discretion of the analyst and depends on the organization circumstances. The CNC project can be considered the less promising among the four studied since it presents higher chances of negative economic potential values for the prices considered.

7.6.5 Cash flow and quantitative risk analysis

Cash flow and quantitative risk analysis were performed for the four case studies. Inputs collected and estimated in previous project steps are used to perform the cash flow assessment, in addition to the financial assumptions suggested in Table 7-7. The minimum product selling price was estimated to satisfy NPV = 0 in all assessments. A comparison between the values estimated using the proposed methodology and the ones estimated in the detailed techno-economic assessments is presented in Table 7-18. Estimated values are very similar, mainly due to small discrepancies in estimations of raw material costs and capital investment values.

The composition of estimated manufacturing costs was evaluated for the four case studies as well. The comparison for CMNF results is illustrated in Figure 7-21. Similar conclusions can be drawn from the early stage and detailed assessments; major contributors to manufacturing costs are pulp, utilities and depreciation. The early-stage cash flow analysis presented similar results to the detailed assessment for the three other case studies. Utility costs were underestimated for LMNP and wood pellets facilities. Results are illustrated in APPENDIX D: Detailed information on proposed method application to case studies.

Table 7-18: Minimum product selling prices estimated using the proposed methodology (early stage assessment) and detailed case studies.

Case study	Estimated minimum product selling price (USD/t)		
	Early stage assessment	Detailed assessment	Difference
CNC	6,843	6,070	+ 13 %
CMNF[a]	2,302	2,440	- 6 %
LMNP[a]	1,288	1,241	+ 4%
Wood pellets	222	203	+ 9 %

[a]For CNC and CMNF the minimum product selling prices are estimated for dry-equivalent material.

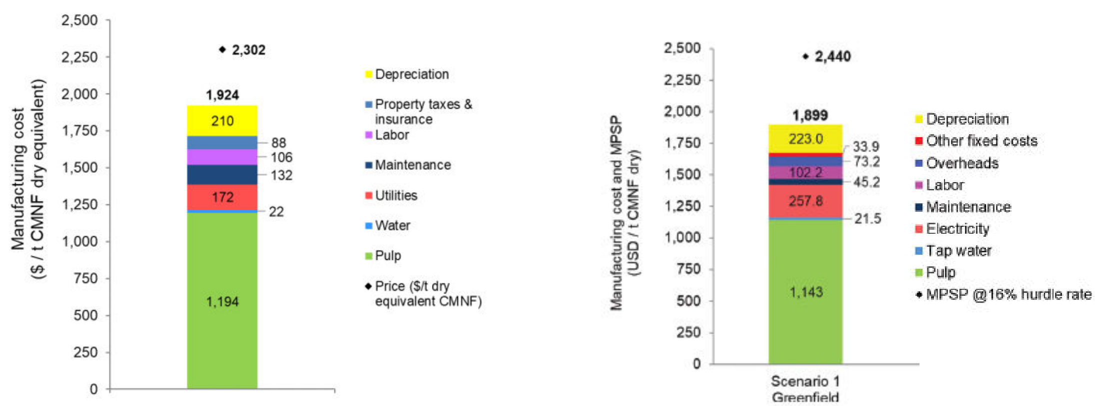

Figure 7-21: Manufacturing cost composition for CMNF – early stage assessment (left), and detailed assessment (right).

Quantitative risk assessment was then performed for the case studies. The assessment for CMNF case study is following described as an illustration of the methodology application. Uncertainties considered for the assessment are related to process conditions, raw materials costs, capital investment value, energy costs and labor costs values (Table 7-19).

Quantitative risk analysis was performed by running a *Monte Carlo* simulation to investigate the impact of uncertainties in manufacturing costs and project NPV. The software *@Risk* was used to perform the assessment. Distribution of manufacturing costs and NPV considering the product price as the MPSP are presented in Figure 7-22. As expected, the ranges of results obtained from the early stage assessment are broader than the detailed assessment results (NPV estimated from early stage methodology varies from - 30 MUSD to 26 MUSD and NPV estimated from detailed assessment methodology varies from -

12 MUSD to 11 MUSD; manufacturing costs estimated from early stage methodology varies from 1,600 USD/t to 2,300 USD/t and manufacturing costs estimated from detailed assessment methodology varies from 1,700 USD/t to 2,000 USD/t). The uncertainties considered and results obtained for the other three case studies are presented in the APPENDIX D: Detailed information on proposed method application to case studies.

Table 7-19: Sources of uncertainty considered for the CMNF case study.

Uncertainty considered	**Range of values**	**Source of information**	**Comments**
Refiner yield	95% – 100%	Pilot plant	Triangular distribution centered at 98%
Raw material costs	985 – 1,081 USD/t	Historical data (RISI) [96]	Distribution curve adjusted to historical data
Capital investment	+ / - 50 % of estimated value	Uncertainty in estimation at TRL 6 (see Table 7-9)	Uniform distribution
Energy costs	10 – 15% (of raw material + labor costs)	Suggested values for energy cost (section 7.3.5.3.3)	Uniform distribution
Labor costs	+ / - 25 % of estimated value	Estimation accuracy (section 0)	Uniform distribution

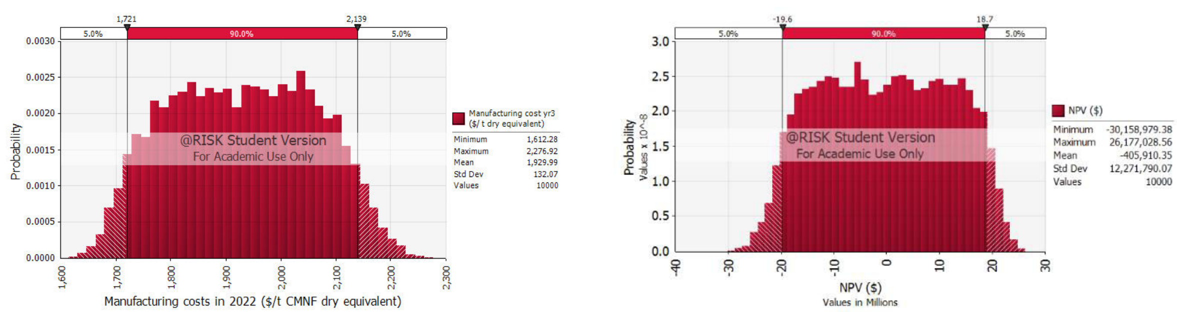

Figure 7-22: Distribution of manufacturing costs (left) and NPV (right) for the CMNF case study.

The last analysis of the quantitative risk assessment consists in the evaluation of market uncertainty in project financial metrics. As discussed in section 7.3.3.1.3, the market uncertainties are predominantly translated into variation in product prices and the quantity of product sold. Table 7-20 illustrate the impact of price variation in NPV values for CMNF, and the impact of product sales is shown in Table 7-21. Information for the other case studies is available in APPENDIX D: Detailed information on proposed method application to case studies. For CMNF case study variations in price present a higher impact on NPV than variations in product sales. The analyst should evaluate possible product prices in subsequent project stages.

Table 7-20: Impact of product price variation in project NPV for CMNF case study.

Case study	Price (USD/ t)	Chance of NPV <0	NPV range (MUSD) – 90% confidence interval
CMNF	2,302 (ref.)	51 %	-30 / +26
	2,500 (+9%)	25%	-18 / + 36
	2,740 (+19%)	< 0.5%	-4 / +49

Table 7-21: Impact of product sales in project NPV for CMNF case study.

Case study	% of sales in first 3 years	Chance of NPV <0	NPV range (MUSD) – 90% confidence interval
CMNF	50%	58%	-36 / +19
	80% (ref.)	49%	-30 / +26
	100%	36%	-25 / +29

The execution of cash flow and quantitative risk analysis at early stages present outputs similar to the ones obtained from detailed assessments. Although higher uncertainties in outputs was expected, the recommended activities for next project steps are similar (for instance for CMNF – evaluate the use of more cost-efficient raw materials, investigate possible product prices for specific applications, and consider a MPSP of USD 2,300 / t in further assessments).

7.7 Limitations of current work

The limitations of current work are following enumerated:

- The method does not account for risks related to the growth and supply of biomass.
- The tools used for capital investment are targeted to greenfield projects. Retrofit or repurposing scenarios were not tested in present work.
- Due to the lack of detailed information of existing biorefineries, methods for CAPEX and OPEX were tested on case studies, precluding its validation using actual project data.

- The proposed methods to estimate capital investment and operational costs rely on the estimation of process steps. Variation on estimated values is expected if the analyst is not aware of the guidelines that define them.

7.8 Conclusions

Despite the growing interest in bio-based projects and the multitude of alternatives to be explored, budget and resources limitations usually prevent the fast development of the bioeconomy at its full potential. Typical techno-economic approaches provide relevant information for investment assessment. However, they involve significant amount of time and resources.

We hereby propose a methodology to evaluate bio-based investment at early stages, saving significant amount of time and resources when assessing project alternatives. The methodology proposed integrates and adapt existing tools to assess investments at early stages in a systematic way and goes beyond techno-economic analysis by including market, financial, and technical factors, as well as quantitative risk analysis.

The first step of the methodology is composed of market, technical, and financial assessments. Market attractiveness score, the technology maturity, and the economic potential of the project are estimated. This information can be used to screen out less attractive project alternatives if necessary. The second step includes a cash flow assessment and quantitative risk analysis. Financial indicators including NPV, IRR, and payback are estimated, as well as the product minimum product-selling price. Project uncertainties are considered in quantitative risk assessment to evaluate project risks. Supporting tools to estimate product prices, capital investment, and operating costs at early stages are provided and save significant time in project evaluation. A checklist covering potential project risks for the bio-based industry is the third and final step of the methodology. It aims to make the analyst aware of factors and risks that can hinder the investment success since the early stages of design.

Four case studies were used to illustrate the attributes of the proposed methodology: cellulose nanocrystals (CNC), cellulose micro- and nanofibrils (CMNF), lignin micro- and nanoparticles (LMNP), and wood pellets. Detailed techno-economic assessments were previously performed for the selected case studies and allowed the comparison between the outcomes of the proposed methodology and the detailed assessments.

It was found that the time necessary to execute the proposed methodology is significantly lower than typical techno-economic assessments, especially for estimating operating costs and capital investment. Fewer data inputs are needed to perform the assessment; a simplified mass balance and block diagram are the main inputs and there is no need to design and perform cost estimation of equipment. Estimated financial metrics using the proposed methodology were very similar to the ones estimated using detailed assessment, although more variation in quantitative risk assessment results was observed for the proposed methodology. The decision-making process was not impacted when the outcomes of the proposed methodology are used instead of outcomes from detailed techno-economic assessments.

The analysis performed herein and outcomes obtained illustrate the potential that the proposed methodology has to improve current practices for early-stage investment assessment, saving time and resources, besides promoting the development of the bio-based industry by guiding investors and researchers to focus efforts in the most promising projects aiming commercialization.

8 FUTURE WORK

The proposed methodology was applied to different case studies and its potential to evaluate projects at early stages was shown and discussed. Nevertheless, there are limitations in the methodology, besides additional areas to be explored and improved. Suggestions for future research are following proposed.

1- Test the proposed methodology for real successes and failures projects

As stated in the limitations section of this dissertation, the methodology was tested on case studies that are available in literature and have detailed estimates available for further comparison, although they were never built. It is suggested that the methodology is tested in known successes cases, such as different pulp and paper facilities, as well as ethanol from sugar cane or from corn. If possible, information from existing organizations could be retrieved, including capital investment and operating costs. Databases as Fisher*Solve* can be used for estimating the manufacturing costs and information of recent investments can be found in media. Information published on literature can be used as well. The results from these assessments can be used to calibrate the methodology regarding the chances of success of an investment.

2- Inclusion of co-location / retrofit / repurpose facilities

Previous studies have shown that investments in co-located / retrofit / repurpose facilities are usually more attractive than greenfield facilities, due to reduced investment costs, less infrastructure needed, as well as lower labor. With the development of the new bio-based industry and decrease of paper consumption in future, the use of existing facilities that process biomass seems to be a feasible and promising project alternative to greenfield facilities. It is suggested that retrofit / co-location / repurpose scenarios are tested and included in the existing methodology.

The major difference when applying the methodology for greenfield or co-location / retrofit/ repurpose projects involves the estimation of capital and operating costs. Existing early-stage capital investment methodologies are focused on greenfield projects. A literature revision on the major savings for co-location situation is suggested, especially if pulp and paper facilities are used, followed by testing selected case studies and further adaptation of the estimation equations.

3- Inclusion of uncertainties related to biomass supply chain in the quantitative risk assessment

The literature review on sources of risk for bio-based investments has showed that the major sources of risks are related to costs, prices, product adoption, technology, and capital investment. There are unique risks in bio-based industry investments that may harm the profitability of an investment. The bio-based industry is dependent on growth and distribution of feedstocks, and the cost of the feedstock may change depending on the collection area or climate conditions, for instance. We believe that climate conditions should not be evaluated on early stages of investment; however, the inclusion of biomass supply chain risks may benefit the investment evaluation and project decision-making.

There are existing publications that relate the cost of feedstock with the collection area. Uncertainties in feedstock costs depending on facility size and area of collection are suggested to be added in the methodology.

4- Improvement of methods to estimate capital investment, labor, and energy costs

As previously discussed, existing methodologies to estimate capital investment and labor costs were aimed for chemical and petrochemical processes. It is suggested that these methodologies are tested for several case studies, in order to verify the accuracy of the method for different types of processes (e.g., liquid based vs. solid based, chemicals production, thermochemical-based processes, pyrolysis-based processes, etc.). Information from previous detailed assessments, such as several NREL reports can be used to test the methods and propose modifications. In addition, it is suggested that the methods to estimate capital and operating costs are tested in new facilities as they are assembled and come to operation. It is believed that with the development of this industry, capital and operating costs can be optimized and minimized, and the methods proposed might need to be adapted accordingly.

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APPENDICES

APPENDIX A: Information on prices and market volumes for different products

Chemical name	Price (USD/t)	Market size (t/yr)	Year	Reference
1,3-propanediol	1,980	150,000	2016	[12]
1,4-butanediol	2,800	1,800,000	2016	[12]
3-hydroxypropionic acid	1,170	3,600,000	2010	[26]
Acetic acid	850	13,000,000	2016	[12]
Acetone	1,350	7,000,000	2016	[12]
Acrolein	1,450	125,000	2010	[26]
Acrylamide	1,862	100,000	2010	[26]
Acrylic acid	2,000	4,500,000	2010	[26]
Acrylonitrile	1,600	7,000,000	2016	[12]
Activated carbon	4,655	1,200,000	2010	[26]
Adipic acid	1,550	2,500,000	2016	[12]
Ammonia	612	122,000,000	2010	[26]
Antibiotics (bulk)	199,500	30,000	2010	[26]
Arginine	26,600	15,000	2010	[26]
Aspartame	39,900	17,000	2010	[26]
Astaxanthine	93,100	42	2010	[26]
Benzene	553	50,000,000	2018	[12]
Butanol	798	1,100,000	2010	[26]
Butyric acid	1,423	50,000	2010	[26]
Caprolactam	2,407	4,000,000	2010	[26]
Carbon fibre	1,596	28,000	2010	[26]
Carboxylic acid	1,064	840,000	2010	[26]
Catechols	5,054	200,000	2010	[26]
Chitin/Chitosan	13,300	20,000	2010	[26]
Citric acid	1,064	1,600,000	2010	[26]
Coenzyme Q10	532,000	150	2010	[26]
Crude Tall Oil (CTO)	599	400,000	2010	[26]
Cyclodextrins	1,330	5,000	2010	[26]
Cyclohexane	851	5,000,000	2010	[26]
Dextran	106,400	200	2010	[26]
D-gluconic acid	1,995	87,000	2010	[26]
Dimethyl ether (DME)	599	150,000	2010	[26]

[12] https://blogs.platts.com/2015/07/14/changing-dynamics-global-benzene-supply/ and https://www.spglobal.com/platts/en/market-insights/latest-news/petrochemicals/010219-us-january-benzene-contract-price-falls-28-cents-to-183-cents-gal-sources [Acessed on December 2018]

Chemical name	Price (USD/t)	Market size (t/yr)	Year	Reference
Epoxy resins	3,392	30,000	2010	[26]
Ethane	32	120,000,000	2010	[26]
Ethanol	636	95,000,000	2018	[13]
Ethylene glycol	1,729	20,000,000	2010	[26]
Ethyl acetate	1,500	2,000,000	2016	[12]
Ethyl lactate	2,150	1,500,000	2016	[12]
Ethyl tert-butyl ether (ETBE)	998	5,750,000	2010	[26]
Ethylene	1,000	130,000,000	2016	[12]
Ethylene oxide	1,862	18,000,000	2010	[26]
Eugenol	4,571	3,500	2005	[399]
Fatty acids	1,100	6,000,000	2016	[12]
Formic acid	1,330	500,000	2010	[26]
Fructose	532	10,100,000	2010	[26]
Fumaric acid	1,962	12,000	2010	[26]
Furfural	850	300,000	2016	[12]
Furfuryl alcohol	466	350	2010	[26]
Gluconic acid	1,995	87,000	2010	[26]
Glucose	625	167,000,000	2010	[26]
Glutamic acid	1,862	1,500,000	2010	[26]
Glycerol (not refined)	399	1,200,000	2010	[26]
Glycerol (refined)	850	2,000,000	2016	[12]
Hydrogen	2,660	54,000,000	2010	[26]
Isoprene	1,300	900,000	2016	[12]
Itaconic acid	2,660	80,000	2010	[26]
Lactate esters	2,660	10,000,000	2010	[26]
Lactic acid	1,790	600,000	2016	[12]
Leucine	665,000	10	2010	[26]
Levulinic acid	10,640	450	2010	[26]
L-Hydroxyphenylalanine	13,300	10,000	2010	[26]
Lysine	2,660	800,000	2010	[26]
Maleic anhydride	1,929	1,600,000	2010	[26]
Malic acid	1,919	25,000	2010	[26]
Malonic acid	31,920	453	2010	[26]
Methane	1,064	60,000,000	2010	[26]
Methanol	500	60,000,000	2016	[12]

[13] https://knect365.com/energy/article/c07f7fba-48fa-464f-9f21-12f913fc67f7/world-ethanol-production-to-expand-steadily-in-2019 and https://www.cepea.esalq.usp.br/en/indicator/ethanol.aspx [Accessed on December 2018]

Chemical name	Price (USD/t)	Market size (t/yr)	Year	Reference
Methionine	26,600	400	2010	[26]
Methyl acetate	532	292,185	2010	[26]
Methyl methacrylate (MMA)	1,809	24,000,000	2010	[26]
Methyl tetrahydrofuran (MTHF)	1,197	13,952,400	2010	[26]
Monosodium glutamate (MSG)	1,995	1,000,000	2010	[26]
Phenol	1,025	10,700,000	2016	[14]
Phenylalanine	13,300	10,000	2010	[26]
Poly-3-hydrozybutyrate (PHB)	11,970	50	2010	[26]
Polyamide	333	6,000,000	2010	[26]
Polyhydroxyalkanoate (PHA)	5,519	29,540	2017	[15]
Polylactic acid	3,325	140,000	2010	[26]
Polyols	2,394	1,600,000	2010	[26]
Polypropylene	1,769	40,000,000	2010	[26]
polyurethanes	3,990	11,600,000	2010	[26]
Polyvynil chloride	1,343	30,000,000	2010	[26]
Propionic acid	1,064	130,000	2010	[26]
Propylene	1,350	70,000,000	2010	[26]
Propylene glycol	1,400	2,757,000	2014	[440]
Propylene oxide	1,596	6,600,000	2010	[26]
Pullutan	11,970	10,000	2010	[26]
Sorbitol	1,500	2,000,000	2016	[12]
Starch	466	58,000,000	2010	[26]
Styrene	1,064	900,000	2010	[26]
Succinate salts	1,463	15,000	2010	[26]
Succinic acid	3,480	50,000	2016	[12]
Tall Oil Fatty Acids (TOFA)	599	400,000	2010	[26]
Tall Oil Pitch (TOP)	532	20,000	2010	[26]
Tall Oil Rosin (TOR)	532	20,000	2010	[26]
Tetrahydrofuran (THF)	3,638	436,000	2010	[26]
Threonine	7,980	30,000	2010	[26]
Toluene	1,031	36,000,000	2010	[26]
Trypthophane	7,980	1,200	2010	[26]
Vanillin	13,300	12,000	2010	[26]
Vinyl acetate	865	5,800,000	2010	[26]

[14] https://mcgroup.co.uk/news/20140131/global-phenol-supply-exceed-107-mln-tonnes.html and http://www.platts.com/news-feature/2015/petrochemicals/global-solvents-overview/solvents-phenol-prices [Accessed on December 2018]
[15] https://www.european-bioplastics.org/market/Bioengineering

Chemical name	Price (USD/t)	Market size (t/yr)	Year	Reference
Vinyl chloride	466	32,000,000	2010	[26]
Vitamin B2	645,050	30,000	2010	[26]
Vitamin C	10,640	80,000	2010	[26]
Xanthan	10,640	20,000	2010	[26]
Xylene (para)	950	30,000,000	2016	[12]

APPENDIX B: Risk assessment survey questionnaire

Information to respondents: NC State University and Duke University are conducting a survey on the use of financial risk assessment for investments in the bio-based industry. It will take 5 - 15 minutes to answer the questionnaire, depending on the level of risk assessment application by the respondent / organization.

Main goals of this survey are: 1) assess sources of uncertainty commonly considered for risk assessment; 2) identify which methods are used for investment risk assessment; and 3) Evaluate how risk assessment is considered for decision-making in investments.

Individual answers will be kept confidential. Respondents will receive a summary of the outcomes according to demographics factors before publication of survey results.

Definitions: RISK is defined as a random event that negatively affects an organization's goals, consequently generating financial losses. RISK ANALYSIS (or RISK ASSESSMENT) is a methodology used to estimate how often an event may happen and the impact of its consequences. In FINANCIAL RISK ASSESSMENT, the impact of different risks on the financials of an investment is evaluated. Safety related risk assessment is not included in this survey.

Any questions: please contact Camilla Abbati de Assis - cabbati@ncsu.edu

Section 1

1.1 Does your organization perform financial risk assessment for investments? This includes quantitative and qualitative methods.

Definitions: Risk Assessment is a methodology used to estimate how often an event may happen and the impact of its consequences. In Financial Risk Assessment, the impact of different risks on the financials of an investment is evaluated. Safety, health and environmental- related risk assessment are not included in this survey.

☐ Frequently (Go to section **2**)

☐ Infrequently (Go to section **2**)

☐ Never used (Go to section **3**)

Section 2: Organizations that perform risk assessment

2.1 Does your organization have a written guideline or procedure on how to perform risk assessment for investments?

☐ Yes

☐ No

2.2 Does your organization have a formally dedicated department / employee to conduct risk assessments for investments?

☐ Yes

☐ No

2.3 How often is risk assessment performed by your organization? (please select only 1 option)

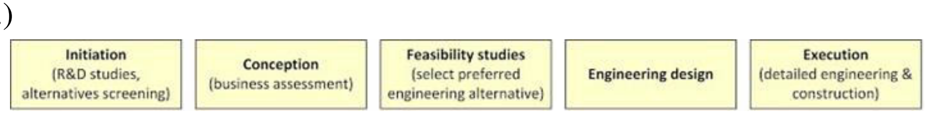
☐ For every investment

☐ Only for investments over a minimum value

☐ Not a defined criteria

☐ Other: ____

2.4 In which project stage(s) does your organization perform risk assessment? (Check all that apply.)



☐ Initiation

☐ Conception

☐ Feasibility studies

☐ Engineering design

☐ Execution

2.5 Which type of methodology does your organization use? (Check all that apply.) P.S.: Some analytical methods, such as what-if analysis, may be classified either as qualitative or quantitative methodology

☐ Qualitative (non-numerical output is assessed, e.g., SWOT analysis - Strengths, Weaknesses, Opportunities, and Threats)

☐ Quantitative (numerical output assessed, e.g., probability assessment)

☐ Qualitative and quantitative assessments combined

☐ Other: ____

2.6 Which software does your organization use to perform risk assessment? (Check all that apply.)

☐ Microsoft Excel spreadsheets

☐ Software developed "in-house"

☐ @Risk (Palisade)

☐ Crystal Ball (Oracle)

☐ Matlab

☐ DPL (Syncopation Software)

☐ Riskturn

☐ None

☐ Other: ____

2.7 Which of the following analytical approach(es) does your organization use to perform risk assessment? (Check all that apply.)

☐ Tornado diagrams

☐ Spider plots

  ☐ Switching value table

  ☐ Probability distribution

  ☐ SWOT Analysis

  ☐ Risk heat map

  ☐ Decision trees

  ☐ What-if analysis

  ☐ Cost-benefit analysis

☐ Worst-case analysis

☐ None

☐ Other: ____

2.8 Identify which specific sources of risk are considered by your organization when performing risk assessment. (Check all that apply.)

☐ Technology (e.g., TRL - technology readiness level)

☐ Financial (e.g., cost of raw materials)

☐ Market and sales (e.g., product adoption)

☐ Operational (e.g., not achieving full capacity at start up)

☐ Engineering (e.g., capital investment higher than forecasted)

☐ Competition (e.g., competition leading to loss in market share)

☐ Resources (e.g., lack of personnel)

☐ Management (e.g., poor management)

☐ Government policies (e.g., subsides are not available)

☐ Timing (e.g., delay in start-up)

☐ Supply chain (e.g., raw material sourcing)

☐ R&D (e.g., intellectual property)

☐ Social (e.g., impact of investment in local community)

☐ Environmental regulations (e.g., use of hazardous materials)

☐ Other: ____

2.9 Select the top 3 sources of risk you believe should be considered by your organization when performing risk assessment.

☐ Technology (e.g., TRL - technology readiness level)

☐ Financial (e.g., cost of raw materials)

☐ Market and sales (e.g., product adoption)

☐ Operational (e.g., not achieving full capacity at start up)

☐ Engineering (e.g., capital investment higher than forecasted)

☐ Competition (e.g., competition leading to loss in market share)

☐ Resources (e.g., lack of personnel)

☐ Management (e.g., poor management)

☐ Government policies (e.g., subsides are not available)

☐ Timing (e.g., delay in start-up)

☐ Supply chain (e.g., raw material sourcing)

☐ R&D (e.g., intellectual property)

☐ Social (e.g., impact of investment in local community)

☐ Environmental regulations (e.g., use of hazardous materials)

☐ Other: ____

2.10 Please list the top 3 benefits of performing risk assessment in your organization.

☐ Reduction of project failures

☐ Development of risk mitigation strategies

☐ Better screening between project alternatives

☐ Better understanding of the risks involved when making a decision

☐ Compliance with regulatory requirements

☐ Consistent data for decision-making (standard procedures used for assessing different projects)

☐ Faster response to unexpected events

☐ Organization image

☐ Allows contingencies for projects

☐ Cost savings by identifying systemic risks and mitigating these at organization level

☐ Other: _______________________________________

2.11 Is your management aware of the benefits of performing risk assessment for the decision-making process?

☐ Yes

☐ No

☐ Not sure

2.12 Which metric does your organization use to assess investment attractiveness? By investment we mean projects of new facilities, revamp projects, and acquisitions of companies. (Check all that apply.)

☐ NPV (Net Present Value)

☐ IRR (Internal Rate of Return)

☐ ROI (Return on Investment)

☐ ROCE (Return on Capital Employed)

☐ Discounted payback

☐ Non-discounted payback

☐ EVA (Economic Value Added)

☐ Hurdle rate

☐ Price-to-earnings ratio

☐ Profitability index

☐ APV (Adjusted Present Value)

☐ Other:____

2.13 Which financial metrics are evaluated during risk assessment? (Check all that apply.)

☐ NPV (Net Present Value)

☐ IRR (Internal Rate of Return)

☐ ROI (Return on Investment)

☐ ROCE (Return on Capital Employed)

☐ Discounted payback

☐ Non-discounted payback

☐ EVA (Economic Value Added)

☐ Hurdle rate

☐ Price-to-earnings ratio

☐ Profitability index

☐ APV (Adjusted Present Value)

☐ Other:____

2.14 How risk assessment outcomes are considered in the investment decision-making process?

	Always considered	Sometimes considered	Never considered
Qualitative risk assessment outcomes (non-numerical outcomes)	☐	☐	☐
Deterministic outcomes (e.g., sensitivity analysis)	☐	☐	☐
Probabilistc outcomes	☐	☐	☐

2.15 Please use this space for any additional comments.

____

Please proceed to section 4

Section 3: Organizations that do not perform risk assessment

3.1 Does your organization have a written guideline or procedure on how to perform risk assessment?

☐ Yes

☐ No

3.2 List possible reasons why your organization is not performing risk assessment for investments. (Check all that apply.)

☐ Unqualified personnel

☐ Tools are not available

☐ Never used before

☐ Procedures are too complicated

☐ Organization is not aware of benefits of performing risk assessment

☐ Other: ____

3.3 Select the top 3 sources of risk you believe should be considered by your organization when performing risk assessment.

☐ Technology (e.g., TRL - technology readiness level)

☐ Financial (e.g., cost of raw materials)

☐ Market and sales (e.g., product adoption)

☐ Operational (e.g., not achieving full capacity at start up)

☐ Engineering (e.g., capital investment higher than forecasted)

☐ Competition (e.g., competition leading to loss in market share)

☐ Resources (e.g., lack of personnel)

☐ Management (e.g., poor management)

☐ Government policies (e.g., subsides are not available)

☐ Timing (e.g., delay in start-up)

☐ Supply chain (e.g., raw material sourcing)

☐ R&D (e.g., intellectual property)

☐ Social (e.g., impact of investment in local community)

☐ Environmental regulations (e.g., use of hazardous materials)

☐ Other: ____

3.4 Which metric does your organization use to assess investment attractiveness? (Check all that apply.)

☐NPV (Net Present Value)

☐ IRR (Internal Rate of Return)

☐ ROI (Return on Investment)

☐ROCE (Return on Capital Employed)

☐ Discounted Payback

☐ Non-discounted payback

☐ EVA (Economic Value Added)

☐ Hurdle rate

☐ Price-to-earnings ratio

☐ Profitability index

☐ APV (Adjusted Present Value)

☐ Other: ____

3.5 Please use this space for any additional comments

____

Section 4: Organization and respondent information

4.1 What is the major industry segment of your organization? (Please check only 1 box)

☐ Fuels Chemicals

☐ Biotech (e.g., enzymes)

☐ Pulp & Paper

☐Personal care

☐ Wood products

☐Other forest products

☐ Forest management

☐ Consulting

☐ Other: ____

4.2 What types of bio-based products is your organization producing or aiming to produce? (Check all that apply.)

☐ Biofuels

☐ Biochemicals

☐ Biomaterials

☐ Pulp and paper

☐ Biotech / enzymes

☐ Forest products (e.g., timber)

☐ Forest management

☐ Other:____

4.3 How many employees are in your organization?

☐ Less than 100

☐ 100 - 1,000

☐ 1,000 to 5,000

☐ 5,000 to 10,000

☐ More than 10,000

4.4 What was your organization's revenue in 2016?

☐ No revenue

☐ Less than USD 1 million

☐ Between USD 1 million and USD 10 million

☐ Between USD 10 million and USD 500 million

☐ Between USD 500 million and USD 1 billion

☐ Between USD 1 billion and USD 10 billion

☐ More than USD 10 billion

☐ No information available

4.5 How would you describe your organization?

☐ Multinational

☐ Local company - U.S.

☐ Local company - other countries

4.6 Where is your organization's headquarters located?

☐ U.S. or Canada

☐ Latin America Europe

☐ Asia Pacific

☐ Africa

4.7 Respondent position ____________________________________

4.8 Respondent organization (this information will be used to assure quality of survey results and will be kept confidential).

____

4.9 To receive survey results before they are published, please enter your email below (optional) ________________

End of questionnaire
Thank you for your participation

APPENDIX C: Supplementary information - capital investment assessment tools

Capital cost estimation equations adjusted to 2016 and U.S. dollars

The selected equations were adjusted to 2016 values, as following illustrated. Values for the Chemical Engineering Plant Cost Index (CEPCI) are found in *Chemical Engineering* magazine [441], and values for exchange rates and location indexes are as used by Tsagkari (2016) [402].

Taylor [413]

- Original equation (1977, UK):

  $ISBL = k_T * \sum_1^N 1.3^{CS} * Q^{0.39}$, in MGBP (GBP stands for Great British Pounds)

  - k_T = 42 kGBP yr / kt
  - Cs = complexity score for each significant process step, detailed information on estimation can be found in Taylor (1977) [413]
  - N = number of significant process steps
  - Q = flowrate (kt/yr)
  - CEPCI (1977) = 204.1
  - CEPCI (2016) = 541.7
  - Location factor UK = 0.9 (base= US, 1977)
  - USD / GBP (1977) = 1.74
- Updated equation (2016):
  - $ISBL = 216.1 * \sum_1^N 1.3^{CS} * Q^{0.39}$, in kUSD
  - Assumed that ISBL = 70% of total investment.

<u>Bridgwater (A)</u> [421] – equation valid for liquid and solid-liquid processes, particularly metal extraction, operating above ambient temperature and pressure, with capacities greater than 10 kt/yr, in a greenfield basis.

- Original equation (1976, UK)
  - $ISBL = 37.7 * N * \left(\frac{Q}{s^{0.5}}\right)^{0.85} * \left(T_{max} * \frac{n}{N}\right)^{-0.17} * \left(P_{max} * \frac{n\prime}{N}\right)^{0.14} * \frac{ENR}{1300}$, in £

  N = number of functional units

Q = plant capacity (t/yr)

s = process conversion (flow of product divided by flow of raw material)

T_{max} = maximum temperature (°C)

P_{max} = maximum pressure (atm)

n and n' = number of functional units operating at T and P greater than $T_{max}/2$ and $P_{max}/2$, respectively

- ENR construction cost index (1969/1970) = 1,300
- ENR construction cost index (2016) = 10,000 [442], [443]
- Location factor UK = 0.97 (base= US, 1976)
- USD / GBP (1976) = 1.8

- Updated equation (2016):
  - $ISBL = 538.1 * N * \left(\frac{Q}{s^{0.5}}\right)^{0.85} * \left(T_{max} * \frac{n}{N}\right)^{-0.17} * \left(P_{max} * \frac{n'}{N}\right)^{0.14}$, in USD
  - Assumed that ISBL = 75% of total investment

<u>Bridgwater (B)</u> [401] – equation valid for liquid and solid-liquid processes

- Original equation (1975, UK)
  - for Q/s > 60,000t/yr: $ISBL = 158 * N * \left(\frac{Q}{s}\right)^{0.675} * \frac{CEPCI\ (2016)}{CEPCI\ (1975)}$
  - for Q/s < 60,000t/yr: $ISBL = 13{,}850 * N * \left(\frac{Q}{s}\right)^{0.30} * \frac{CEPCI\ (2016)}{CEPCI\ (1975)}$
  -

N = number of functional units

Q = plant capacity (t/yr)

s = process conversion (flow of product divided by flow of raw material)

CEPCI (1975) = 182.4

CEPCI (2016) = 541.7

Location factor UK = 0.95 (base= US, 1975)

- USD / GBP (1975) = 2.21

- Updated equation (2016):

for Q/s > 60,000t/yr: $ISBL = 1{,}092 * N * \left(\frac{Q}{s}\right)^{0.675}$, in USD

for Q/s < 60,000t/yr: $ISBL = 95{,}687 * N * \left(\frac{Q}{s}\right)^{0.3}$, in USD

Bridgwater (C) [401] – this equation is based on the same set of data used for Bridgwater (B), but a linear regression model is used.

- Original equation (1975, UK)

  $ISBL = \left[401{,}600 + 1.304 * \left(\frac{Q}{s}\right)\right] * N * \frac{CEPCI\ (2016)}{CEPCI\ (1975)}$, in GBP

  N = number of functional units

  Q = plant capacity (t/yr)

  s = process conversion (flow of product divided by flow of raw material)

  CEPCI (1975) = 182.4

  CEPCI (2016) = 541.7

  - Location factor UK = 0.95 (base= US, 1975)
  - USD / GBP (1975) = 2.21

- Updated equation (2016):

  $ISBL = \left[2{,}774{,}547 + 9.01 * \left(\frac{Q}{s}\right)\right] * N$, in USD

Bridgwater (D) [401] – equation valid for Q/s > 60,000 t/yr, using the same set of data from Bridgwater (B), but accounting for temperature and presser to increase correlation.

- Original equation (1975, UK)

$$ISBL = 193 * N * \left[\left(\frac{Q}{s}\right)^{0.665}\right] * \left[e^{2.58*E-7*Q}\right] * \left[T_{max}{}^{0.022}\right] * \left[P_{max}{}^{-0.064}\right] * \frac{CEPCI\ (2016)}{CEPCI\ (1975)}$$

  N = number of functional units

  Q = plant capacity (t/yr)

  s = process conversion (flow of product divided by flow of raw material)

  T_{max} = maximum temperature (°C)

  P_{max} = maximum pressure (atm)

  CEPCI (1975) = 182.4

CEPCI (2016) = 541.7

- Location factor UK = 0.95 (base= US, 1975)
- USD / GBP (1975) = 2.21

- Updated equation (2016):

$ISBL = 1{,}333 * N * \left[\left(\frac{Q}{s}\right)^{0.665}\right] * [e^{2.58*E-7*Q}] * \left[T_{max}{}^{-0.022}\right] * \left[P_{max}{}^{-0.064}\right]$, in USD

- Assumed that ISBL = 75% of total investment

Klumpar *et* al. (A and B) [417] – equation based on 20 plants involving solids, liquids, gases, and the combination of them, and considered especially facilities involving the extraction of natural resources and related technologies. The authors claimed to cover a wider range of capacities and process than other studies, particularly solids processing facilities (ore and coal beneficiation, coal and oil shale conversion, and extractive metallurgy).

- Original equation (1981, US)

$ISBL = 1{,}800 * F * N * G^{v}$, in USD

$F = 2 * 10^{T+P+M}$

$T = 1.8E-4 * (t-27), for\ t \geq 27℃$, $T = 2.0E-3 * (t-27), for\ t \geq 27℃$

$P = 0.1 * \log(p)\ , for\ p \geq 1bar$, $P = 0.1 * \log\left(\frac{1}{p}\right), for\ p < 1bar$

F = complexity factor, no dimension

T = temperature factor, no dimension

P = pressure factor, no dimension

t = temperature, °C

p = pressure, bar

M = material construction factor, no dimension (varies from 0 to 0.4, table available in original article)

N = number of process modules

G = average throughput, kg/h (sum of all module throughputs divided by the number of modules; the module throughput is the sum of individual flowrates of all module inlet and outlet streams divided by two).

$v = 0.57$ for equation (A) – constant exponent, and $v = 0.83x_1 + 1.05\ x_2 + 0.59\ x_3 + 0.47\ x_4 + 0.59\ x_5 + 1.07\ x_8 + 0.60\ x_9 + 0.83\ x_{11} + 0.40\ x_{12}$ for equation (B). The constant exponent in (A) is replaced by an exponent computed for each facility, which is the weighted average of individual exponents for each module, weighted by the number of modules.

x_i = number of process modules of type I divided by the total number of process modules (see Klumpar *et* al. 1983, [417])

- Updated equation (2016):
  $ISBL = 3{,}283 * F * N * G^{v}$, in USD
  - Assumed that ISBL = 75% of total investment

Petley [419]:

- Original equation (1988, West Germany)
  $ISBL = 55{,}882 * Q^{0.44} * N^{0.486} * T_{max}{}^{0.038} * P_{max}{}^{-0.02} * F_m{}^{0.341}$, in USD

Q = facility capacity (t/yr)

N = number of functional units

T_{max} = maximum operating temperature (K)

P_{max} = maximum operating pressure (bar)

F_m = factor for materials of construction: carbon steel= 1; stainless steel (400 series)= 1.28; stainless steel (300 series)= 1.5; Hastelloy C= 1.54; Titanium, tantalum= 2

CEPCI (1988) = 342.5

CEPCI (2016) = 541.7

- Location factor Germany = 1.03 (base= US, 2011)

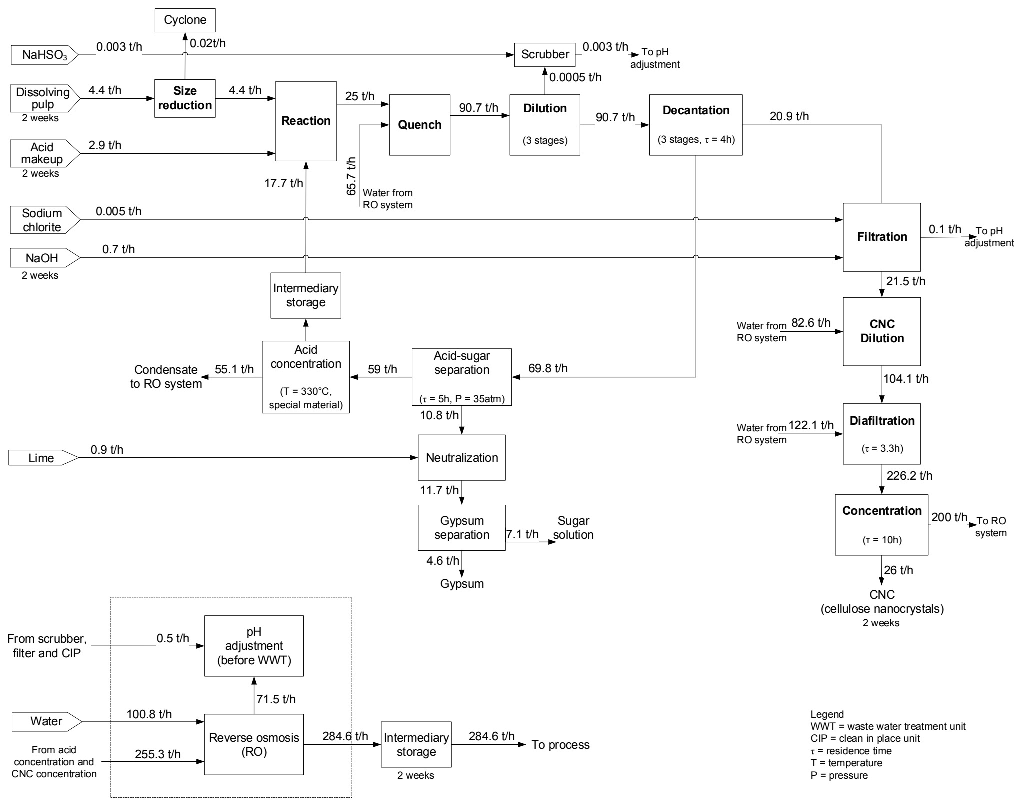
- Updated equation (2016)
  $ISBL = 85{,}809 * Q^{0.44} * N^{0.486} * T_{max}{}^{0.038} * P_{max}{}^{-0.02} * F_m{}^{0.341}$, in USD

Application of the methods for case studies

The flowsheets below were used to calculate the capital investment. In all cases, if no process information is available, then it means that: residence time (τ) ≤ 3h, temperature (T) is between 20°C and 500°C, Pressure (P) is between 1 and 10 atm, and storage time ≤ 1 week.

1- Cellulose nanocrystals (CNC)

Flowsheet:



Process steps considered:

Taylor: 1) Storage of dissolving pulp, 2) Storage of recycled acid, 3) Storage of acid makeup, 4) Storage of water, 5) Storage of sodium chlorite, 6) Storage of sodium bisulfite, 7) Storage of sodium hydroxide, 8) Storage of lime, 9) Storage of cellulose nanocrystals (CNC), 10) Storage of gypsum, 11) Storage of water recycle, 12) Storage of sugar solution, 13) Size reduction, 14) Cyclone, 15) Reaction, 16) Quench, 17) Dilution, 18) Scrubber, 19) Decanters, 20) Filter, 21) Dilution CNC, 22) Diafiltration, 23) CNC concentration, 24) Acid-sugar separation, 25) Acid concentration, 26) Neutralization, 27) Gypsum separation, 28) Adjustment of pH of the effluent, 29) Reverse osmosis

Bridgwater (A-D) and Petley: 1) Size reduction, 2) Cyclone, 3) Reaction, 4) Quench, 5) Dilution, 6) Scrubber, 7) Decanters, 8) Filter, 9) Dilution CNC, 10) Diafiltration, 11) CNC concentration, 12) Acid-sugar separation, 13) Acid concentration, 14) Neutralization, 15) Gypsum separation, 16) Adjustment of pH of the effluent, 17) Reverse osmosis

Klumpar: 1) Storage of acid makeup, 2) Storage of water, 3) Storage of sodium hydroxide, 4) Storage of lime, 5) Storage of CNC, 6) Storage of gypsum, 7) Size reduction, 8) Reaction, 9) Quench, 10-12) Dilution (3x), 13-15) Decantation (3x), 16) Filtration, 17) Dilution CNC, 18) Diafiltration, 19) CNC concentration, 20) Acid-sugar separation, 21) Acid concentration, 22) Neutralization, 23) Gypsum separation, 24) Pulp handling

For the method proposed by Taylor [413], the following table including the complexity scores is shown below. There might be small differences between the calculated value below and the value in the dissertation due to adjusted curves to estimate the costliness index.

Process step number	Complexity score (CS)						Costliness index (1.3^CS)
	Throughput ratio	Material of construction	Reaction / Storage time	Pressure / Temperature	Other	Total score	
1	-3	1	1	0	1	0	1.0
2	0.5	2	0	0	0	2.5	1.9
3	-3	2	1	0	0	0	1.0
4	2.5	1	0	0	0	3.5	2.5
5	-3	1	0	0	0	-2	0.6
6	-3	1	0	0	0	-2	0.
7	-3	1	1	0	0	-1	0.8
8	-3	1	0	0	0	-2	0.6
9	0	1	1	0	0	2	1.7
10	-3	1	0	0	0	-2	0.6
11	4.5	1	1	0	0	6.5	5.5
12	-2.5	1	0	0	0	-1.5	0.7
13	-3	1	0	0	0	-2	0.6
14	-3	1	0	0	0	-2	0.6
15	0	3	0	0	0	3	2.2
16	2.5	3	0	0	0	5.5	4.2
17	2.5	3	0	0	2	7.5	7.2
18	-3	2	0	0	0	-1	0.8
19	2.5	1	0.5	0	2	6	4.8
20	-0.5	1	0	0	0	0.5	1.1
21	2.5	1	0	0	0	3.5	2.5
22	4.5	1	0	0	0	5.5	4.2
23	4.5	1	2	0	2	9.5	12.1
24	1.5	2	1	2	2	8.5	9.3
25	2	3	0	0	1	6	4.8
26	-1.5	2	0	0	1	1.5	1.5
27	-1.5	1	0	0	1	0.5	1.1
28	2	1	0	0	0	3	2.2
29	5	1	0	0	1	7	6.3
						Total	**83.0**

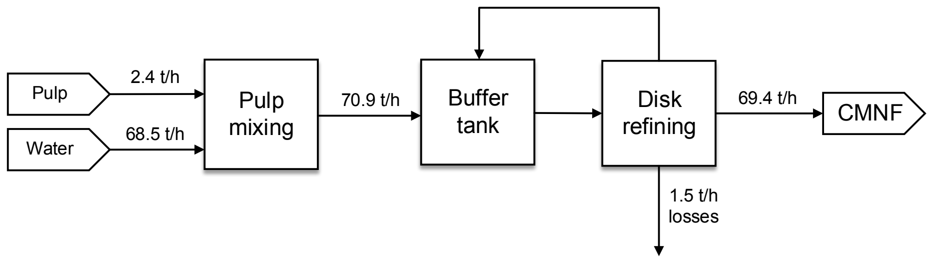
$$Investment\ (OSBL) = (216.1 * \sum (1.3)^{CS} * Q^{0.39}) * 1.3$$

$$Q = 205.3\ kt/yr$$

$$Investment\ (OSBL) = \ (216.1 * 83.0 * 205.3^{0.39}) * 1.3$$

2- Cellulose micro- and nanofibrils (CMNF)

Flowsheet:



Process steps considered:

Taylor: 1) Pulp mixing, 2) Disk refiner, 3) Storage of pulp, 4) Storage of water, 5) Storage of cellulose micro- and nanofibers (CMNF), 6) Intermediate handling (buffer)

Bridgwater (A-D) and Petley: 1) Pulp mixing, 2) Disk refining

Klumpar: 1) Pulp handling, 2) Pulp dilution, 3) Disk refining, 4) Storage of water, 5) Storage of cellulose micro- and nanofibers (CMNF)

For the method proposed by Taylor [413], the following table including the complexity scores is shown below. There might be small differences between the calculated value below and the value in the dissertation due to adjusted curves to estimate the costliness index.

Process step number	**Complexity score (CS)**						**Costliness index (1.3^CS)**
	Throughput ratio	**Material of construction**	**Reaction / Storage time**	**Pressure / Temperature**	**Other**	**Total score**	
1	0	1	0	0	0	1	1.3
2	0	1	0	1	2	4	2.8
3	-3	0	1	0	0	-2	0.6
4	0	1	1	0	0	2	1.7
5	0	1	1	0	0	2	1.7
						Total	**10.3**

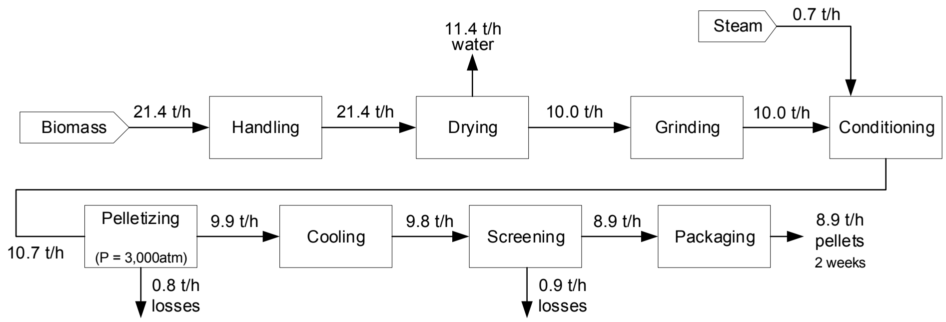
$$Investment\ (OSBL) = (216.1 * \sum (1.3)^{CS} * Q^{0.39}) * 1.3$$

$$Q = 566.7\ kt/yr$$

$$Investment\ (OSBL) = (216.1 * 10.3 * 566.7^{0.39}) * 1.3$$

3- Wood pellets

Flowsheet:



Process steps considered:

Taylor: 1) Feedstock handling, 2) Drying, 3) Grinding, 4) Conditioning, 5) Pelletizing, 6) Cooling, 7) Screening, 8) Final product storage, 9) Biomass storage

Bridgwater (A-D) and Petley: 1) Feeding, 2) Drying, 3) Grinding, 4) Conditioning, 5) Pelletizing, 6) Cooling, 7) Screening

Klumpar: 1) Feeding, 2) Drying, 3) Grinding, 4) Conditioning, 5) Pelletizing, 6) Cooling, 7) Screening, 8) Storage

For the method proposed by Taylor [413], the following table including the complexity scores is shown below. There might be small differences between the calculated value below and the value in the dissertation due to adjusted curves to estimate the costliness index.

Process step number	Complexity score (CS)						Costliness index (1.3^CS)
	Throughput ratio	Material of construction	Reaction / Storage time	Pressure / Temperature	Other	Total score	
1	2	0	0	0	0	2	1.7
2	2	0	0	0	1	3	2.2
3	0.2	0	0	0	0	0.2	1.1
4	0.2	0	0	0	0	0.2	1.1
5	0.2	0	0	5.5	0	5.7	4.5
6	0.2	0	0	0	0	0.2	1.1
7	0.2	0	0	0	0	0.2	1.1
8	0.2	0	1	0	0	1.2	1.4
						Total	**15.4**

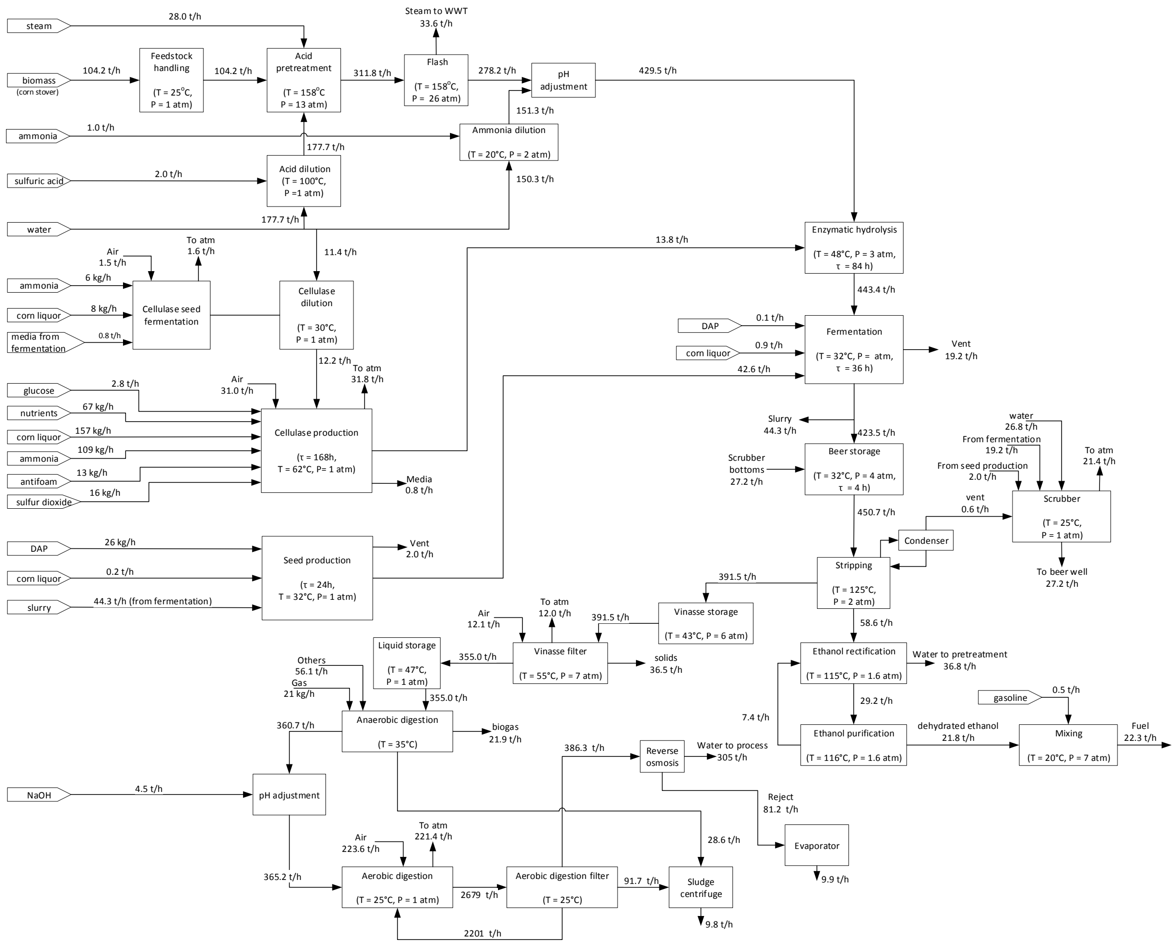
$$Investment\ (OSBL) = (216.1 * \sum (1.3)^{CS} * Q^{0.39}) * 1.3$$

$$Q = 75\ kt/yr$$

$$Investment\ (OSBL) = (216.1 * 15.4 * 75^{0.39}) * 1.3$$

4- Ethanol from corn stover

Flowsheet:



Process steps considered:

<u>Taylor</u>: 1) Biomass storage, 2) Ammonia storage, 3) Sulfuric acid storage, 4) water storage (new), 5) water storage (recycled), 6) Corn liquor storage, 7) Glucose storage, 8) sulfur dioxide storage, 9) DAP storage, 10) Storage of slurry from fermentation, 11) NaOH storage, 12) Gasoline storage, 13) Ethanol storage, 14) Fuel storage, 15) Feedstock handling, 16) Pretreatment with acid, 17) Acid dilution for pretreatment, 18) Flash, 19) pH adjustment, 20) Ammonia dilution, 21) Cellulase seed fermentation, 22) Cellulase production, 23) Cellulase dilution, 24) Enzymatic hydrolysis, 25) Fermentation, 26) Beer storage, 27) Seed production, 28) Stripping, 29) Scrubber, 30) Ethanol rectification, 31) ethanol purification, 32) Mixer (ethanol and gasoline), 33) Intermediate vinasse storage, 34) Vinasse filter, 35) Liquid storage, 36) Anaerobic digestion, 37) pH adjustment with

caustic, 38) Aerobic digestion, 39) Sludge centrifuge, 40) Reverse osmosis, 41) Evaporator, 42) Air compressor to aerobic digestion

Bridgwater (A-D) and Petley: 1) Feedstock handling, 2) Pretreatment with acid, 3) Acid dilution for pretreatment, 4) Flash, 5) pH adjustment, 6) Ammonia dilution, 7) Cellulase seed fermentation, 8) Cellulase production, 9) Cellulase dilution, 10) Enzymatic hydrolysis, 11) Fermentation, 12) Beer storage, 13) Seed production, 14) Stripping, 15) Scrubber, 16) Ethanol rectification, 17) ethanol purification, 18) Mixer (ethanol and gasoline), 19) Vinasse filter, 20) Anaerobic digestion, 21) pH adjustment with caustic, 22) Aerobic digestion, 23) Sludge centrifuge, 24) Reverse osmosis, 25) Evaporator, 26) Air compressor to aerobic digestion

Klumpar: 1) Feedstock handling, 2) Pretreatment, 3) Enzymatic hydrolysis, 4) Fermentation, 5) Stripping, 6) Ethanol rectification and purification, 7) Final product mixing, 8) Sulfuric acid dilution, 9) Ammonia dilution, 10) Celllulase production, 11) Vinasse filter, 12) Anaerobic digestion, 13)Aerobic digestion, 14) Sludge filter, 15) Biomass storage, 16) Sulfuric acid storage, 17) Process water storage, 18) Corn liquor storage, 19) Gasoline storage, 20) Fuel storage

For the method proposed by Taylor [413], the following table including the complexity scores is shown below. There might be small differences between the calculated value below and the value in the dissertation due to adjusted curves to estimate the costliness index.

Process step number	Complexity score (CS)						Costliness index (1.3^CS)
	Throughput ratio	Material of construction	Reaction / Storage time	Pressure / Temperature	Other	Total score	
1	3	1	0	0	1	5	3.7
2	-3	1	0	0	0	-2	0.6
3	-3	1	0	0	0	-2	0.6
4	1	1	0	0	0	2	1.7
5	5	1	0	0	0	6	4.8
6	-3	1	0	0	0	-2	0.6
7	-3	1	0	0	0	-2	0.6
8	-3	1	0	0	0	-2	0.6
9	-3	1	0	0	0	-2	0.6
10	1.2	1	0	0	0	2.2	1.8
11	-3	1	0	0	0	-2	0.6
12	-3	1	0	0	0	-2	0.6
13	0	1	0	0	0	1	1.3
14	0	1	0	0	0	1	1.3
15	2.9	1	0	0	0	3.9	2.8
16	5	1	0	1	0	7	6.3
17	4	1	0	0	0	5	3.7
18	5	1	0	0	0	6	4.8
19	5.7	1	0	0	0	6.7	5.8
20	3.6	1	0	0	0	4.6	3.3
21	-3	1	0	0	0	-2	0.6
22	1.5	1	7.5	0	0	10	13.8
23	-1	1	0	0	0	0	1.0
24	5.5	1	6.5	0	0	13	30.3
25	5.8	1	4.8	0	0	11.6	21.0
26	5.8	1	0.5	0	0	7.3	6.8
27	1.3	1	4	0	0	6.3	5.2
28	5.8	1	0	0	0	6.8	6.0
29	1.5	1	0	0	0	2.5	1.9
30	2	1	0	0	0	3	2.2
31	0.5	1	0	0	0	1.5	1.5
32	0	1	0	0	0	1	1.3
33	5.5	1	0	0	0	6.5	5.5
34	5.3	1	0	0	0	6.3	5.2
35	5.1	1	0	0	0	6.1	5.0
36	5.3	1	0	0	0	6.3	5.2
37	5.2	1	0	0	0	6.2	5.1
38	9	1	0	0	0	10	13.8
39	3.1	1	0	0	0	4.1	2.9
40	5.5	1	0	0	0	6.5	5.5
41	2.5	1	0	0	0	3.5	2.5

Process step number	Complexity score (CS)						Costliness index (1.3^CS)
	Throughput ratio	Material of construction	Reaction / Storage time	Pressure / Temperature	Other	Total score	
42	1.5	1	0	0	0	2.5	1.9
						Total	**190.2**

$$Investment\ (OSBL) = (216.1 * \sum (1.3)^{CS} * Q^{0.39}) * 1.3$$

$$Q = 187\ kt/yr$$

$$Investment\ (OSBL) = \ (216.1 * 190.2 * 187^{0.39}) * 1.3$$

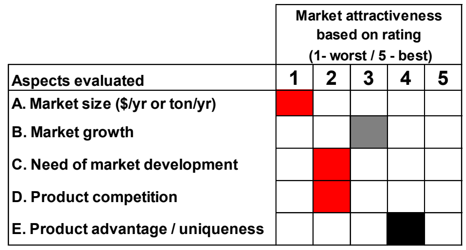
APPENDIX D: Detailed information on proposed method application to case studies

1- Market assessment:

Cellulose nanocrystals

Market evaluation XXX Input values

#	Market aspects	Rating	Comments
A.	Market size ($/yr or ton/yr)	1	Less than 100 MUSD/yr
B.	Market growth	3	CNC expected growth is lower than CMNF
C.	Need of market development	2	Very few applications available
D.	Product competition	2	CNC may displace existing products
E.	Product advantage / uniqueness	4	Renewable, nanoscale, high strength, etc.
Total score (0 - worst / 1- best)		**0.48**	= sum of ratings / 25



Suggested rates

#A - Market size ($/yr or ton/yr)
1 Very small / Inexistent
2 Small
3 Medium
4 Large
5 Very large

#B - Market growth
1 Decreasing
2 Low growth
3 Average growth
4 High growth
5 Very high growth

#C - Need of market development
1 Extensive customer educational program
2 Significant customer education
3 Moderate customer resistance
4 Low customer resistance
5 Ready customer acceptance

#D - Competition with other products
1 Very high - pulverized market, several alternatives available
2 High - alternatives available
3 Moderate - some alternatives available
4 Low - very few competitors
5 Inexistent

#E - Product advantage / uniqueness
1 Very inferior
2 Inferior
3 Similar
4 Superior
5 Very supperior

Cellulose micro- and nanofibrils

Market evaluation | XXX | Input values

#	Market aspects	Rating	Comments
A.	Market size ($/yr or ton/yr)	1	Less than 100 MUSD/yr, 13.8kt/yr for nanocellulose
B.	Market growth	4	Expected 22.1% CAGR (2015-2020) for nanocellulose
C.	Need of market development	3	Few applications available - customer education needed
D.	Product competition	2	CNC may displace existing products
E.	Product advantage / uniqueness	4	Renewable, nanoscale, high strength, etc.
Total score (0 - worst / 1- best)		0.56	= sum of ratings / 25

Aspects evaluated	Market attractiveness based on rating (1- worst / 5 - best) 1	2	3	4	5
A. Market size ($/yr or ton/yr)	■				
B. Market growth				■	
C. Need of market development			■		
D. Product competition		■			
E. Product advantage / uniqueness				■	

Suggested rates

#A - Market size ($/yr or ton/yr)
1 Very small / Inexistent
2 Small
3 Medium
4 Large
5 Very large

#B - Market growth
1 Decreasing
2 Low growth
3 Average growth
4 High growth
5 Very high growth

#C - Need of market development
1 Extensive customer educational program
2 Significant customer education
3 Moderate customer resistance
4 Low customer resistance
5 Ready customer acceptance

#D - Competition with other products
1 Very high - pulverized market, several alternatives available
2 High - alternatives available
3 Moderate - some alternatives available
4 Low - very few competitors
5 Inexistent

#E - Product advantage / uniqueness
1 Very inferior
2 Inferior
3 Similar
4 Superior
5 Very supperior

Lignin micro- and nanoparticles

Market evaluation | XXX | Input values

#	Market aspects	Rating	Comments
A.	Market size ($/yr or ton/yr)	1	Inexistent
B.	Market growth	2	Expected low growth in coming years
C.	Need of market development	1	Extensive customer education program needed, applications are being developed in laboratory scale
D.	Product competition	2	LMNP will substitute other products
E.	Product advantage / uniqueness	4	renewable, nanoscale, high stiffness, antioxidant, low toxicity, low density, UV absorbance
Total score (0 - worst / 1 - best)		**0.40**	= sum of ratings / 25

Market attractiveness based on rating (1- worst / 5 - best)

Aspects evaluated	1	2	3	4	5
A. Market size ($/yr or ton/yr)	■				
B. Market growth		■			
C. Need of market development	■				
D. Product competition		■			
E. Product advantage / uniqueness				■	

Suggested rates

#A - Market size ($/yr or ton/yr)
1 Very small / Inexistent
2 Small
3 Medium
4 Large
5 Very large

#B - Market growth
1 Decreasing
2 Low growth
3 Average growth
4 High growth
5 Very high growth

#C - Need of market development
1 Extensive customer educational program
2 Significant customer education
3 Moderate customer resistance
4 Low customer resistance
5 Ready customer acceptance

#D - Competition with other products
1 Very high - pulverized market, several alternatives available
2 High - alternatives available
3 Moderate - some alternatives available
4 Low - very few competitors
5 Inexistent

#E - Product advantage / uniqueness
1 Very inferior
2 Inferior
3 Similar
4 Superior
5 Very supperior

Wood pellets

Market evaluation XXX Input values

#	Market aspects	Rating	Comments
A.	Market size ($/yr or ton/yr)	4	Large - 20 billion USD WW, 26 Mt/ yr in 2015
B.	Market growth	3	10 - 14% annually
C.	Need of market development	5	Ready customer acceptance - commercial product available
D.	Product competition	3	Alternatives for energy generation are available (gas, oil, etc.)
E.	Product advantage / uniqueness	3	Renewable source of energy, advantage: regulations may allow consumption
Total score (0 - worst / 1 - best)		0.72	= sum of ratings / 25

Aspects evaluated	Market attractiveness based on rating (1- worst / 5 - best)				
	1	2	3	4	5
A. Market size ($/yr or ton/yr)					
B. Market growth					
C. Need of market development					
D. Product competition					
E. Product advantage / uniqueness					

Suggested rates

#A - Market size ($/yr or ton/yr)
1 Very small / Inexistent
2 Small
3 Medium
4 Large
5 Very large

#B - Market growth
1 Decreasing
2 Low growth
3 Average growth
4 High growth
5 Very high growth

#C - Need of market development
1 Extensive customer educational program
2 Significant customer education
3 Moderate customer resistance
4 Low customer resistance
5 Ready customer acceptance

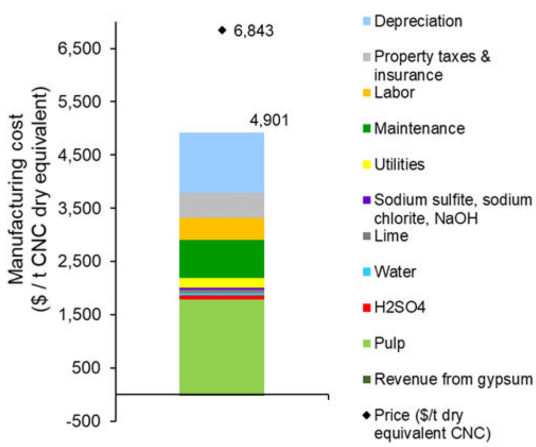
#D - Competition with other products
1 Very high - pulverized market, several alternatives available
2 High - alternatives available
3 Moderate - some alternatives available
4 Low - very few competitors
5 Inexistent

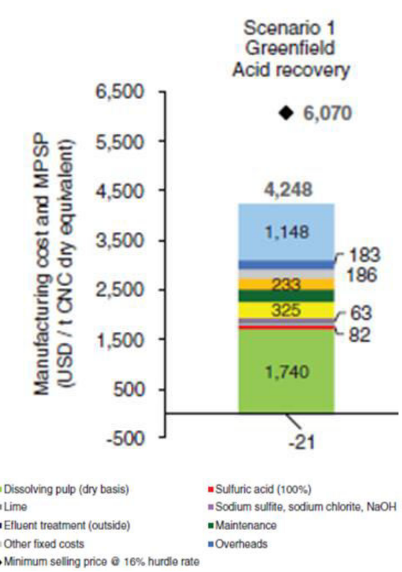
#E - Product advantage / uniqueness
1 Very inferior
2 Inferior
3 Similar
4 Superior
5 Very supperior

2- Cash flow assessment

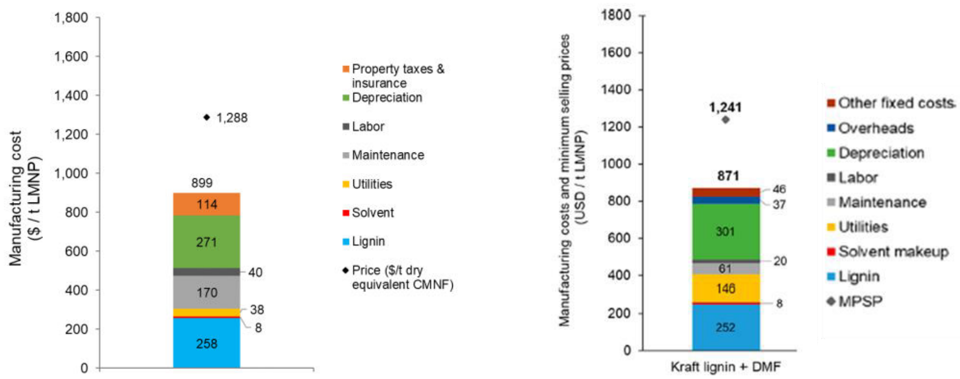
a. Composition of manufacturing costs

CNC – Early stage assessment (left) vs. detailed assessment (right) [121]

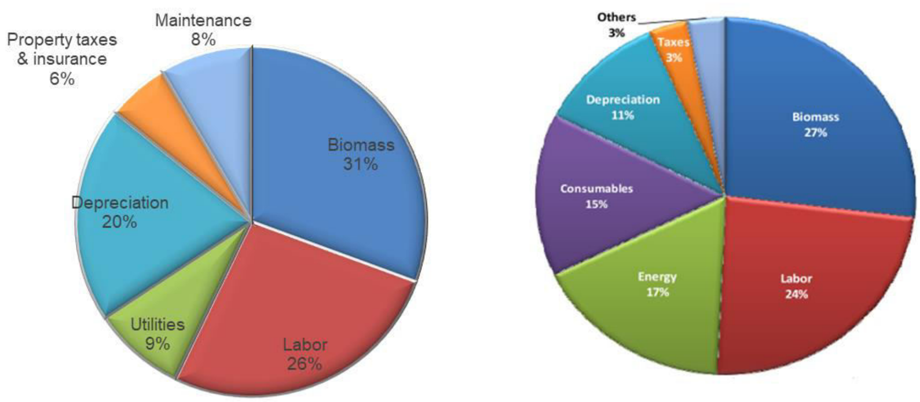




LMNP – Early stage assessment (left) vs. detailed assessment (right) [429]



Wood pellets – Early stage assessment (left) vs. detailed assessment (right) [420]

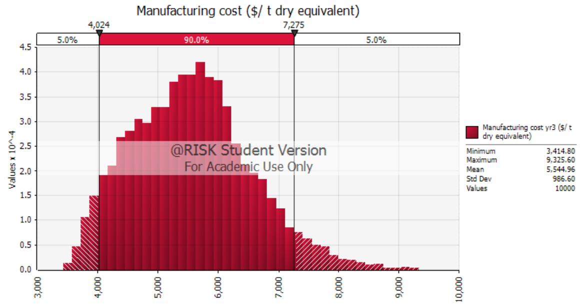


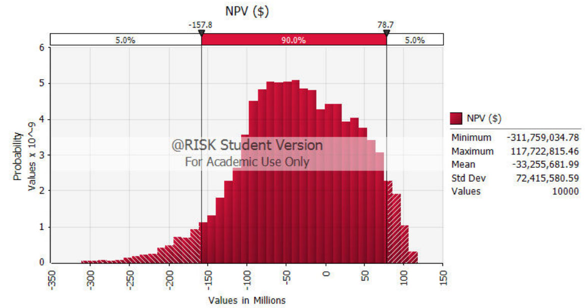
b. Quantitative risk assessment

CNC – Uncertainties considered

Uncertainty considered	Range of values	Source of information	Comments
Hydrolysis yield	45% – 55%	Pilot plant	Triangular distribution centered at 50%
Raw material costs	707 – 2,198 USD/t	Historical data (RISI) [96]	Distribution curve adjusted to historical data
Capital investment	+ / - 50 % of estimated value	Uncertainty in estimation at TRL 6 (see Table 7-9)	Uniform distribution

CNC – manufacturing costs (left) and MPSP distribution (right). CNC prices fixed as the MPSP.





Manufacturing cost ranges

- Early stage assessment: 3,400 – 9,300 USD/t (dry equivalent)
- Detailed assessment: 3,160 – 6653 USD/t (dry equivalent)

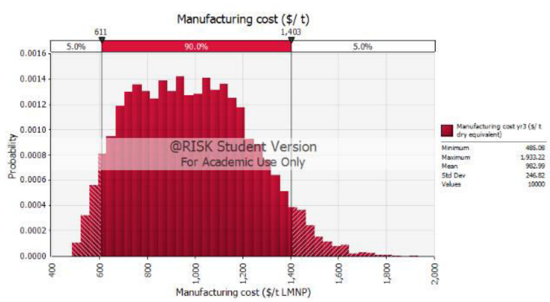
Project NPV

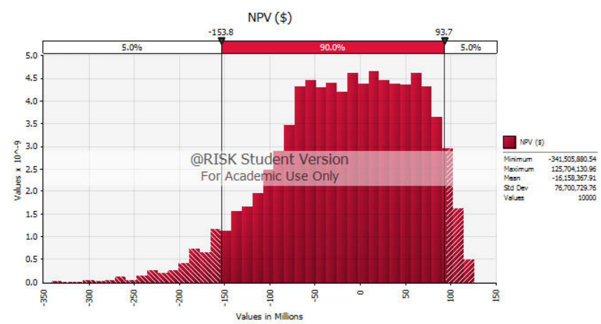
- Early stage assessment: -312 – 118 MUSD
- Detailed assessment: -145 – 67 MUSD

LMNP – Uncertainties considered

Uncertainty considered	Range of values	Source of information	Comments
Lignin concentration	2% - 10%	Laboratory data	Triangular distribution centered at 6%
Separator efficiency	95% – 100%	Assumed for industrial scale facility	Triangular distribution centered at 99%
Lignin cost	250 – 500 USD/t	Literature [178]	Triangular distribution skewed to the left
Capital investment	+ / - 70%	Uncertainty in estimation at TRL 4 (see Table 7-9)	Uniform distribution

LMNP – manufacturing costs (left) and MPSP distribution (right). LMNP prices fixed as the MPSP.

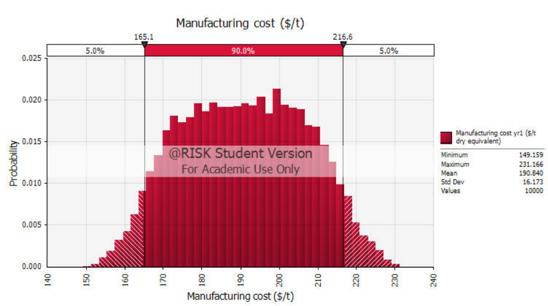


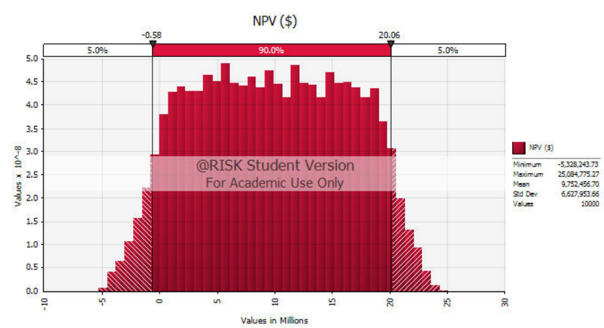


Wood pellets – Uncertainties considered

Uncertainty considered	Range of values	Source of information	Comments
Pelletizer efficiency	83% - 100%	Assumed	Triangular distribution centered at 92%
Biomass cost	57 – 69 USD/t (dry equivalent)	Literature [420]	Triangular distribution centered at 99%
Capital investment	+ / - 50%	Uncertainty in estimation at TRL 9 (see Table 7-9)	Uniform distribution
Energy costs	10 – 15% (of raw material + labor costs)	Suggested values for energy cost (section 7.3.5.3.3)	Triangular skewed to the right
Labor costs	+ / - 25 % of estimated value	Estimation accuracy (section 0)	Uniform distribution

Wood pellets – manufacturing costs (left) and MPSP distribution (right). Wood pellets prices fixed as the average market price (276 USD/t [420]).





Impact of price variation in project NPV

Case study	Price (USD/ t)	Chance of NPV <0	NPV range (MUSD) – 90% confidence interval
CNC	5,500 (-16%)	92 %	- 250 / +12
	6,603 (ref.)	65 %	-160 / + 79
	7,500 (+13%)	49 %	-119 / + 110
LMNP	800 (-37%)	93%	-274 / + 5
	1,288 (ref.)	55%	-154 / + 94
	2,200 (+70%)	3%	+26 / + 258
Wood pellets	235 (-15%)	53%	-11 / + 10
	276 (ref.)	7%	-0.6 / + 20
	317 (+15%)	0%	+10 / + 30

Impact of product sales in project NPV

Case study	Price (USD/ t)	Chance of NPV <0	NPV range (MUSD) – 90% confidence interval
CNC	50%	75%	-185 / +53
	80%	65%	-160 / +79
	100%	58%	-145 / +93
LMNP	50%	62%	-180 / 76
	80%	55%	-154 / +94
	100%	49%	-137 / 105
Wood pellets	50%	44%	-10 / +12
	80%	21%	-4 / +17
	100%	7%	-0.6 / +20