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Techno-economic analysis and life cycle assessment of manufacturing a cellulose nanocrystal-based hybrid membrane

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ABSTRACT

Moisture-selective polymer-based membranes can be a promising method for energy saving in drying systems of different industries that vent moisture vapor-rich air to the atmosphere, such as wood drying, biorefinery, food processing, and pharmaceutical industry. Developing a sustainable product with bio-based materials reduces the environmental impacts. This study assessed the techno-economic feasibility and life-cycle environmental impacts of producing a novel cellulose nanocrystal/polydimethylsiloxane hybrid moisture-selective membrane. The cradle-to-gate assessment was facilitated by developing an industrial-scale membrane production process model guided by optimized experimental results. The estimated plant capital, operating cost, and annual revenue of a 10 MT/day capacity cellulose nanocrystal/polydimethylsiloxane membrane production plants were $136 million, $139 million, and $198 million respectively. The estimated minimum selling price of the final product, 1 m^2 80 μm thick cellulose nanocrystal/polydimethylsiloxane membrane was $3.68/$m^2$, which is lower or comparable to the current alternative market retail price. The environmental impacts of the cellulose nanocrystal/polydimethylsiloxane production process were lower for all evaluated environmental impact categories, with an estimated global warming impact of 8.7 kg CO_2 eq/m^2 of 80 μm thick cellulose nanocrystal/polydimethylsiloxane membrane, representing a 12 % reduction compared to polydimethylsiloxane membrane production without cellulose nanocrystal. The small addition of cellulose nanocrystal to the polydimethylsiloxane membrane provided relatively lower environmental impacts with a similar cost and thus ought to be the preferred choice.

1. Introduction

Wood processing industries use thermal energy to dry wood products for dimensional stability before using them for constructing buildings, furniture, and other products. For the wood industry, wood drying tends to be one of the highest energy consumers even though its primary source is woody biomass (Puettmann et al., 2010; Puettmann and Milota, 2017; Sahoo et al., 2019). Conventional steam kiln (also known as heat-and-vent kiln) drying is the most common technique used by wood processing industries to dry lumber and other solid wood products (Bergman, 2021; Meng et al., 2019), mainly due to their large capacity, flexible drying schedules for various wood species, and high efficiency of drying time, compared with other drying processes such as vacuum drying (Espinoza and Bond, 2016; Lyon et al., 2021), solar drying (Khouya, 2022), super-critical drying, dehumidification kiln drying, and microwave drying (Chuchala et al., 2020). It was estimated that the conventional kiln drying process accounts for 50–70 % of total energy consumption for lumber production in softwood sawmills (Bergman and Bowe, 2010; He et al., 2016; Milota and Puettmann, 2017; Puettmann, 2020) and an even higher percentage for hardwood sawmills (Bergman and Bowe, 2008, 2012; Denig et al., 2000; Hubbard et al., 2020; Heidari et al., 2023). However, approximately 20 % of the energy (i.e., heat) is lost in traditional ventilation, which is due to the direct exhaust of hot and moist air derived from force-drying the freshly-sawn lumber (Garrahan, 2008; Meng et al., 2019). Different energy recovery methods have been developed and used to recover the heat and water from outlet exhaust, such as organic Rankine cycle, absorption systems, condensation methods, waste heat boilers, and heat exchangers, but these

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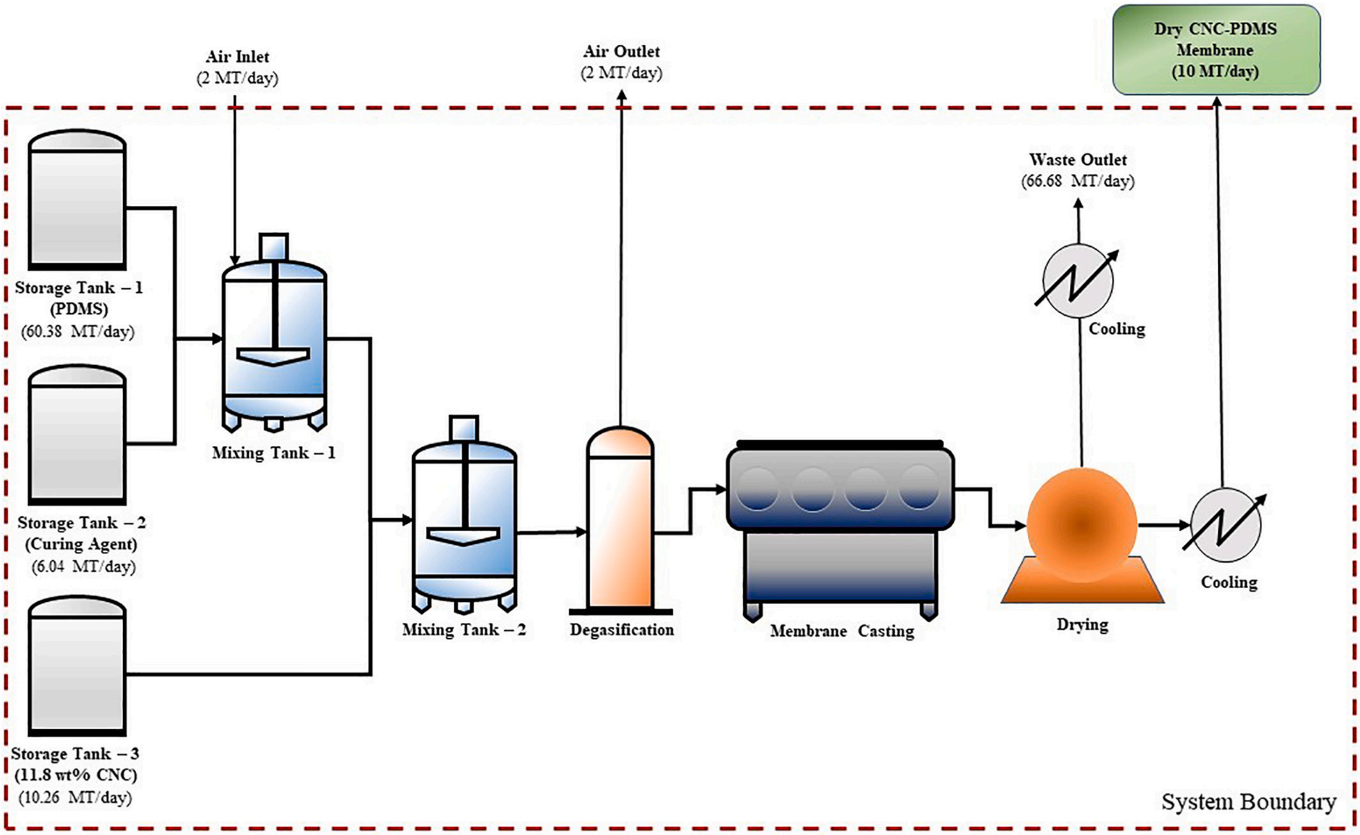


Fig. 1. Process flow of cellulose nanocrystal/polydimethylsiloxane membrane production.
Note: PDMS: polydimethylsiloxane/CNC: cellulose nanocrystal.

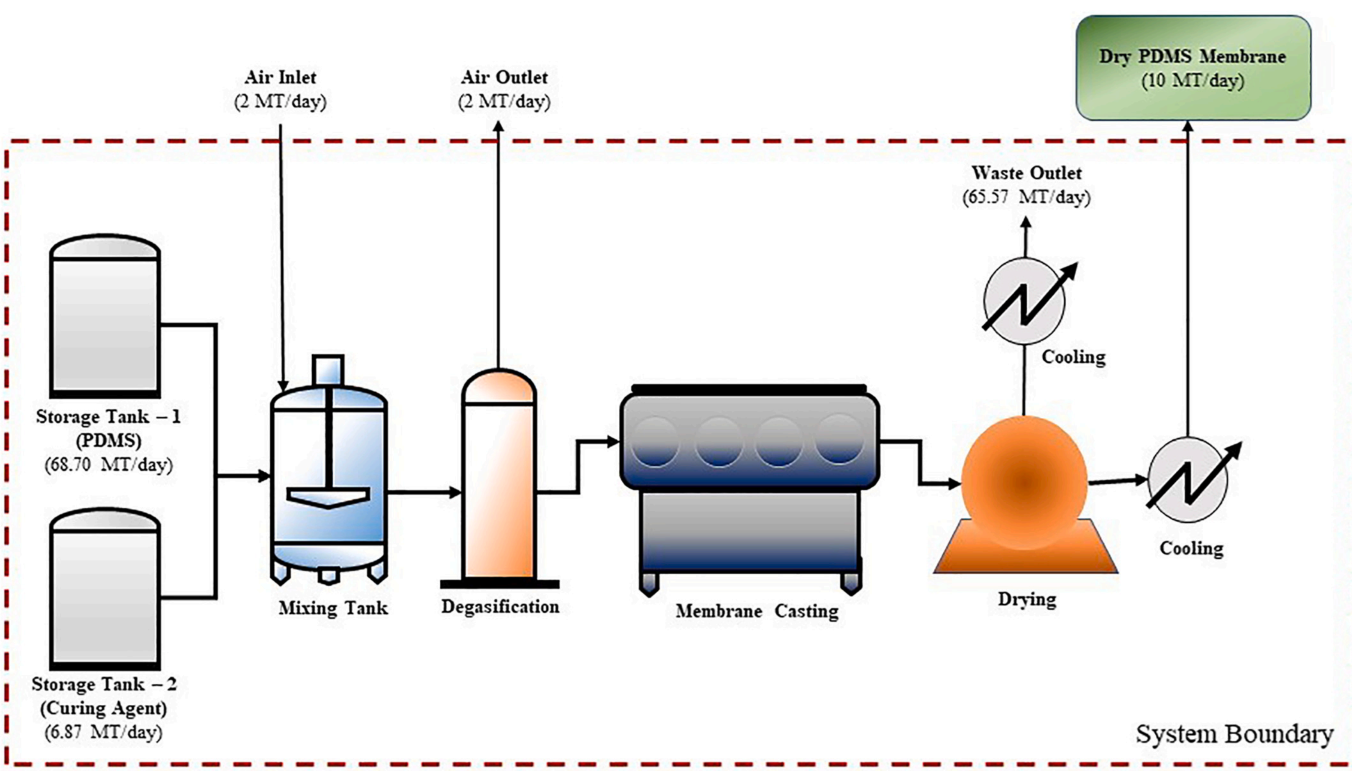


Fig. 2. Process flow of polydimethylsiloxane membrane production.
Note: PDMS: polydimethylsiloxane.

Table 1
Minimum, base, and maximum values of raw materials, tax, and project lifetime used for the sensitivity analysis.

Variables	Minimum value	Base value	Maximum value
PDMS ($/kg)	2.38	4.75	7.13
Curing Agent ($/kg)	2.50	5.00	7.50
CNC ($/kg)	4.37	8.73	13.09
Tax rate (%)	10	21	30
Project lifetime (yr)	15	20	25

Table 2
Life cycle inventory process and database used for membrane fabrication.

Material	Life cycle inventory database
Polydimethylsiloxane	Ecoinvent 3: polydimethylsiloxane {GLO}|market for polydimethylsiloxane|APOS, U
Curing Agent (Sylgard 184)	Curing Agent (developed proxy)
Cellulose nanocrystals	Gu et al., 2015 (USDA CNC pilot plant)
Water	DATASMART (US EI 2.2): water, deionised, at plant/US* US-EI U
Steam	DATASMART (US EI 2.2): steam, for chemical processes, at plant/US US-EI U
Electricity	DATASMART (US EI 2.2): electricity, medium voltage, at grid, Wisconsin/US US-EI U
Wastewater	Ecoinvent 3: wastewater, average {RoW}|market for wastewater, average|APOS, U

methods are either expensive as they require a large surface area, or the efficiency of energy recovery is greatly affected by environmental conditions. For example, the energy recovery efficiency of heat exchangers is very low if the vents are open to get fresh moist air on rainy/snowy days. Thus, the development of a high-efficiency, low-cost heat recovery technology is necessary for improving the sustainability of conventional kiln-based wood drying (Zhao et al., 2017).

One of the most efficient technologies to recover heat and water from exhaust air steam is membrane separation technology (Zhao et al., 2017). This isothermal air dehumidification process has been

Table 3
Equipment cost (SuperPro built-in cost model) for 10 MT/day of membrane.

Description	Cellulose nanocrystal/ polydimethylsiloxane ($)	Polydimethylsiloxane ($)
Membrane casting machine	14,806,000.00	14,676,000.00
Drum dryer	306,000.00	304,000.00
Flat bottom tank	34,000.00	34,000.00
Flat bottom tank	34,000.00	34,000.00
Flat bottom tank	34,000.00	0.00
Degasifier	10,000.00	10,000.00
Heat exchanger	8000.00	8000.00
Heat exchanger (waste outlet)	90,000.00	78,000.00
Tumble mixer	5000.00	5000.00
Tumble mixer	4000.00	0.00
Unlisted equipment	3,832,000.00	3,788,000.00
Total	19,163,000.00	18,937,000.00

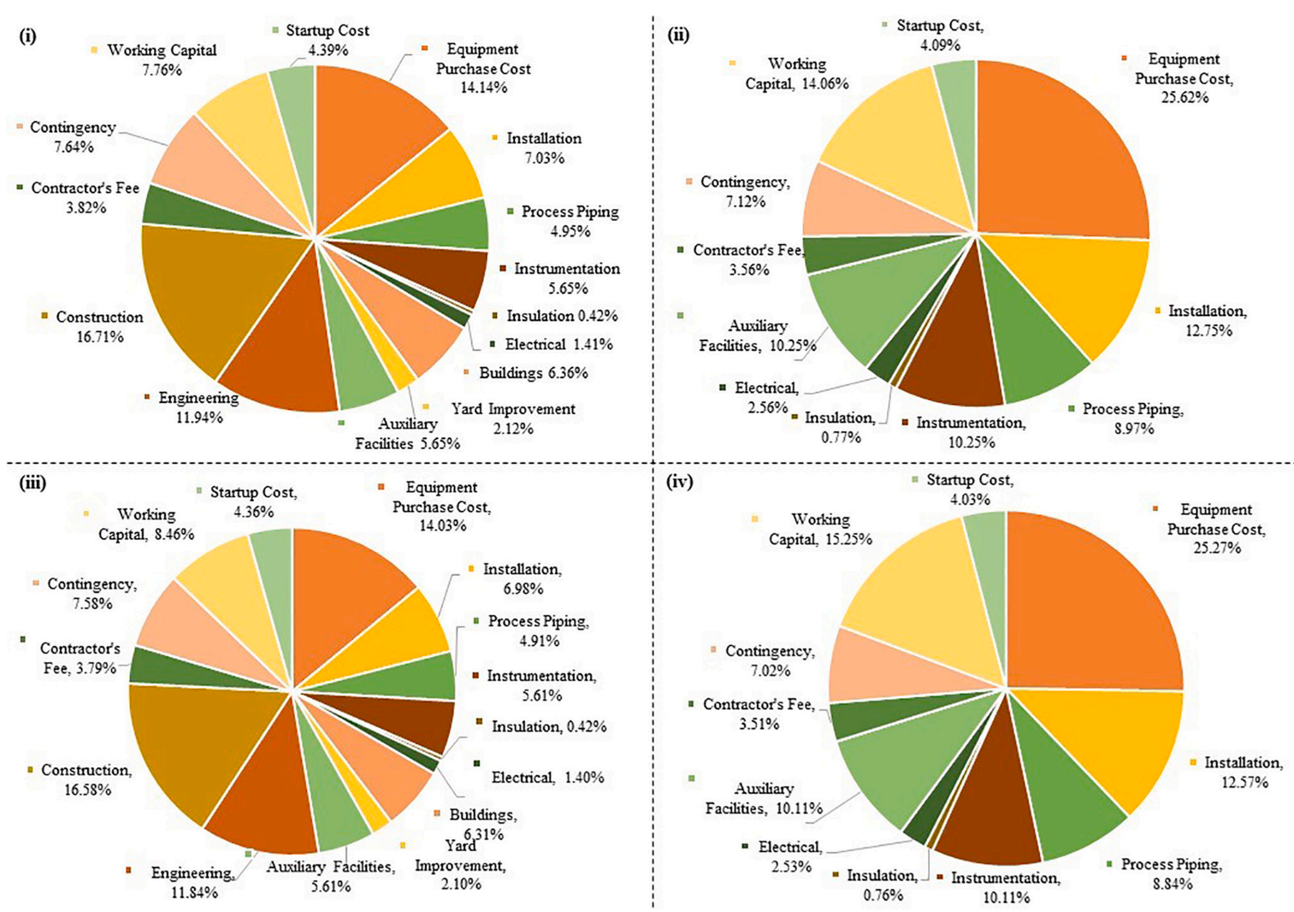


Fig. 3. Capital investment of membrane preparation (i) cellulose nanocrystal/polydimethylsiloxane membrane preparation (greenfield) - $135,564,000 (ii) cellulose nanocrystal/polydimethylsiloxane membrane preparation (expanding in an existing plant) - $74,786,000, (iii) polydimethylsiloxane membrane preparation (greenfield) – $135,000,000, and (iv) polydimethylsiloxane membrane preparation (expanding in an existing plant) – $74,941,000.

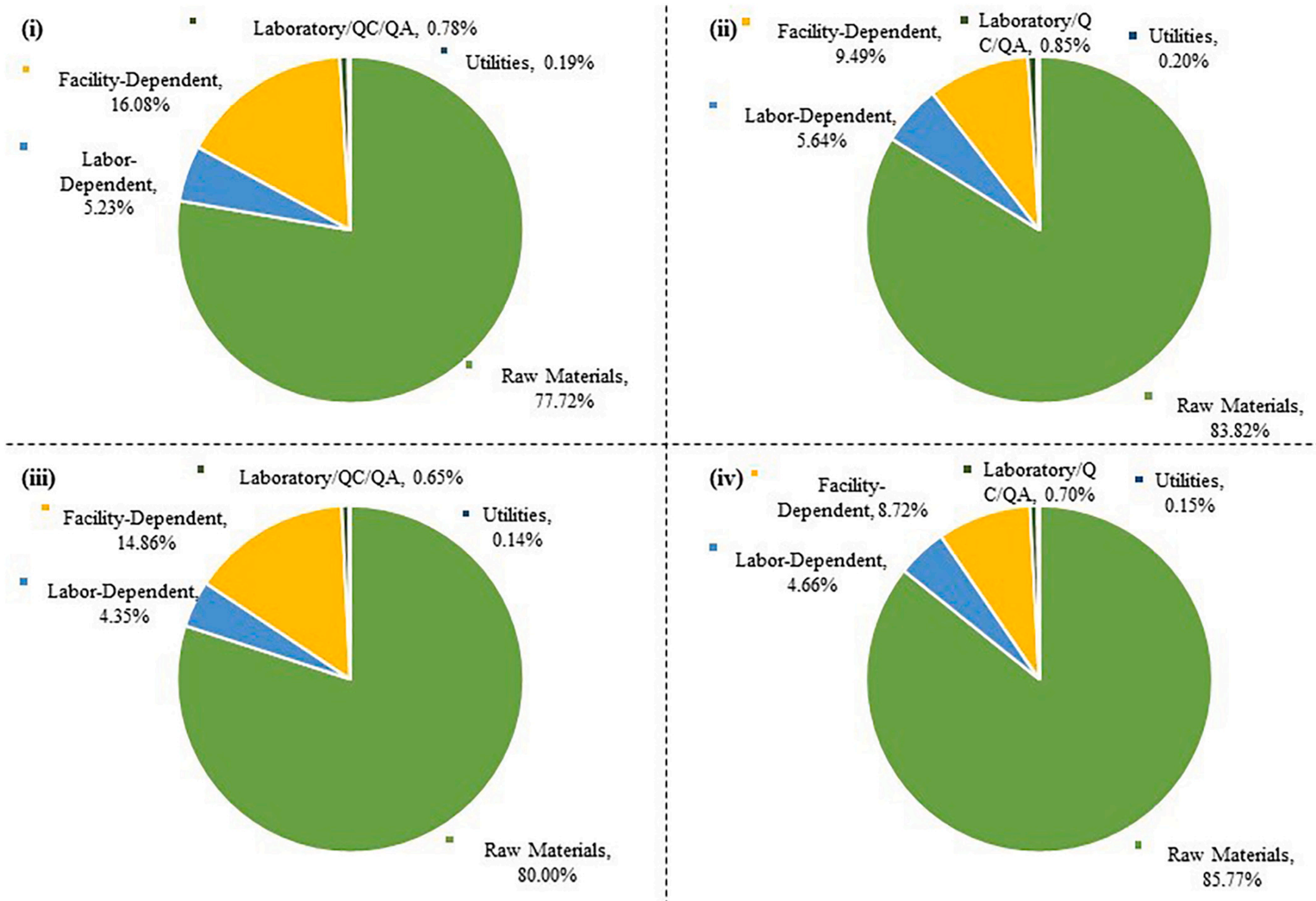
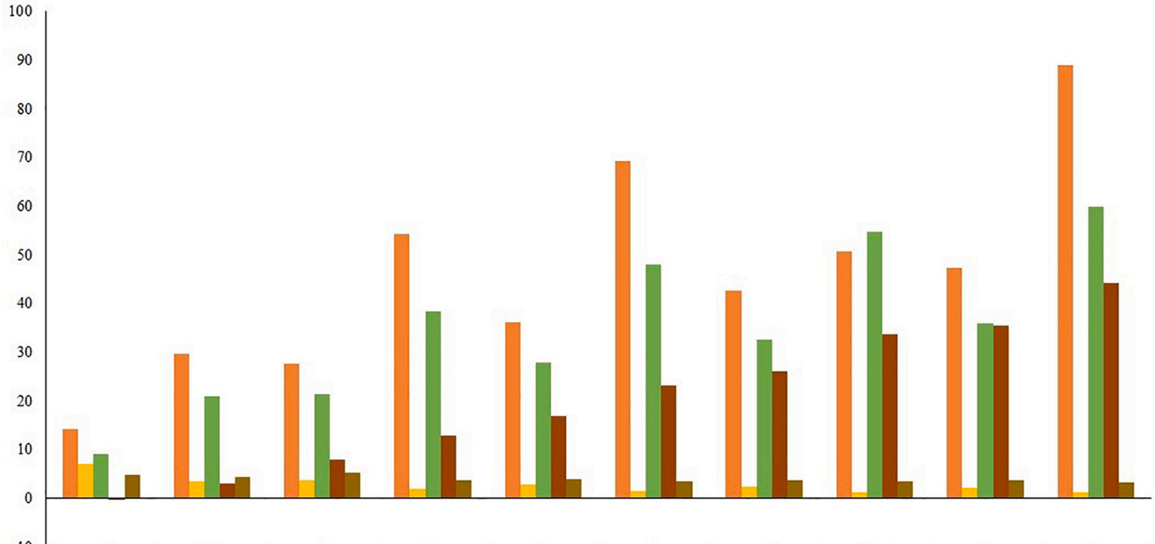


Fig. 4. Annual operating cost of membrane preparation (i) cellulose nanocrystal/polydimethylsiloxane membrane preparation (greenfield) - $139,119,000 (ii) cellulose nanocrystal/polydimethylsiloxane membrane preparation (expanding in an existing plant) - $128,989,000, (iii) polydimethylsiloxane membrane preparation (greenfield) – $148,785,000 and (iv) polydimethylsiloxane membrane preparation (expanding in an existing plant) – $138,775,000.

Table 4
Economic summary of the membrane production process.

Description	Cellulose nanocrystal/ polydimethylsiloxane (Greenfield)	Cellulose nanocrystal/polydimethylsiloxane (expanding in an existing plant)	Polydimethylsiloxane (Greenfield)	Polydimethylsiloxane (expanding in an existing plant)
Capital investment ($)	135,564,000.00	74,786,000.00	135,000,000.00	74,941,000.00
Operating cost ($/yr)	139,119,000.00	128,989,000.00	148,785,000.00	138,775,000.00
Revenues ($/yr)	197,921,000.00	197,921,000.00	197,921,000.00	197,921,000.00
Cost basis annual rate (kg/yr)	3,298,680.00	3,298,680.00	3,298,680.00	3,298,680.00
Net unit production cost ($/kg)	42.17	39.10	45.10	42.07
Unit production revenue ($/kg)	60.00	60.00	60.00	60.00
Gross margin (%)	29.71	34.83	24.83	29.88
Return on investment (%)	42.61	80.59	37.04	70.02
Payback time (Yr)	2.35	1.24	2.70	1.43
IRR (after taxes) (%)	32.53	54.81	28.87	49.44
NPV (at 10.0 % interest) ($)	260,994,000.00	335,868,000.00	209,492,000.00	314,361,000.00
MSP of membrane ($/m^2)	3.68	3.35	3.93	3.60

successfully used in different fields such as food, pharmaceutical and chemical industries, wastewater treatment, desalination and bio-refineries. The membrane types are grouped into dense (0.1 nm) and porous (0.1 μm) categories based on their pore structure. Dense membranes are used in energy recovery ventilators due to their efficiency, high permeability, high water selectivity, easy scale-up, low cost, and



	2.5		5		7.5		10		12.5	
	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)
Return On Investment (%)	14.11	29.64	27.67	54.24	36.17	69.34	42.61	50.59	47.43	88.92
Payback Time (Year)	7.09	3.37	3.61	1.84	2.76	1.44	2.35	1.24	2.11	1.12
IRR (After Taxes) (%)	9.13	20.88	21.33	38.33	27.89	47.97	32.53	54.81	35.89	59.82
NPV (at 10.0% Interest) (10M$)	-0.34	2.90	7.84	12.81	16.78	23.10	26.10	33.59	35.49	44.12
MSP ($/m sq)	4.88	4.29	5.22	3.69	3.85	3.47	3.69	3.35	3.59	3.28

Fig. 5. Estimated effects on the profitability factors and minimum selling price of changes on plant capacity (MT/day) for producing cellulose nanocrystal/polydimethylsiloxane membranes, (i) cellulose nanocrystal/polydimethylsiloxane membrane preparation (greenfield), (ii) cellulose nanocrystal/polydimethylsiloxane membrane preparation (expanding in an existing plant).

low carbon footprint (Baldinelli et al., 2019). It was reported that the membrane-based process consumes less than 90 % of energy compared to the conventional distillation technique (Liang et al., 2019). Different polymeric membranes such as nitrocellulose, polyethylene, cellulose acetate, polysulfone hollow fiber, polyamide, polyimide, polyacrylonitrile polypropylene and polydimethylsiloxane (PDMS) are used for water and gas separation processes (Liang and Chung, 2018; Sidhikku Kandath Valappil et al., 2021).

This study selected the PDMS membrane due to its good chemical resistance and processability. Commercially, the PDMS polymer membrane is widely used for water, gas, and vapor separation, which is the most gas-permeable polymer membrane due to flexible siloxane linkage and adequate water/nitrogen selectivity (Liang and Chung, 2018). Different material combinations of PDMS membranes have been used for different applications such as zeolitic imidazole frameworks-PDMS (Şahin et al., 2020), glass wool-polydopamine-PDMS (Kang et al., 2019), and PDMS-ceramic (Chen et al., 2019). Targeting wood drying applications, Alikhani et al. conducted a lab-scale experiment to investigate the dehumidification efficiency of pure PDMS dense membrane under simulated drying conditions and suggested that this membrane separation technique can be used as a pre-drying process to enhance wood drying efficiency (Alikhani et al., 2020). Different PDMS-coated and mixed matrix membranes were developed and used for enhancing the water vapor and volatile organic compound separation performance. For example, Liang et al. (Lejarazu-Larrañaga et al., 2022) developed a PDMS-coated polyacrylonitrile (PAN) hollow fiber membrane to separate water vapor from moist air and gases. The PDMS-coated PAN membrane showed better performance than the PAN membrane, which was more stable and had a water vapor removal rate of 65 % from moist air.

Nanocellulose materials, such as cellulose nanofiber (CNF) and cellulose nanocrystal (CNC), have been widely used as reinforced nanofillers or additives in different applications, due to their high mechanical stability, low thermal expansion, non-toxicity, large surface area, high strength, biodegradability, and renewability. CNCs are produced from different sources such as lignocellulosic sources, animal, algae, and bacteria sources using different methods of acid hydrolysis, mechanical method, oxidation method, ionic liquid treatment, subcritical water hydrolysis and enzyme hydrolysis (Trache et al., 2017). CNCs have been used in different industrial applications such as biomedical engineering, wastewater treatment, energy and electronics, oil and gas, food industries, painting and coating, and construction (Grishkewich et al., 2017). CNCs have also been used in films and membranes in biosensors and wastewater treatment to reduce the use of non-biodegradable materials (Gomri et al., 2022). Xia et al. developed a multilayer sandwiched membrane ((Si-CNC)-PDMS-(Si-CNC)) with improved storage modulus, barrier performance, optical scattering, and hazing. Boron nitride nanosheet-CNC/PDMS matrix membrane shows high thermal stability than pure PDMS membrane (Zhang et al., 2021). Li et al. developed a synthesis process to fabricate CNC-PDMS hybrid membrane materials with the intention to increase its water vapor permeability and found that adding 1 % by weight of CNC in PDMS could increase the water vapor transmission rate at room temperature by about 20 % to 30 % (Li et al., 2021).

When applying the moisture-selective PDMS membrane in wood drying processes that use conventional temperatures of 43 °C to 82 °C (Simpson, 1991), the water vapor permeability at elevated temperatures needs to be investigated. Currently, there is a lack of information on the moisture separation of PDMS membranes at such temperatures. Research on the measurement of the water vapor and gas permeability of synthesized CNC-PDMS membrane materials at 25 °C, 50 °C, and 80 °C was investigated through laboratory experiments by the experimental research group at the University of Maine, which results are briefly discussed in the Subsection of 3.1. The economic and environmental impact analysis is important to find the membrane market sustainability. Techno-economic analysis (TEA) and lifecycle assessment (LCA) of membrane production were not discussed much previously and very few studies are available. Hong et al. (2023) discussed the TEA and LCA of polyimide flat sheet membranes with green solvent based on a lab-scale model (Hong et al., 2023).

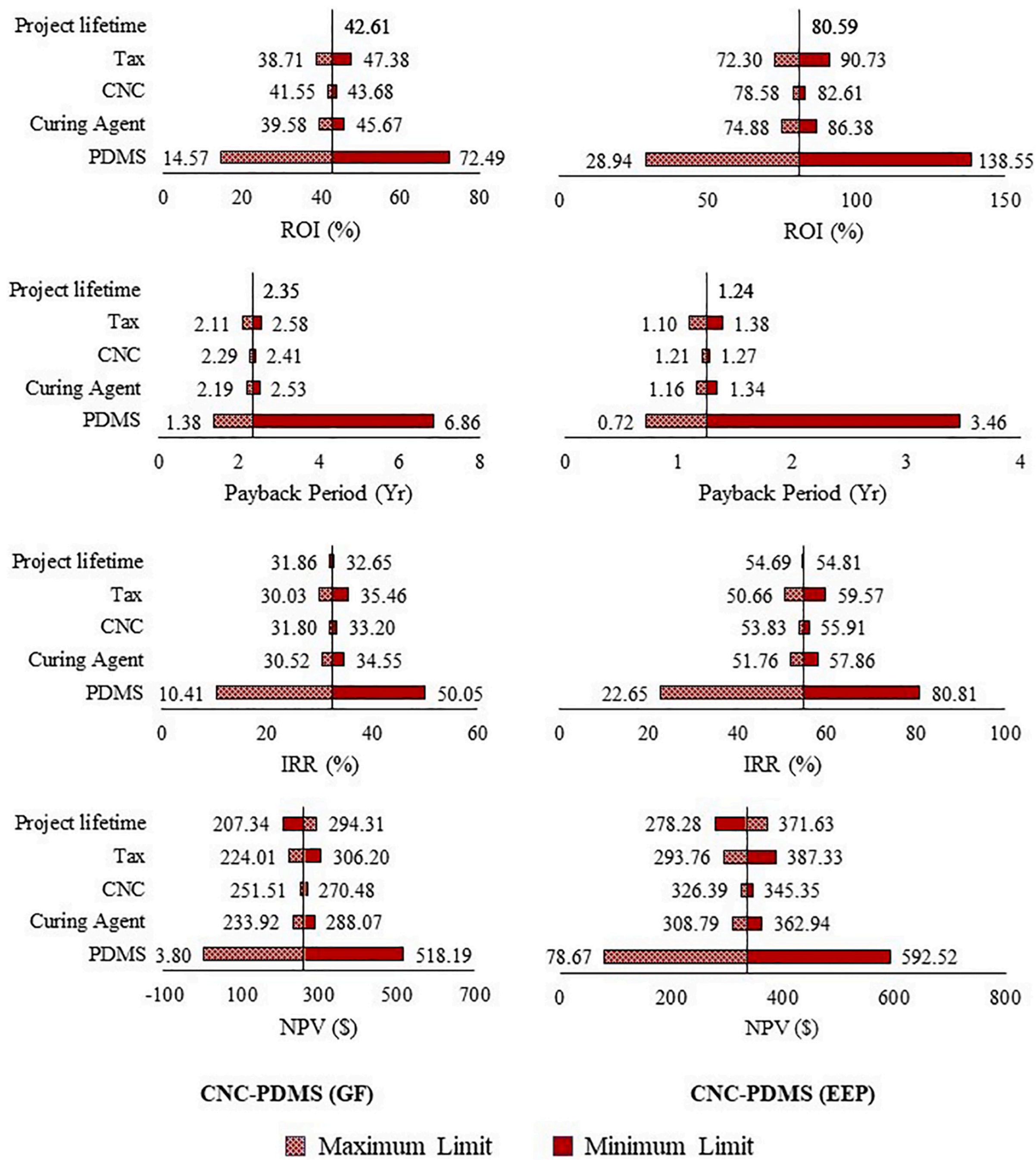


Fig. 6. The effects of changes in economic variables on various measures of profitability factors for greenfield (GF) (left) and expanding in an existing plant (EEP) (right) cellulose nanocrystal/polydimethylsiloxane production scenarios.
Note: PDMS: polydimethylsiloxane/CNC: cellulose nanocrystal.

The laboratory experiments provided information on the optimized processes needed to develop an industrial-scale process model of novel CNC-PDMS production and to understand the financial viability and environmental performance of the entire CNC-PDMS production process, which are two major focuses of this study. This study developed an industrial scale process model of the CNC-PDMS production and subsequently evaluated its technical and financial viability through techno-economic analysis (TEA) and its environmental performance through life cycle assessment (LCA). TEA helps guide decisions about investing in further research or commercialization of innovations and LCA helps understand the environmental burden of producing a product through its entire life cycle. Performing TEA and LCA in the early stages of development can provide developers and their customers with information on economic and technical feasibility and environmental impact as the products are developed. In this study, membrane performance was not included and will be published as a separate work in the future. But this work helps to further membrane-related economic and environmental studies.

2. Materials and methods

Using data and information from experiments and industry, a process simulation modeling approach was used to model the CNC-PDMS membrane manufacturing and its scale-up analysis. For the optimal scale, the TEA and cradle-to-gate LCA methods were used to estimate the financial performance indicators and life cycle environmental impacts,

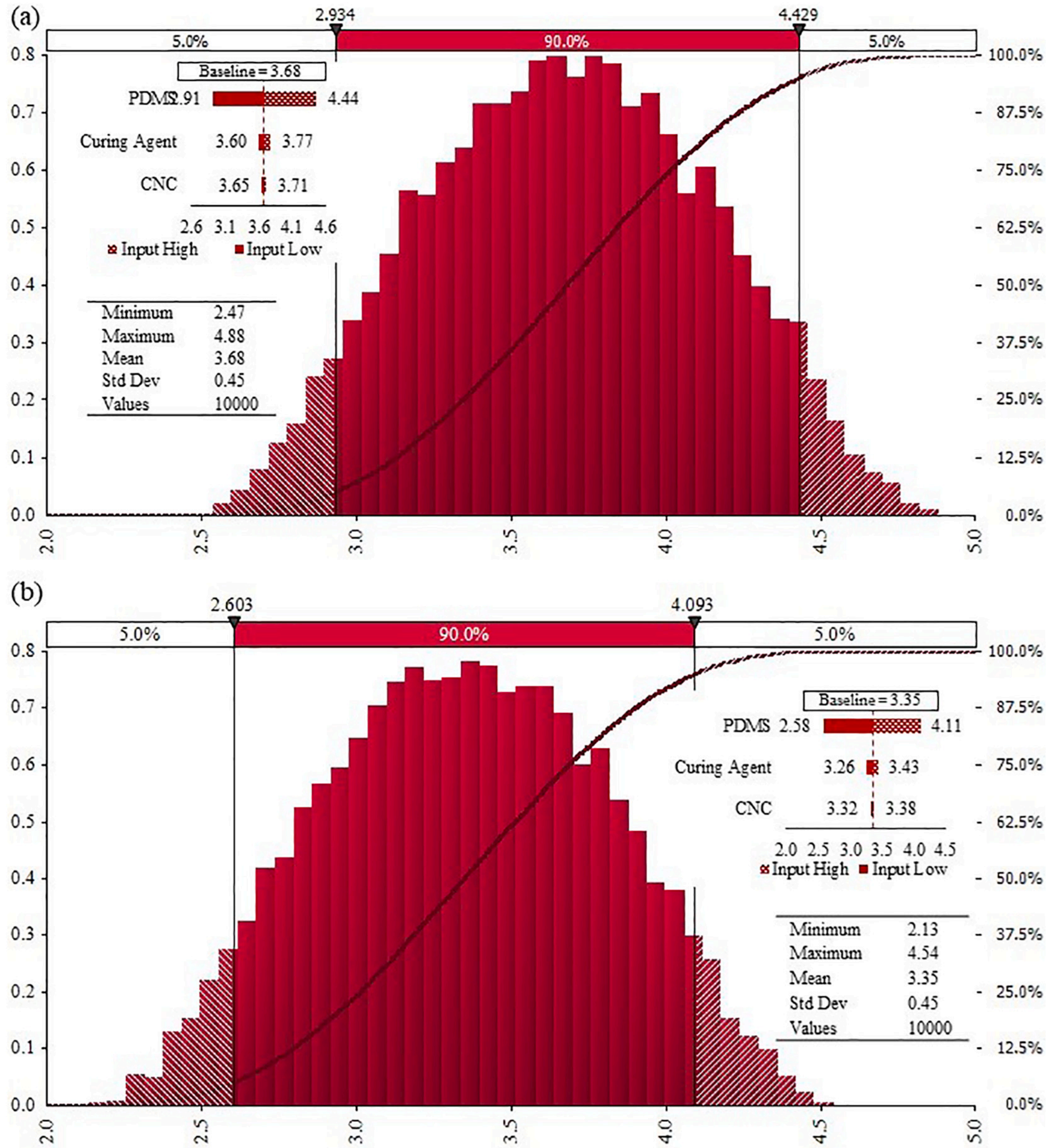
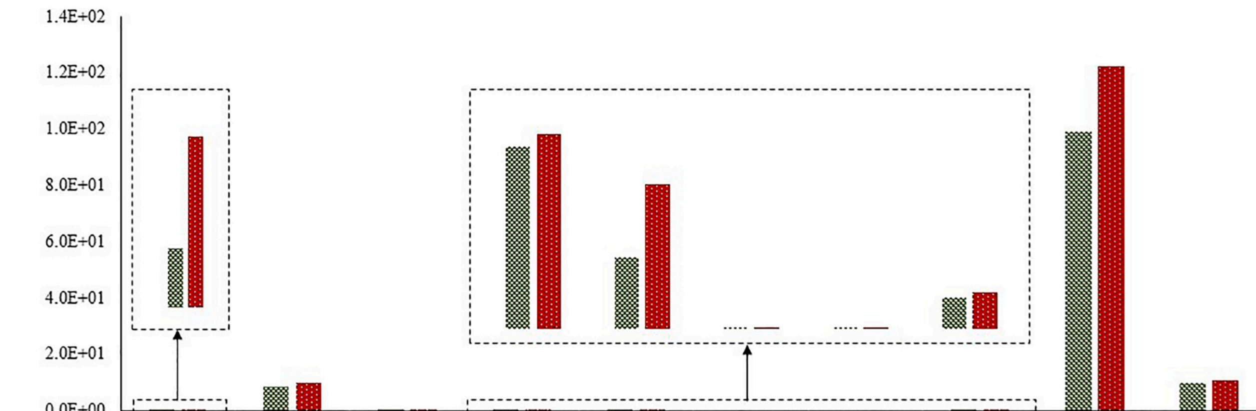


Fig. 7. Uncertainty on the estimated MSP based due to changes in prices of polydimethylsiloxane, curing agent, and cellulose nanocrystal (a) cellulose nanocrystal/polydimethylsiloxane actual scenario (b) cellulose nanocrystal/polydimethylsiloxane greenfield scenario.
Note: PDMS: polydimethylsiloxane/CNC: cellulose nanocrystal.

Table 5
Input and output materials and energy consumption per m^2 of cellulose nanocrystal/polydimethylsiloxane membrane production.

Material/energy	Unit	1 m^2 of PDMS-CNC Membrane			1 m^2 of PDMS Membrane		
		Input	Output (wastewater outlet)	Output (product steam)	Input	Output (wastewater outlet)	Output (product steam)
Polydimethylsiloxane	kg	0.4983			0.5668		
Curing agent (Sylgard 184)	kg	0.0495			0.0569		
Cellulose nanocrystals	kg	0.0099					
Water	kg	0.0751					
Membrane	kg			0.0825			0.0825
Total (material)	kg	0.6328			0.6237		
Steam	kg	0.2888			0.2327		
Electricity	kW-h	0.0157			0.0124		
Wastewater	l		0.5654			0.5577	



	Ozone depletion	Global warming	Smog	Acidification	Eutrophication	Carcinogenics	Non carcinogenics	Respiratory effects	Ecotoxicity	Fossil fuel depletion
CNC-PDMS	8.2E-03	8.7E+00	6.1E-01	4.9E-02	1.9E-02	4.0E-07	1.9E-06	8.6E-03	99.04	10.08
PDMS	9.3E-03	9.9E+00	7.1E-01	5.3E-02	3.9E-02	5.4E-07	3.8E-06	1.0E-02	122.49	10.93

Fig. 8. Estimated cradle-to-gate life cycle impacts of cellulose nanocrystal/polydimethylsiloxane and polydimethylsiloxane membranes.
Note: PDMS: polydimethylsiloxane/CNC: cellulose nanocrystal.

respectively for the CNC-PDMS membrane.

2.1. Lab-scale cellulose nanocrystal/polydimethylsiloxane membrane production

The synthesis method of CNC-PDMS membrane materials followed the solution casting method described in (Li et al., 2021) with a modification of increasing the CNC concentration to 2 % by weight. A 2 % concentration of CNC is the optimal ratio of adding CNC to PDMS, which is being reported in detail in a separate article in progress by the experimental research group. A brief description of the synthesis method is provided below:

PDMS prepolymer and curing agent were mechanically mixed at a ratio of 10:1 by weight using a magnetic stirrer plate at 125 rpm for 5 min at room temperature. An appropriate amount of CNC suspension with a solid content of 11.8 % was added to the mixture, ensuring CNC solids were 2 % of the weight of PDMS prepolymer. The mixture with added CNC was then mixed for 1 h using the magnetic stirrer plate at 125 rpm and room temperature. The mixed solution was degassed for 45 s. The degassed solution was cast on a Teflon plate using a casting knife adjusted to obtain a nominal thickness of 150 μm (wet film thickness). The wet membrane samples were dried under vacuum at a vacuum pressure of 88 kPa for 1 h. Lastly, the semi-cured membrane was further dried in an oven at 50 °C for 24 h.

2.2. Techno-economic analysis of polydimethylsiloxane membrane and cellulose nanocrystal/polydimethylsiloxane membrane production

The process and costs related to the membrane preparation process were modeled using SuperPro Designer v12 software based on the optimized experimental results and industrial data (Canizales et al., 2020). The process flow of CNC-PDMS and PDMS membrane preparation were developed and shown in Figs. 1 and 2. In this study, the plant production capacity was assumed at 10 MT of membrane per day with the plant running time of 7920 h/yr and the plant's lifetime of 20 years. Currently, a few large industries annually produce 5 million m^2 membrane (approximately 1.5 MT/day), based current market we assumed 10 MT per day as per future aspects in this study. The income tax rate was set at 21 % (IRS, 2017). The cost of the general equipment in the process was determined using the SuperPro Designer equipment cost database (Canizales et al., 2020), and the cost of the membrane casting equipment was obtained from MEMS-Wellspring Expand Co., Ltd., South Korea (MEMS-Wellspring Expand Co., Ltd., South Korea, 2022). The cost of PDMS base ($4.75/kg) and curing agent ($5/kg) was collected from the e-commerce website (https://www.alibaba.com/, 2022) and the CNC price ($8.73/kg) data was collected from peer-reviewed literature (Bondancia et al., 2020). The price of the membrane was assumed to be $60/kg ($5/m^2 of 80 μm thick membrane) based on commercial price (MEMS-Wellspring Expand Co., Ltd., South Korea, 2022; Shielding Solutions Limited, 2022). Detailed economic data and information used in the analysis are presented in Tables 1 and 2. In this study, two process flows with two different scenarios were evaluated including (i) CNC-PDMS membrane preparation (greenfield), (ii) CNC-PDMS membrane preparation (expanding in an existing plant), (iii) PDMS membrane preparation (greenfield), and (iv) PDMS membrane preparation (expanding in an existing plant). Scenarios (ii) and (iv) denoted that the plant was constructed at the existing production location, and therefore the costs of building construction and yard improvement, and the construction and engineering fees were considered zero.

In techno-economic analysis, capital investment, operating costs, and profitability factors such as the return on investment (ROI), payback period, internal rate of return (IRR), and net present value (NPV) were calculated (Rajendran and Han, 2023). Capital investment mainly depends on equipment cost and the costs of plant construction and development, which includes direct fixed capital, working capital, and startup cost. Direct fixed cost includes the direct costs associated with equipment, installation, and project development; indirect cost, which includes fees associated with engineering and construction; and other cost, which includes contractor's fees and contingency costs. The operating cost includes facility-dependent costs, labor, laboratory, utilities, and some miscellaneous costs (Naveenkumar and Baskar, 2020, 2021a). A sensitivity analysis was carried out to understand the robustness of the estimated profitability factors and to identify the key variables affecting the results. In sensitivity analysis, the plant capacity, raw material cost, tax and project lifetime were varied, and the corresponding changes in profitability factors were investigated (Naveenkumar and Baskar, 2019, 2021b). Next, the minimum selling price (MSP) of the final product, 1 m^2 of 80 μm thick CNC-PDMS membrane was calculated and compared with the PDMS membrane. The MSP is an indicator of product sustainability in the current market, as it indicates the minimum price that a provider can sell while still covering the costs of its production. Finally, a Monte Carlo simulation was applied to determine the uncertainty of the estimated MSPs of CNC-PDMS membranes under the actual and greenfield process scenario. A Monte Carlo simulation was conducted to gauge the uncertainty in the estimated MSP given the variation in prices of PDMS, curing agent and CNC by ±50 % (Table 1). The Monte Carlo

Table 6
Contribution analysis of environmental impacts of cellulose nanocrystal/polydimethylsiloxane and polydimethylsiloxane membrane production, cradle-to-gate, mass allocation.

Impact category	Unit	PDMS		Curing Agent		Water		Steam		Electricity		CNC		Wastewater		Total	
		CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS	CNC-PDMS	PDMS
Ozone depletion	kg CFC-11 eq	7.5×10^{-3}	8.6×10^{-3}	6.6×10^{-4}	7.5×10^{-4}	2.9×10^{-14}	0.0	4.1×10^{-12}	3.3×10^{-12}	4.0×10^{-10}	3.2×10^{-10}	1.1×10^{-8}	0.0	2.6×10^{-11}	2.5×10^{-8}	8.2×10^{-3}	9.3×10^{-3}
Global warming	kg CO2 eq	$7.7 \times 10^{+0}$	$8.8 \times 10^{+0}$	6.7×10^{-1}	7.7×10^{-1}	8.1×10^{-8}	0.0	7.6×10^{-5}	6.1×10^{-5}	1.2×10^{-2}	9.4×10^{-3}	2.9×10^{-1}	0.0	3.1×10^{-4}	3.1×10^{-1}	$8.7 \times 10^{+0}$	$9.9 \times 10^{+0}$
Smog	kg O3 eq	5.5×10^{-1}	6.2×10^{-1}	4.8×10^{-2}	5.5×10^{-2}	3.9×10^{-9}	0.0	1.4×10^{-6}	1.1×10^{-6}	4.9×10^{-4}	3.9×10^{-4}	1.7×10^{-2}	0.0	2.9×10^{-5}	2.8×10^{-2}	6.1×10^{-1}	7.1×10^{-1}
Acidification	kg SO2 eq	4.0×10^{-2}	4.6×10^{-2}	3.5×10^{-3}	4.0×10^{-3}	3.3×10^{-10}	0.0	1.8×10^{-7}	1.4×10^{-7}	5.5×10^{-5}	4.3×10^{-5}	5.3×10^{-3}	0.0	2.8×10^{-6}	2.7×10^{-3}	4.9×10^{-2}	5.3×10^{-2}
Eutrophication	kg N eq	1.7×10^{-2}	2.0×10^{-2}	1.5×10^{-3}	1.7×10^{-3}	1.8×10^{-10}	0.0	1.6×10^{-8}	1.3×10^{-8}	3.2×10^{-5}	2.5×10^{-5}	5.0×10^{-4}	0.0	1.8×10^{-5}	1.8×10^{-2}	1.9×10^{-2}	3.9×10^{-2}
Carcinogenics	CTUh	3.6×10^{-7}	4.1×10^{-7}	3.1×10^{-8}	3.6×10^{-8}	6.2×10^{-15}	0.0	4.6×10^{-13}	3.7×10^{-13}	5.3×10^{-10}	4.2×10^{-10}	8.2×10^{-9}	0.0	9.7×10^{-11}	9.6×10^{-8}	4.0×10^{-7}	5.4×10^{-7}
Non carcinogenics	CTUh	1.7×10^{-6}	1.9×10^{-6}	1.5×10^{-7}	1.7×10^{-7}	2.9×10^{-14}	0.0	1.5×10^{-12}	1.2×10^{-12}	1.8×10^{-9}	1.4×10^{-9}	8.6×10^{-8}	0.0	1.7×10^{-9}	1.7×10^{-6}	1.9×10^{-6}	3.8×10^{-6}
Respiratory effects	kg PM2.5 eq	7.7×10^{-3}	8.7×10^{-3}	6.7×10^{-4}	7.7×10^{-4}	2.7×10^{-11}	0.0	1.7×10^{-8}	1.3×10^{-8}	3.3×10^{-6}	2.6×10^{-6}	3.0×10^{-4}	0.0	5.3×10^{-7}	5.2×10^{-4}	8.6×10^{-3}	1.0×10^{-2}
Ecotoxicity	CTUe	$9.0 \times 10^{+1}$	$1.0 \times 10^{+2}$	$7.8 \times 10^{+0}$	$9.0 \times 10^{+0}$	4.4×10^{-7}	0.0	3.8×10^{-5}	3.1×10^{-5}	4.3×10^{-2}	3.4×10^{-2}	9.6×10^{-1}	0.0	1.1×10^{-2}	$1.1 \times 10^{+1}$	$9.9 \times 10^{+1}$	$1.2 \times 10^{+2}$
Fossil fuel depletion	MJ surplus	$8.6 \times 10^{+0}$	$9.8 \times 10^{+0}$	7.6×10^{-1}	8.7×10^{-1}	1.1×10^{-7}	0.0	1.7×10^{-4}	1.4×10^{-4}	1.1×10^{-2}	8.5×10^{-3}	7.1×10^{-1}	0.0	2.8×10^{-4}	2.7×10^{-1}	$1.0 \times 10^{+1}$	$1.1 \times 10^{+1}$

Note: PDMS: polydimethylsiloxane/CNC: cellulose nanocrystal.

simulation assumed a Program (or Project) Evaluation and Review Technique (PERT) distribution with 10,000 iterations.

2.3. Life cycle assessment of polydimethylsiloxane membrane and cellulose nanocrystal/polydimethylsiloxane membrane production

The environmental impacts of the CNC-PDMS and PDMS membrane production processes were estimated using the cradle-to-gate LCA method based on the ISO 14040 and 14044 standards (ISO, 2006a, 2006b). Using the optimal plant scale, this was facilitated by developing a life cycle inventory (LCI) flows using the data and information on input and output of the process mass and energy flows. In this study, DATASMART (2022) and Ecoinvent 3 databases (Wernet et al., 2016) were used for background LCI data. The cradle-to-gate environmental impacts of CNC-PDMS and PDMS membrane production processes were estimated using SimaPro 9.3 LCA software (PRé Consultants, 2021) under 10 impact categories including ozone depletion, global warming (GW), smog, acidification, eutrophication, carcinogenics, non-carcinogenics, respiratory, ecotoxicity and fossil fuel depletion following the tool for the reduction and assessment of chemical and other environmental impacts (TRACI) 2.1 methodology (Bare, 2011). The scope of the LCA in this study was to calculate the cradle-to-gate environmental impacts of CNC-PDMS membrane production considering 1 m^2 of the membrane at the plant output gate as a functional unit. The life cycle inventory database is shown in Table 2.

3. Results and discussion

Along with economic and life-cycle environmental impacts were presented based on a commercial-scale operation of 10 MT/day production of the final product, 1 m^2 of 80 μm thick CNC-PDMS and PDMS thick membranes. The CNC-PDMS membrane had an average thickness of 80 μm when the wet film thickness was 150 μm. Because of the homogeneous distribution of CNC in PDMS, the CNC-PDMS membrane samples were semi-transparent.

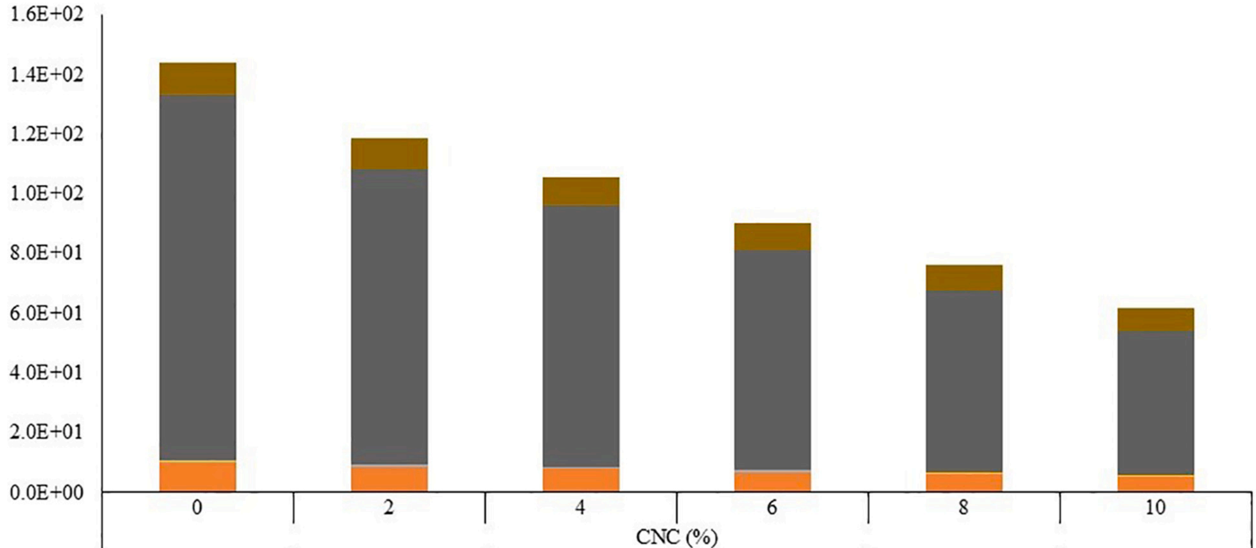
3.1. Process flow description

In the CNC-PDMS process flow, 10 MT/day of the membrane was produced from 60.38 MT/day of PDMS, 6.04 MT/day of curing agent and 12.26 MT/day of CNC (11.8 % wt. solids). The process resulted in an annual production of 3300 MT of membrane, which did not include membrane cutting and packing. In the PDMS process flow, 10 MT/day of the membrane was produced from 68.70 MT/day of PDMS and 6.87 MT/day of curing agent. In this process, CNC was not used, and a mixing unit function was eliminated, except that the process is like CNC-PDMS. Around 66.68 MT/day (86.96 %) and 65.57 MT/day (86.77 %) of input materials were evaporated in the drying process of the CNC-PDMS and PDMS membranes, respectively. The evaporated materials were condensed and outputted as waste material. The waste material comprised of used PDMS and curing agent was sent to a waste treatment facility because these two compounds were not able to be separated for reuse at this time. The impacts from treating the waste were included in the analysis.

3.2. Economic analysis

3.2.1. Capital investment

Fig. 3 shows detailed capital investment under four scenarios of membrane production. The estimated capital investment for a 10 MT/day membrane manufacturing plant in the four scenarios was $136 million, $75 million, $135 million, and $75 million, respectively. The equipment cost was the base for all cost calculations (Table 3). Around 78 % of the total equipment cost was shared by the membrane casting machine. Because a slow membrane process requires large size equipment, it increases the cost of the membrane casting machine as well as



	0	2	4	6	8	10
Fossil fuel depletion	1.1E+01	1.0E+01	9.6E+00	8.9E+00	8.3E+00	7.8E+00
Ecotoxicity	1.2E+02	9.9E+01	8.8E+01	7.4E+01	6.1E+01	4.9E+01
Respiratory effects	1.0E-02	8.6E-03	7.9E-03	6.9E-03	6.1E-03	5.2E-03
Non carcinogenics	3.8E-06	1.9E-06	1.8E-06	1.6E-06	1.4E-06	1.2E-06
Carcinogenics	5.4E-07	4.0E-07	3.6E-07	3.1E-07	2.6E-07	2.2E-07
Eutrophication	3.9E-02	1.9E-02	1.7E-02	1.5E-02	1.3E-02	1.1E-02
Acidification	5.3E-02	4.9E-02	4.9E-02	4.8E-02	4.7E-02	4.6E-02
Smog	7.1E-01	6.1E-01	5.5E-01	4.8E-01	4.2E-01	3.5E-01
Global warming	9.9E+00	8.7E+00	7.9E+00	7.0E+00	6.1E+00	5.2E+00
Ozone depletion	9.3E-03	8.2E-03	7.2E-03	5.9E-03	4.8E-03	3.7E-03

Fig. 9. The effect on environmental impacts of increasing the percent of CNC on PDMS membrane, cradle-to-gate.

overall equipment cost. The plan was developed at the existing industrial location, so the costs associated with building, yard improvement, engineering, and construction were zero. While the costs of construction and equipment were the top contributors to capital investment in actual scenarios (scenarios (i) and (iii)), the cost of equipment dominated in the greenfield scenarios (scenarios (ii) and (iv)). As expected, the greenfield scenarios resulted in a substantial reduction in capital investment (by around 45 %) compared to the actual scenarios. The capital investment of the PDMS plant was lower than CNC-PDMS plant due to the reduction of unit operations.

3.2.2. Operating cost

A detailed breakdown of the estimated operating costs of membrane production is shown in Fig. 4. The annual operating costs of the plant in the four scenarios were $139 million, $129 million, $149 million, and $139 million, respectively, which included the costs associated with the raw materials, labor, facility-dependent, laboratory, and utilities. The cost of raw materials was the largest contributor to total operating costs. For example, the PDMS cost covered 87.5 % in scenarios (i) and (ii), and 90.5 % in scenarios (iii) and (iv). Apart from raw material cost, facility-dependent and labor cost also contributed somewhat to total operating costs. The facility-dependent cost included maintenance, depreciation, insurance, local taxes, and factory expense, which depends on direct fixed capital cost. While the large numbers or sizes of equipment increased annual maintenance costs, the continuous process resulted in reduced labor costs.

3.2.3. Profitability and minimum selling price

The modeled plant annually produced 3300 MT of the membrane with annual revenue of $197.92 million. The estimated economic metrics such as gross margin, ROI, payback period, IRR and NPV are shown in Table 4. Scenario (ii) showed the highest gross margin, ROI, IRR, NPV and lowest payback period among all scenarios due to low capital investment and operating costs. The estimated MSPs of 1m^2 of 80 μm thick membrane in the four scenarios were about $3.68, $3.35, $3.93, and $3.60 respectively. Note that 1 kg is equal to 12 m^2 of the 80 μm thick membrane. The addition of CNC increases the membrane performance and reduces the amount of PDMS, resulting in a relatively lower estimated MSP of CNC-PDMS membrane (scenarios i and ii) compared to PDMS membrane (scenarios iii and iv). Scenarios (ii) and (iv) further reduced the estimated MSP of membranes by 8–9 % compared to scenarios (i) and (iii). The commercial price of PDMS membrane is very high currently as it is a specialty material. Its cost varies depending on the quantity and thickness, with the cost increasing with decreasing thickness of the membrane. Reducing the thickness of the membrane increases the production time. The current commercial market retail price of a 1 m^2 80 μm thick membrane is around $112, which will most likely reduce in the future with increased economies of scale (Shielding Solutions Limited, 2022) The PDMS membrane is mostly produced on a lab-scale and pilot-scale and therefore estimated industrial-scale manufacturing costs are critical for future industry endeavors. Sanchis-Perucho et al. (2020) assumed that the price of 1 m^2 of PDMS membrane was €30. Raw materials pricing is one of the major factors determining the MSP of the products, which was also found true in this study. The next section presents the results of the sensitivity analysis to understand the effects of changes in PDMS price on the estimated MSP of the membrane.

3.3. Sensitivity analysis

In sensitivity analysis, different variables such as plant capacity, raw material price, tax, and project lifetime were varied, and their effects on profitability factors were analyzed. The sensitivity analysis was carried out only for the CNC-PDMS scenarios (scenarios i and ii). The effect on the profitability of changes in plant capacity was evaluated by varying plant capacity from 2.5 to 12.5 MT/day with an increment of 2.5 MT/day. While the increment of plant capacity increased the capital investment and operating cost of membrane production, it also increased the profitability and reduced the MSP of the membrane due to increased economy of scale. The opposite effect was observed with lower plant capacities. For example, scenario (i) showed a negative NPV when the plant capacity was 2.5 MT/day (Fig. 5). In most cases, the lower plant capacity was not economically feasible and resulted in higher MSP of the membranes.

Similarly, the effects on profitability factors of changes in the costs of raw materials were evaluated by varying the prices of PDMS, curing agent and CNC by ±50 %, and the results indicated that the profitable factors were most sensitive to the assumed PDMS prices (Fig. 6). Likewise, the sensitivity of lower and higher taxes rates (10 % and 30 %) and project lifetime (15 and 25 years), indicated that tax reduction and subsidies would help develop an economically viable plant and that longer-term projects would improve the profitability factors, especially the IRR and NPV.

A PERT distribution was assumed as it represents a continuous probability distribution defined by the minimum, most likely and maximum values that a variable can take. Fig. 7 shows the results of the simulation summarized in terms of the probability density, cumulative curve, and statistical results. As shown in Fig. 7, the estimated 90 % confidence interval of CNC-PDMS membrane's MSP in scenario (i) fell between $2.93/kg (lower bound) to $4.43/kg (upper bound). Similarly, the estimated 90 % confidence interval of the CNC-PDMS membrane's MSP in scenario (ii) was between $2.60/kg to $4.09/kg. The PDMS price was the key factor impacting the uncertainty of the estimated MSP of the membrane.

3.4. Life-cycle environmental impact analysis

The amounts of input materials and energy needed for the preparation of 1 m^2 of CNC-PDMS and PDMS membranes are shown in Table 5. These data are based on a large-scale SuperPro Designer database. The production of 1 m^2 of CNC-PDMS membrane required 0.4983 kg of PDMS, 0.0495 kg of curing agent (Sylgard 184), 0.0099 kg of CNC, 0.0751 kg of water, 0.2888 kg of steam and 0.0157 kWh of electricity. PDMS is a major compound used in membrane production, and the needed amounts of PDMS and curing agent increase in the absence of CNC in the membrane production process. The information on curing agent (Sylgard 184) is not available in the SimaPro database libraries and therefore was developed based on Palchesko et al. (Palchesko et al., 2012) and the DOW® Safety data sheet (DOW, 2019). The curing agent contains xylene (0.19 %), ethylbenzene (0.10 %), dimethyl methylhydrogen siloxane (55 %), dimethylvinyl-terminated dimethyl siloxane (15 %), dimethylvinylated and trimethylated silica (10 %), and tetramethyl tetravinyl cyclotetrasiloxane (1 %). Xylene and ethylbenzene are available in the SimaPro database library, US EI 2.2 while other chemicals are not available in any of the SimaPro libraries. Therefore, PDMS was used as a proxy for other chemicals. In the LCA of the curing agent, the production process energy usages were not included.

In cradle-to-gate LCA analysis, ecotoxicity, fossil fuel depletion and global warming were showing large impacts. The estimated ecotoxicity of 1 m^2 CNC-PDMS and PDMS membrane production processes were 99.0 and 122.5 CTUe respectively. The addition of CNC reduces ecotoxicity by 19 %. The PDMS is the major contributor to ecotoxicity. Dimethyldichlorosilane and potassium hydroxide are used to produce PDMS, which require a large amount of chemicals and industrial processes leading to higher ecotoxicity. The estimated fossil fuel depletion of 1 m^2 CNC-PDMS and PDMS membrane production processes were 10.1 and 10.9 MJ surplus respectively. The addition of CNC reduces fossil fuel depletion by 7.8 %. The utilization of steam and electricity in the CNC-PDMS membrane production process was higher than in the PDMS membrane production process due to extra unit operation and water content (11.8 % CNC solution). So, the fossil fuel depletion of steam and electricity in the CNC-PDMS membrane process is higher than in the PDMS membrane process. The estimated GW impacts of 1 m^2 CNC-PDMS and PDMS membrane production processes were 8.7 and 9.9 kg CO_2 eq, respectively, indicating an improvement of 12 % for CNC-PDMS membrane. The analysis indicated that the PDMS was the largest contributor to most of the impact categories. For example, in producing CNC-PDMS, the contribution of the PDMS in ozone depletion, global warming (GW), smog, acidification, eutrophication, carcinogenics, non-carcinogenics, respiratory, ecotoxicity and fossil fuel depletion were 92.02, 88.75, 89.42, 81.91, 89.38, 89.95, 87.67, 88.80, 91.06 and 85.31 % respectively. The detailed environmental impacts by impact categories are shown in Fig. 8 and Table 6. Because a very small quantity of CNC was used in the CNC-PDMS membrane production, it resulted in a small reduction in environmental impact categories.

3.4.1. Sensitivity analysis of CNC on PDMS membrane

The addition of small amount of CNC solution (2 %) in producing PDMS resulted in a small reduction in the cradle-to-gate environmental impacts. A sensitivity analysis was conducted to understand how the environmental impacts change when increasing the percentage addition of CNC solution (Fig. 9). The addition of CNC solution reduced the PDMS and curing agent volume and accordingly reduced other input materials, proportionately reducing the environmental impacts. The sensitivity analysis indicated that increasing CNC solution from 2 % to 10 % reduced the ecotoxicity, fossil fuel depletion and GW impacts by 50.94, 23.04 and 39.89 % respectively. However, the acidification was reduced to only 5.87 % due to generally higher acidification impacts of CNC production (Gu et al., 2015; Rajendiran et al., 2023) than PDMS (PRé Consultants, 2021).

4. Conclusions

This study assessed the techno-economic feasibility and life-cycle environmental impacts of adding CNC to modify PDMS membranes, i.e., the manufacturing process of CNC/PDMS hybrid membrane materials. The assessment was facilitated by developing an industrial-scale CNC-PDMS membrane production process model guided by the optimized experimental results. By performing TEA and LCA in the early stages of product development, this study provided critical information needed by the investors interested in investing at the commercial scale CNC-PDMS production technology as well as the regulators and general consumers interested in understanding the environmental impacts of such technology.

The analysis found that adding even a small amount of CNC would improve the financial and environmental performances of the PDMS membrane. For example, the economic analysis finds that the CNC-PDMS membrane (0.0099 kg of CNC per m^2 of PDMS membrane) would reduce the MSPs by 8 to 9 % compared to the PDMS membrane. In addition, the estimated MSPs of the 1 m^2 80 μm thick CNC-PDMS membrane ($3.35/$m^2$ in expanding in an existing plant and $3.68/$m^2$ in a greenfield plant) were lower than the current commercial market retail price ($112/$m^2$). These MSPs are likely to reduce further with the likely increased economy of scale and reduced cost of materials over time.

Adding CNC to PDMS membrane also improved environmental performance. For example, the CNC-PDMS membrane production process showed reductions in all evaluated impact categories, compared to the PDMS membrane. The GW impact of 1 m^2 80 μm thickness CNC-PDMS membrane was estimated at 8.7 kg CO_2 eq, which was 12 % lower than the PDMS membranes GW impact. Because the PMDS was the largest contributor to all impact categories, replacing the PDMS with biobased polymers would likely achieve larger reductions in the environmental impacts.

Furthermore, as discussed earlier in the introduction section, the energy loss through the ventilation of conventional steam kiln is high to

20 %. By fabricating a CNC/PDMS hybrid membrane-based isothermal air dehumidification system and implementing it in the steam kiln, energy consumption can be greatly reduced. This could be achieved by separating dry air from the humid and hot exhaust air, rerouting the dry, hot air back into the kiln, and minimizing the energy needed to heat another cold air stream coming from the environment.

CRediT authorship contribution statement

Naveenkumar Rajendran: Conceptualization, Methodology, Resources, Modeling, Validation, Visualization, Writing – original draft, Writing – review & editing. **Troy Range:** Formal Analysis, Resources, Writing – review & editing, Visualization and Funding Acquisition. **Richard Bergman:** Formal Analysis, Resources, Writing – review & editing, Visualization and Funding Acquisition. **Prakash Nepal:** Validation, Writing – review & editing, Visualization. **Nasim Alikhani:** CNC/PDMS membrane material preparation and experimental results discussion, Writing- draft, review & editing. **Ling Li:** CNC/PDMS membrane introduction, material preparation and experimental results discussion, Writing- review & editing, Funding Acquisition. **Shane R. O'Neill:** Writing – review & editing. **Jinwu Wang:** Writing – review & editing.

Declaration of competing interest

There are no conflicts to declare.

Data availability

The models that support the findings of this study are available from the corresponding author, upon reasonable request for non-commercial use.

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