



# Comparing the financial costs and carbon neutrality of polyester fibres produced from 100% bio-based PET, 100% recycled PET, or in combination

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## Abstract

The rise of fast fashion has led to challenges in sustainable production and recycling of polyester textile waste. Bio-based polyethylene terephthalate (bio-PET) and the enzymatic hydrolysis of PET textiles may offer two solutions for bio and circular clothing. This study designed and simulated scaled enzymatic hydrolysis of fossil PET into ethylene glycol (r-EG) and purified terephthalic acid (r-PTA), the production of bio-EG and bio-PTA from the wheat straw ethanol (EtOH) and corn stover isobutene (IBN), respectively, and the production of PET polyester textile fibres from these monomers. The research goal was to determine whether bio-PET, r-PET, or their mixture achieves better positive profitability and NPV<sub>2023</sub> and carbon neutrality in textile fibres. The financial returns and carbon emissions for r-PET fibres with a bio-PET content of 0%, 20%, 40%, 60%, 80% to 100% was estimated for scenario 1 (a newly constructed plant), scenario 2 (no capital costs for the EtOH or IBN processes), and scenario 3 (no capital costs for the EtOH, IBN, and enzymatic hydrolysis processes). While scenario 1 was not able to generate positive net profits or NPV<sub>2023</sub>, scenarios 2 and 3 were able to attain financial sustainability when the bio-PET content was  $\leq 40\%$ . On the other hand, increasing the amount of bio-PET content in the polyester fibre from 0 to 100 wt.% decreased its carbon footprint from 2.99 to 0.46 kg CO<sub>2</sub>eq./kg of PET fibre.

**Keywords** Polyester (PET) textiles · Polyester (PES) · Chemical recycling · Isobutene · Ethanol · 100% bio-PET · Life cycle analysis · Circular economy · Bioeconomy

## Abbreviations

AD	Anaerobic digestion	CHP	Combined heat and power
ALP	Annual loan payment (\$/year)	CO <sub>2</sub>	Carbon dioxide
AOC	Annual operating cost (\$/year)	CPI	Consumer price index
BHET	Bis(2-hydroxyethyl) terephthalate	CtEG	Coal-to-ethylene glycol
BOKU	Universität für Bodenkultur (University of Natural Resources and Life Sciences)	C-to-G	Cradle-to-gate
BTX	Benzene, toluene, xylene	DC	Direct cost (\$)
CEAP	Circular economy action plan	DFC	Direct fixed capital (\$)
CEBC	Centre for Environmentally Beneficial Catalysis	DIB	Diisobutene
		DMF	Dimethylformamide
		DMO	Dimethyl oxalate
		EG	Ethylene glycol
		EH	Enzymatic hydrolysis
		EO	Ethylene oxide
		EPC	Equipment purchase cost (\$)
		EPR	Extended producer responsibility
		ET	Ethylene
		EtOH	Ethanol
		FOC	Fixed operating cost (\$)
		GHG	Greenhouse gas

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GWP	Global warming potential (kg CO <sub>2</sub> eq./kg)
HMF	Hydroxymethylfurfural
<i>I</i>	Discount rate (%)
IBN	Isobutene (or isobutylene or 2-methylpropene)
IC	Indirect cost (\$)
IVET	Institut für Verfahrens und Energietechnik (Institute of Chemical and Energy Engineering)
LCA	Life cycle analysis
LCI	Life cycle inventory
MSE-bio/(r)-PET-fibre Ref.	Microsoft Excel bio/(recycled) PET-fibre Refinery Tool
MTO	Methyltrioxorhenium
NCF	Net cash flows (\$)
NPV <sub>2023</sub>	Net present value 2023 (\$)
NREL	National Renewable Energy Laboratory
PES	Polyester
PET	Polyethylene terephthalate
PTA	Purified terephthalic acid
SPD	SuperPro Designer
Suppl. Doc.	Supplementary document
TA	Terephthalic acid
USD, \$	United States dollar (\$)
VOC	Variable operating cost (\$)
WC	Working capital (\$)

## 1 Introduction

Clothing serves many roles as means of comfort and protection from the elements and pathogens, and even as a social device for expressing our physicality, status, identity, and more. While historically silk, cotton, to wool fibres were once treasured commodities and our clothing options were reduced to a few garments, rapid global industrialisation and the invention of polyester have made clothing cheap, abundant, and dispensable. With the widespread acceptance of “fast fashion” in the West, it has been estimated on average each person in Europe uses an average of 26 kg of textiles and disposes of up to 15 kg as waste (85% being clothing) per year [1, 2], with roughly 1/3 collected, ~20% recycled, 10–20% incinerated, and 60–70% exported to Africa and Asia [3]. While the direct effects of textile waste in Europe are not felt, annual textile purchases add 270 kg of CO<sub>2</sub> per EU consumer, or globally 10% of annual carbon emissions [4]. It is estimated the average T-shirt uses roughly 2700 L of fresh water, with industry annually consuming roughly

93 billion m<sup>3</sup> of water, 20% of global water pollution (e.g. from dyes and chemicals), and 35% of global microplastic emissions are linked to clothing manufacture and use. As it stands, around 87% of clothing fibres are incinerated and/or disposed of in landfills [5] and in Europe, approximately only 1% of recycled clothing fibres are inputted in new clothes [6]. With this insane amount of wastefulness and pollution, clear and definitive measures for textile waste reduction and circular re-utilisation are still not clear and not definitively set in EU policies or industry standards. For example, the EU Commissions’s Single-Use Plastic Directive (EU) 2019/904 only indicates a desire to reduce microplastics in textile and clothing items, to mitigate environmental pollution, [7] and the 2020 circular economy action plan (CEAP) only outlines goals such as sustainably made textiles with eco-design (e.g. recycled fibres, non-toxic chemicals), extended producer responsibility (EPR), to reuse practices (e.g. renting to repair) [8]. One of the primary issues with textiles today is that nearly 60% are made from synthetic plastic fibres like polyethylene terephthalate (PET) polyester [9] produced from fossil hydrocarbons, which along with having a high carbon footprint (e.g. 81.62 kgCO<sub>2</sub>eq./T-shirt) [10], emit as much as 500,000 tonnes of microplastic fibres into the ocean per year from regular washing and wear [11], and outliving their original owner 1000 years or more as they do not break down naturally in the environment [12]. Europe still lacks basic technology, facilities, and strategies to process large quantities of textile waste effectively and economically due to the complex characteristics of textiles (e.g. dyes to fibre used) which require sorting, preparation, and cleaning [13]. As well, depending on the condition of the clothing and who collects it, the clothing will be incinerated or burned if processed in municipal waste, salvaged for materials by a collector, handed off to a new user by charities, or exported to African and Asian nations, sabotaging domestic production and increasing textile waste in the developing world [6]. While it is a more sustainable practice according to the EU’s waste hierarchy to reuse textile clothing secondhand, over recycling fibres directly, to reduce resource consumption and waste output, nearly 25–50% of collected waste clothes are not reusable, and they must be treated through some form of mechanical or chemical recycling to a simpler form or monomers to be of value [6]. The conventional method of plastic and PET recycling is the mechanical route of collecting the plastic waste and grinding it into bits prior to sorting by plastic-type (e.g. PET, polyethylene, polystyrene) typically through flotation separation or other means with the PET plastic bits decontamination via washing with chemicals (e.g. tetrachloroethylene or sodium hydroxide and detergent at temperatures of around 80 °C) and then washed with water to remove all impurities before extrusion. All of which entails the deterioration of the PET’s

melt viscosity and molecular weight meaning additives to resins are required to compensate and restore the PET's quality [14, 15].

To compensate for the losses during conventional mechanical recycling processes, plastics from bio-renewable material rather than fossil hydrocarbons and bio-based recycling methods may help improve the sustainability of PET polyester textile clothing. While bio-PET exists, generally, it consists of roughly 30 wt.% ethylene glycol (EG), synthesised from bio-ethanol dehydration into ethylene, while the remaining 70 wt.% is derived from terephthalic acid (TA) from fossil naphtha [16]. In 2020, market research suggests that the present annual production of EG (~28 million tonnes) would not be adequate to meet the demand of over 50 million tonnes in the next 20 years [16]. Presently, the industry manufacture of bio-EG is still hindered due to the high temperatures involved in the production of the intermediate ethylene oxide (EO) resulting in the loss of process control and highly undesired by-product formation (e.g. CO<sub>2</sub> and water) [17]. Subsequently, there is high water consumption for EO hydrolysis into EG, with non-optimal yields (e.g. 90–92% EO conversion) and the energy intensity involved in EG distillation [18–21]. To transcend these lingering issues, alternative innovations like Shell's OMEGA process can react CO<sub>2</sub> with EO to form ethylene carbonate for hydrolysis into EG at nearly 98% selectivity [21]. The

primary drawback is that ethylene oxide is typically fossil hydrocarbon derived, and the CO<sub>2</sub> used in the process is not sequestered but released after hydrolysis. Another example of scaled and demonstrated carbon-based ethylene glycol (c-EG) production is the coal-to-ethylene glycol (CtEG) technology in operation across 15 plants in China, with individual annual capacities reaching as high as 300,000 tonnes of c-EG [22]. In summary, the CtEG process begins with the gasification of coal into syngas (i.e. hydrogen and carbon monoxide mixture), separation of the hydrogen and carbon monoxide, conversion of the carbon monoxide into dimethyl oxalate (DMO), and the hydrogenation of the DMO with the hydrogen into EG. Due to its use of fossil coal and the high CO<sub>2</sub> emissions released during processing (e.g. 3.2 t CO<sub>2</sub>/t<sub>EG</sub>), the CtEG technology is contributing to new carbon emissions to the environment and is not sustainable [19, 23].

New bio-TA pathways are presently being pursued by American corporations such as the Coca-Cola Company to Procter & Gamble for future commercialisation of 100% PET bottles [16, 24]. Two main pathways being seriously considered for bio-TA production can be summarised as direct TA routes and indirect p-xylene routes depicted in Fig. 1. Direct TA routes include the fermentation of sugars into isoprene followed by cycloaddition of isoprene with acrylic acid to form 4-methylcyclohexane-3-carboxylic acid which is oxidised into TA [25],

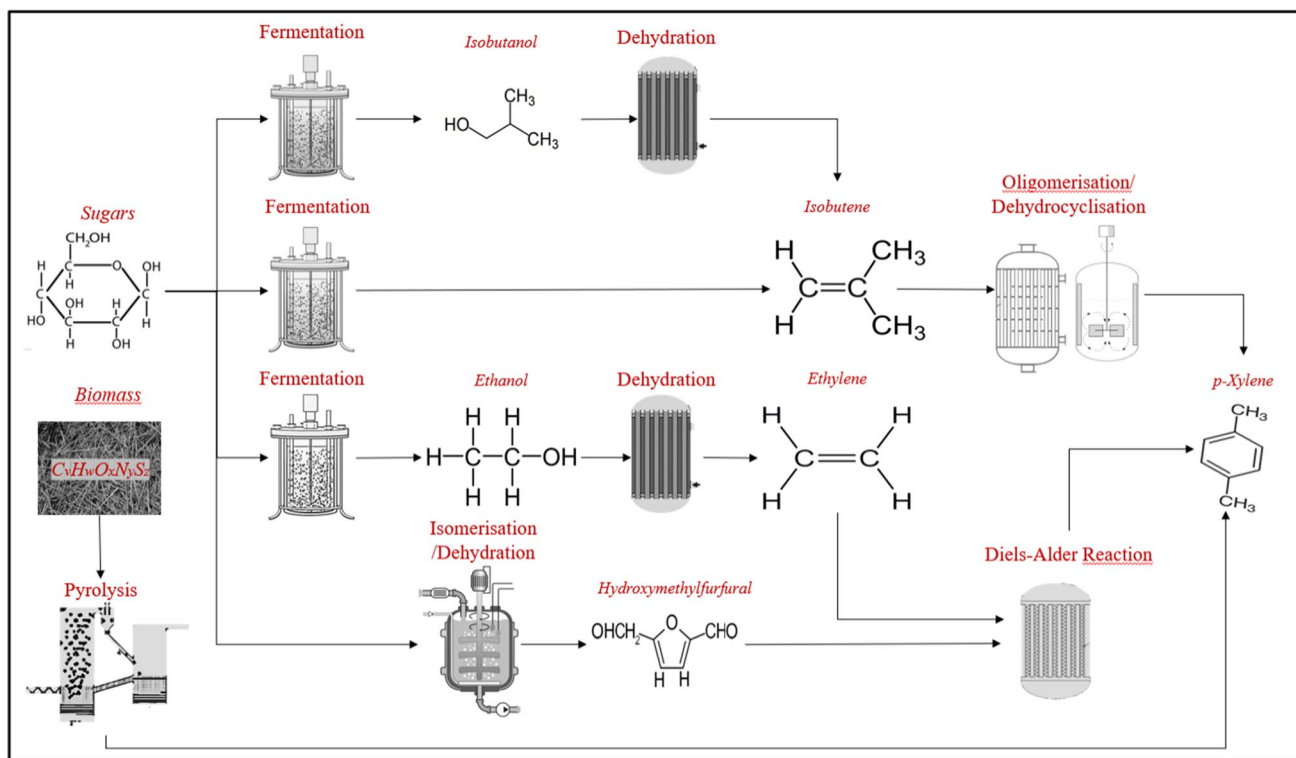


Fig. 1 Indirect pathways via p-xylene for terephthalic acid production

the second being the synthesis and dehydrogenation of limonene into p-cymene and its oxidation into TA [26], and lastly, via acid catalysed dehydration of C<sub>5</sub> sugars (e.g. xylose) into furfural followed by the furfural's oxidation and dehydration into maleic anhydride followed by a reaction with furan and then dehydration to yield phthalic anhydride and later PTA [27]. As these routes are mostly in the experimental phase, the indirect p-xylene routes (Fig. 1) are the most successful and demonstrated to date and consist of four main process routes. These routes convert isobutanol into isobutene (or isobutylene or 2-methylpropene), fructose into hydroxymethylfurfural (HMF), and ethanol into ethylene (ET) before conversion into p-xylene and then to PTA [28, 29]. Other studies have examined the potential of acquiring p-xylene through the benzene-toluene-xylene (BTX) processing of pyrolysis aromatics; however, after distillation of the aromatics, the yields of p-xylene are too low to be practical for large-scale purposes [30]. While most research on obtaining isobutene is via microbial fermentation and synthesis and dehydration of isobutanol into isobutene (IBN) [31], bio-isobutanol production is hindered by low yields since the isobutanol generated is toxic to the microbes and the process requires constant vacuum stripping throughout fermentation which consumes high energy [32]. Alternatively, the fermentation of isobutane and its catalytic dehydrogenation into IBN also suffers from high energy intensity and non-efficient conversion rates [33]. Yet, promising developments have been made in direct bio-IBN production. For example, the French company Global Bioenergies's pilot-scale plant manufactures roughly 2000 tonnes of IBN per year [34–36] by fermenting wheat straw hydrolysate with a genetically engineered strain of *Escherichia coli* [37–41]. The main drawback of this process is the fact IBN yields are lower than what is required to be economical at < 2–4 g<sub>IBN</sub>/L/h with the reaction favouring roughly 2/3 wt. carbon dioxide relative to 1/3 wt. IBN [37, 38].

With the need for sustainable production of polyester textiles and recycling methods, the first goal of this research study is to determine how economic returns, in terms of profits and return on investment in the form of NPV<sub>2023</sub>, and the global warming potential (GWP) in kg CO<sub>2</sub>eq./kg of PET polyester fibres could be improved when considering polyester textile fibres produced with either bio-polyethylene terephthalate (bio-PET) or recycled fossil polyethylene terephthalate (r-PET), or a combination of the two. To estimate and access the significance of bio-PET vs. r-PET in textiles, this research study modelled and simulated in the biochemical engineering software SuperPro Designer; the large-scale process conversion of a wheat straw ethanol (EtOH) and a corn stover isobutene (IBN) biorefinery's allocation of

EtOH and IBN for ethylene glycol (bio-EG) and purified terephthalic acid (bio-PTA) production, respectively; the enzymatic hydrolysis (EH) recycling of fossil PET textiles into ethylene glycol (r-EG) and purified terephthalic acid (r-PTA); and the production of PET polyester fibres from these chemicals. The energy and material data from the simulation, as well as capital and operational cost data, were then inputted in the Microsoft Excel bio/(recycled) PET-fibre Refinery Tool (MSE-bio/(r)-PET-fibre Ref.) to determine the financial returns and carbon emissions for six different PET polyester fibres with bio-PET content of 0%, 20%, 40%, 60%, 80% to 100%. As well, three scenarios were analysed for financing. Scenario 1 assumes the plant is newly constructed and must pay off all its capital expenses; scenario 2 assumes the ethanol plant and the isobutene plant are already constructed, operational, and their capital expenses are already covered; and scenario 3 assumes the ethanol plant, the isobutene plant, and the PET recycling plant are already constructed, operational, and their capital expenses are covered. The second goal of this research is to freely supply the public with the data and calculations from the simulations, excel tool, and literature utilised in this study as a resource and reference for their own academic to professional interests leading towards the creation of more sustainable and affordable bio and circular textiles.

## 2 Methodology

### 2.1 Process data and materials

#### 2.1.1 Overview

As shown in Fig. 2, to measure the economic effects and the carbon emissions of different combinations of recycled fossil polyethylene terephthalate (r-PET) and bio-polyethylene terephthalate (bio-PET) compositions in polyester (PES) fibres, a concept plant was designed for the production of bio-purified terephthalic acid (bio-PTA), the production of bio-ethylene glycol (bio-EG), the enzymatic hydrolysis (EH) recycling of waste fossil-PET textiles into PTA and EG, and the production of PET fibres from either bio and/or recycled PTA and EG. The plant's production scale was set to be ~ 3965 tonnes of PET fibres per year. As indicated in Table 1, six different polyester fibre blends with 100 to 0% bio-PET content, with the remaining content being r-PET, were analysed. To provide sufficient income to the plant, due to the high costs of new process innovation and development, the facility's ethanol (EtOH) and isobutene (IBN) production were scaled to convert 632,002 t/year of corn stover and 820,836 t/year wheat straw into 129,939 t of EtOH and 102,781 t of

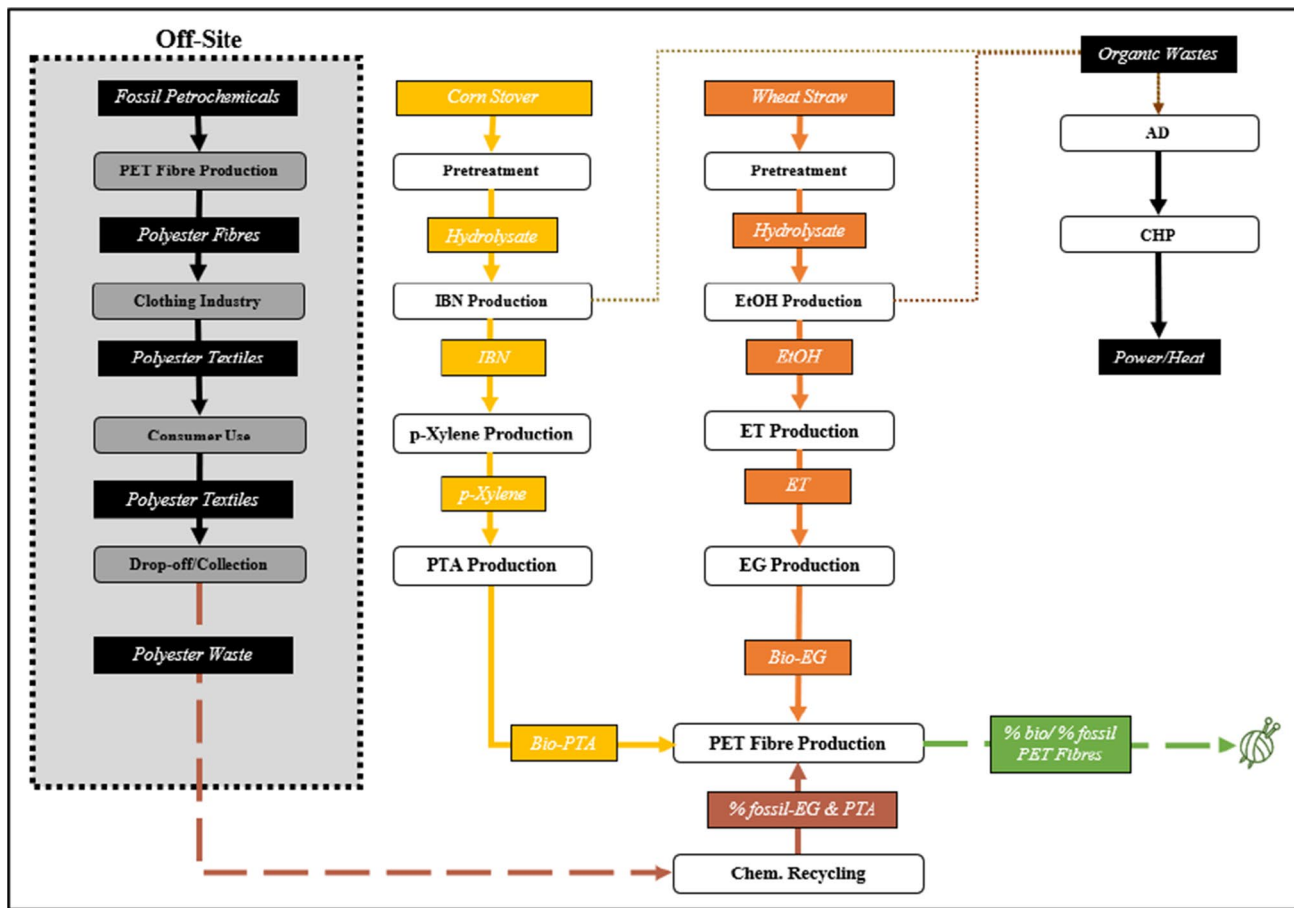


Fig. 2 Bio-circular production and recycling of textiles and carbon emission process pathway

Table 1 EtOH and IBN sold or used in bio-PET fibre (at scale of 3965 t of PET fibres/year)

Fibre #	Fibre types		Main chemicals utilised or sold			
	Bio-PET Wt.% content	r-fossil PET	IBN for PTA kg/year	IBN sold	EtOH for EG kg/year	EtOH sold
1	100%	0%	7,826,055	94,955,057	9,090,627	111,848,730
2	80%	20%	6,260,844	96,520,268	7,272,501	113,666,855
3	60%	40%	4,695,633	98,085,479	5,454,376	115,484,981
4	40%	60%	3,130,422	99,650,690	3,636,251	117,303,106
5	20%	80%	1,565,211	101,215,901	1,818,125	119,121,231
6	0%	100%	0.00	102,781,112	0.00	120,939,257

IBN per year with the surplus EtOH and IBN not used in production sold for additional revenue. Likewise, on-site bioenergy was integrated to reduce fossil energy consumption and costs. As shown in Fig. 2, the bioenergy is produced from the conversion of the bio-wastes into biogas in an anaerobic digester (AD) and the biogas’s combustion in a combined heat and power (CHP) unit for electricity and heating. The financial costs and revenues, and life cycle impacts (LCA) impacts for the upstream processes for bio-PTA, bio-EG, enzymatic hydrolysis (EH) recycling

of fossil-based polyester textiles (e.g. dashed brown-white boxes/arrows), and PET production are within the scope of analysis. However, although the production and use of fossil PET polyester textiles are not accounted for in the facility’s ledger, the carbon impacts incurred from shipping the PET polyester fibres (i.e. the grey area processes labelled “Off-site”) were assessed. To ascertain the economic and carbon impacts, first data and literature were researched and collected to design and simulate the equipment processes’ material and energy flows.



### 2.1.2 Bio-purified terephthalic acid (PTA) production

Following Fig. 2, the upstream processes involved in the manufacture of bio-purified terephthalic acid (bio-PTA) include the pretreatment of corn stover into sugary hydrolysate, the production of isobutene (IBN) through sugar fermentation, and extraction from the CO<sub>2</sub>. The processing equipment, procedures, methods, and technical–economic parameters (e.g. equipment power consumption, capital, and labour costs) for pretreatment were modelled to resemble the National Renewable Energy Laboratory’s (NREL) past studies on corn stover ethanol and hydrocarbon biorefineries [40, 42]. The design and modelling data, as well as the capital and fixed operational costs (e.g. labour), for IBN production, build upon the authors’ at the University of Natural Resources and Life Sciences (BOKU) Institute for Chemical and Energy Engineering (IVET), in association with the Energie Institut in Linz, Austria, past research and biorefinery model which produces roughly 102,956 t<sub>IBN</sub>/year from corn stover sugars [43]. In this process model, organic matter and wastewater separated from the feedstock after pretreatment conditioning, as well as unreacted sugars and nutrients from IBN production, are utilised for biogas production in the AD. The biogas, along with the filtered lignin from pretreatment, is combusted in the combined heat and power (CHP), for on-site bioenergy [37, 39, 40]. As is planned in Table 1, surplus IBN is sold for revenue while the remainder is converted into p-xylene. P-xylene production in Fig. 2 is an adapted model of GEVO Inc.’s process technology presently in commercial use [44–46]. P-xylene production is performed through the oligomerisation of the IBN into diisobutene (DIB). After purification, the DIB is converted into a pure stream of p-xylene [28, 45, 46]. Techno-economic costs for p-xylene production, namely the equipment, labour costs, and other direct (e.g. installation, piping, electrical) and indirect (e.g. contingency, engineering) capital costs, were derived from the University of Pennsylvania study on the scaled conversion of 500,000 tonnes of IBN/year into p-xylene through GEVO Inc.’s patented technology [46]. While the production of purified terephthalic acid (PTA) typically employs the standard Amoco® process, this involves oxidating p-xylene through the input of corrosive catalysts (e.g. sodium bromide) as promoters in expensive alloy-covered reactors [24]. Alternatively, to improve this process, SABIC’s ionic liquid patented technology, which contains organic cation and bromide anion (1-ethyl-3-methylimidazolium bromide), was modelled to avoid this issue [29, 47]. The engineering design, process conditions, installed equipment, and labour costs were sourced from the University of Pennsylvania’s publication on the production of 800 million lbs (362.87 million kg) of PTA/year using the SABIC technology [47]. Direct

cost and indirect cost factors were referenced from a study on the production of PTA using p-xylene sourced from miscanthus gasification and BTX synthesis [48].

### 2.1.3 Bio-ethylene glycol (EG) production

Following Fig. 2, the first process leading up to the manufacture of ethylene glycol (EG) is the pretreatment of wheat straw biomass via mechanical grinding/milling, thermal acid steam explosion, and enzymatic hydrolysis to render monomer sugar hydrolysate. The scale of production was set at 80,203 kg/h of waste wheat straw. In ethanol (EtOH) production, the wheat straw hydrolysate is then fermented into EtOH, and the EtOH is extracted and purified to 99% proof from the beer broth through distillation and filtration [40]. The processing equipment, procedures, methods, and technical–economic parameters (e.g. equipment electricity to costs) for transforming wheat straw into sugar hydrolysate and the hydrolysate’s fermentation and purification into EtOH were modelled to resemble the NREL’s past studies on corn stover to algae ethanol biorefineries [40, 42, 49]. Other supplementary academic research was also referenced for the processing of wheat straw biomass [50–57]. Similar to the IBN production model, the residual organic matter and the wastewater recovered after distillation are transferred to the AD for biogas production, along with the wastewater and organic solids acquired from pretreatment, and the biogas and lignin are combusted as fuels in the combined heat and power (CHP) system to generate electricity and steam heating for the refinery [39, 40]. Given the amount of EtOH needed for the plant’s bio-PET production, a majority of the EtOH is sold while the remainder is utilised for ethylene (ET) production (see Table 1). ET production consists of catalytic dehydration of the ethanol (EtOH) into ethylene (ET) and the ET’s purification via washing and gas distillation [58–60]. The machinery modelling, the material and energy consumption, performance efficiency, and the overall process design for ET production were sourced from relevant examples, blueprints, and descriptions available in scientific literature [59–61]. The costs for the main equipment and other associated related direct and indirect capital cost factors were acquired from scientific literature and techno-economic studies [59–61]. Referencing Fig. 2, two main pitfalls affect the efficiency of ethylene glycol (EG) production. The precursor for EG, ethylene oxide (EO), is formed through an exothermic reaction of ET and oxygen under high temperatures. This leads to a loss of control, the formation of high quantities of CO<sub>2</sub> and water, and product losses due to the EO combining with the oxygen [17]. To transcend this issue, a new production methodology was modelled based on the latest technical tests and findings of the Centre for Environmentally Beneficial Catalysis (CEBC), where hydrogen peroxide is utilised as the oxidant (rather than oxygen),

along with a methyltrioxorhenium (MTO) catalyst, using lower temperatures but high pressure (~40 °C, 50 bar) [17] [62]. These conditions greatly improve the safety, ease, and efficiency of the production with around 90% of the ethylene converted into EO which is then separated from the water, unreacted ethylene, solvents, and hydrogen peroxide through simple distillation and flash columns [62]. Capital costs and operational costs were derived from two techno-economic studies on the scaled CEBC production process for EO [17, 62]. Referencing Fig. 2, EG production entails the hydrolysis of EO to yield EG by mixing the EO with a large portion of water at elevated temperature and pressure [19]. The unreacted water is separated from the EG through multi-effect evaporation and dehydration columns, and the EG is then distilled from the by-products. The operating conditions and the equipment parameters for EG production were modelled to mimic academic sources and industry patented technology [18–21, 63]. The primary technical design (e.g. equipment processes), capital expenditure, and fixed operating costs (e.g. labour) were based on a research study on the economic potential of EG plant of an annual capacity of 200,000 tonnes [62].

#### 2.1.4 Polyester textile chemical recycling

For the chemical recycling of the polyester fibres, the NREL's 2021 large-scale research study on a facility's enzymatic hydrolysis of polyethylene terephthalate (PET) bottle flakes into terephthalic acid (TA) and ethylene glycol (EG) was the main source for the process model design, material, labour, to equipment costing. When information was lacking, additional sources from associated studies were referenced regarding details such as chemical reactions, batch processing, to chemical load rate [65]. This process technology was considered an appropriate example given the current state of development and the challenges facing large-scale PET EH recycling. For example, the study uses cutinase enzymes, capable of conversion yields above 90.0%, as they can handle the high crystallinity of PET wastes (e.g. 30.0–40.0% for bottles to fibres) and high heat (e.g. ~70 °C), meaning they can take advantage of PET's glass transition temperature [39, 66]. As well, the process takes extra steps to address performance inhibitors like contaminants (e.g. additives like pigments and dyes) with an activated carbon column and from acidification, due to the ester-bond hydrolysis, by pH neutralisation of the solution [39, 66]. As the NREL's study focuses on PET bottle chips, an additional mechanical pretreatment step was added for crushing and shredding the polyester textiles into bits before biochemical treatment [66]. As well, the modified model was also scaled down by a factor of 100 to handle a maximum of roughly ~3965 tonnes of PET/year rather than the 396,481,142 done by the NREL to match the maximum capacity of the ethanol (EtOH) and

isobutene (IBN) plants for bio-PTA and EG and recycled EG and recycled PTA mixing [64]. Additionally, considering the PET flakes recycled in the NREL's study are for PET bottles and not polyester textiles and the study focuses primarily on the TPA and not the recycled EG, this study performed its own process simulation and LCA calculations using a sampled global warming potential factor for end-of-life polyester textiles (30 kg CO<sub>2</sub> eq./kg) from the European Publication Office [67].

#### 2.1.5 Polyethylene terephthalate (PET)/polyester fibre production

PET production consists of the preparation of the bio and/or recycled ethylene glycol (EG) and purified terephthalic acid (PTA) their esterification into bis(2-hydroxyethyl)terephthalate (BHET), BHET polymerisation into polyethylene terephthalate (PET), and the forming of the PET polyester fibres [68–71]. Six different PET polyester fibres of varying mixtures of bio-PTA and bio-EG to recycled PTA and recycled EG content were analysed in this study as outlined in Table 1. This process also involves high temperatures and vacuum pressure to allow venting, distillation, and recovery of the EG for reuse and is done in a series of reactors to maximise yields of PET [69, 71]. All equipment and their respective processing parameters and technical characteristics (e.g. heating, pressure, materials, electricity consumption) mirror the data, descriptions, and accompanying engineering diagrams provided by industry and academic experimental research [68, 69, 72, 73]. Immediately, after the formation of the PET resin, it is spun, filtered, and extruded into polyester fibres using a spinning extruder [70, 71]. Since useful techno-economic research studies or industry reports were not available, the capital costs of the equipment were sampled from data provided in alternative bio-plastic studies operating identical machinery [74, 75], and the cost of PET spinning extruder was assumed similar to a model for sale on Alibaba [76]. The corresponding installation, piping, engineering, and construction costs were taken from default quotes in SuperPro Designer.

#### 2.2 Process design and simulation modelling

Pertaining to Fig. 2, the modelled processes for isobutene (IBN) production, p-xylene production, purified terephthalic acid (PTA) production, ethanol (EtOH) production, ethylene (ET) production, ethylene glycol (EG) production, the chemical recycling (Chem. Recycling) of fossil polyethylene terephthalic (PET) textiles, and the PET polyester fibre production were simulated in the biochemical engineering software SuperPro Designer to calculate the material and energy flow balances for each of the equipment machinery operations. The written detailed technical description along

**Table 2** Data location per process or product

MSE-bio/(r)-PET-fibre Ref. file					
Process	Material flow data (sheet names)	Energy-utilities data (sheet name)	Flow totals and costs (sheet name)	Products	LCA-GWP (sheet name)
Wheat straw pretreatment	W.S. Pretreat	Equip.\$&P	Oper.\$&Flow	100% bio-PET fibres	LCA-Bio100%
EtOH production	bio-EG			80% bio-PET fibres	LCA-Bio80%
ET production	bio-EG			60% bio-PET fibres	LCA-Bio60%
EG production	bio-EG			40% bio-PET fibres	LCA-Bio40%
Corn stover pretreatment	C.S. Pretreat			20% bio-PET fibres	LCA-Bio20%
IBN production	bio-PTA			0% bio-PET fibres	LCA-Bio0%
P-xylene production	bio-PTA				
PTA production	bio-PTA				
PET production	PET				
PET Chem. recycling	r-Chem				
Anaerobic digestion	Energy				
Combined heat and power	Energy				

with the engineering diagrams for each of the processes simulated in SuperPro Designer is available in the supplementary Microsoft Word file. To overview the material and energy flows for each of these processes, see Table 2 for the location in Microsoft Excel bio/(recycled) PET-fibre Refinery Tool (MSE-bio/(r)-PET-fibre Ref.).

## 2.3 Financial and carbon footprint tool

### 2.3.1 Overview

With the completion of the SuperPro Designer simulations, each of the modelled process's material and energy data in Fig. 2, their corresponding equipment and machinery, direct and indirect capital cost factors, the price for materials and energy, and their respective kg CO<sub>2</sub> eq. factors were uploaded into the Microsoft Excel bio/(recycled) PET-fibre Refinery Tool (MSE-bio/(r)-PET-fibre Ref.) tool. Table 2 outlines the general location of the material and energy flow balances, along with their associated prices, kg CO<sub>2</sub>eq. factors, and the aggregated costs and carbon emissions in the tool file for each of the processes and the six types of PET fibres in Table 1. A 20-year period, with 2 years assumed for construction, 18 years of manufacture (i.e. earning period (*k*)), and 7880 h of operation/year, was assumed. The MSE-bio/(r)-PET-fibre Ref. tool contains various embedded financial formulas, developed from SuperPro Designer's [77] and Aspen Plus's [78] techno-economic calculation methodologies, for calculating the total fixed capital investment (TFCI), annual operating costs (AOC), variable operating costs (VOC), fixed operating costs (FOC), revenues, gross

profits, net profits, net present value (NPV), payback period, and break-even point with the input of material, energy, and cost data detailed in Table 3. The tool was also modified to allow the user to estimate the economic impacts of altering the scale of corn stover IBN and wheat straw EtOH output and/or the output of PET fibres. The tool offers other features for predicting the profitability and NPV<sub>2023</sub> via different funding options (e.g. annual loan payments vs. grants), and it contains a built-in sensitivity analysis and a Monte Carlo simulator for uncertainty analysis for finances. Additionally, the MSE-bio/(r)-PET-fibre Ref. tool life cycle analysis (LCA) template sheets automatically compile material and energy balances for each of the processes in life cycle inventory (LCI) tables, and with the uploaded CO<sub>2</sub> eq. factors allocate carbon emissions based on the weight mass fraction of the product (functional unit) and by-product(s) produced. The tool's LCA methodology conforms with the ISO 14040 [79] and 14,044 [80] standards and was used to calculate the CO<sub>2</sub> eq. per process and kg of PET fibre and material and energy consumption comparisons per process and product. The location of each of the six PET fibre's LCA, LCI, GWP datasets, assumptions, unavailable factors, and minor materials that were cut off is available in Table 2.

### 2.3.2 Measures

Three financial scenarios were developed for analysis. Excluding the grey processes labelled off-site, scenario 1's finances include all the processes shown in Fig. 2, while scenario 2 excludes the pretreatment processes and IBN and EtOH production, and scenario 3's excludes the



**Table 3** Financial calculations and data locations

ID	Item	Calculation	MSE-bio/(r)-PET-fibre Ref. file (sheet name)
A	Annual operating cost (AOC)	AI + AII	Finances
AI	Variable operating cost (VOC)	SUM(AI-1:AI-3)	Finances
AI-1	Materials	See MSE-bio/(r)-PET-fibre Ref. sheet	Oper.\$&Flow
AI-2	Utilities	See MSE-bio/(r)-PET-fibre Ref. sheet	Oper.\$&Flow
AII	Fixed operational cost (FOC)	SUM(AII-1:AII-2)	Finances
AII-1	Labour	See MSE-bio/(r)-PET-fibre Ref. sheet	Oper.\$&Flow
AII-2	Depreciation ( $r = 5\%$ , $t = 15$ yrs.)	$((EPC + \text{installation}) - (r \times DC)) / t$	Finances
B	Total fixed capital investment (TFCI)	b + bIII	Finances
b	Direct fixed capital (DFC)	SUM(bI:bII)	Finances
bI	Direct costs (DC)	SUM(bI-1:bI-8)	Finances
bI-1	Equipment purchase cost (EPC)	Base cost $\$ \times \left( \frac{\text{new size}}{\text{base size}} \right)^n \times \left( \frac{CPI}{CPI_0} \right)$	Equip.\$&P
bI-2	Installation	Lang factor $\times$ EPC	Equip.\$&P
bI-3	Piping	Lang factor $\times$ EPC	Finances
bI-4	Instrumentation and controls	Lang factor $\times$ EPC	Finances
bI-5	Electrical	Lang factor $\times$ EPC	Finances
bI-6	Buildings	Lang factor $\times$ EPC	Finances
bI-7	Land improvement	Lang factor $\times$ EPC	Finances
bI-8	Auxiliary facilities	Lang factor $\times$ EPC	Finances
bII	Indirect cost (IC)	SUM(bII-1:bII-3)	Finances
bII-1	Prorateable expenses	Lang factor $\times$ DC	Finances
bII-2	Engineering and construction fees	Lang factor $\times$ DC	Finances
bII-3	Project contingency	Lang factor $\times$ DC	Finances
bIII	Working capital (WC)	$5\% \times DFC$	Finances
C	Annual loan payment (ALP), $i = 4\%$ and $t = 15$ yrs	$TFCI \times (1 - \%Grant) \times (i / (1 - (1 + i)^{-t}))$	Finances
a	Product operating cost (POC)	$= \frac{AOC}{\text{Product kg/yr.}}$	Graph analysis
ai	Product variable cost (PVC)	$= \frac{VOC}{\text{Product kg/yr.}}$	Graph analysis
b	Total product cost (TPC)	$= \frac{\text{Annual loan payment} + AOC}{\text{Product kg/yr.}}$	Graph analysis
D	Net profit	$= \text{Total gross profit} - \text{taxes} - \text{total loan payment} + \text{depreciation}$	Finances
DI	Gross profit	$= \text{Annual revenues} - AOC$	Finances
F	Net present value ( $NPV_{2023}$ ) $i = 5\%$ , $N = 20$ yrs	$= \sum_k^N \frac{NCF}{(1+i)^k} - (TFCI_{Loan})$	Finances
G	Sensitivity analysis	See MSE-bio/(r)-PET-fibre Ref. sheet	Sens. analysis
H	Monte Carlo analysis	See MSE-bio/(r)-PET-fibre Ref. sheet	Monte Carlo

pretreatment processes, isobutene (IBN) production, ethanol (EtOH) production, and PET enzymatic hydrolysis (EH) recycling (Chem. Recycling). The “cradle-to-gate” LCA system boundaries for the PET fibres include all processes depicted in Fig. 2. For each process, the respective material and energy flow and the subsequent cost (\$ USD) and kg CO<sub>2</sub> eq. emission were then set relative to the functional units: 1 kg<sub>100%bio-PET</sub>, 1 kg<sub>80%bio-PET</sub>, 1 kg<sub>60%bio-PET</sub>, 1 kg<sub>40%bio-PET</sub>, 1 kg<sub>20%bio-PET</sub>, and 1 kg<sub>0%bio-PET</sub>. The material and energy pricing and CO<sub>2</sub> factors were extracted from various datasets and literature sources for Western

Europe, and the summed impacts for the VOC and the carbon emissions are available in the respective sheets in Table 2. As mentioned in all scenarios, the plant produces on-site energy from the bio-wastes collected from IBN and EtOH production which partially covers a percentage of the plant’s electricity and steam heat needs. However, while the plant sells its mid-pressure (MP) and high-pressure (HP) steam heat to the grid, in all scenarios, extra electricity and low-pressure (LP) steam are taken from the grid which incurs added operational costs. For the ease of carbon emission calculation, it was assumed that the

facility would use only electricity and steam heat from the grid. Due to the lack of available information and their low significance on costs and carbon emissions, some minor material items (e.g. boiler chemicals, catalysts, to certain nutrients) were presumed negligible and not considered in the analysis. For VOCs like the material and utility costs and FOCs like labour (e.g. the specific workforce, hours, and salaries), this information is available in MSE-bio/(r)-PET-fibre Ref. tool in sheets specified in Table 2. The depreciation of the installed capital equipment was calculated using the straight line formula for a period of 15 years (Table 3). Direct costs (DC) such as equipment purchase costs (EPC) per process were scaled based on the formula in Table 3 [81]. The base cost, size (e.g. in m<sup>3</sup>/h or kg/h), and the scaling factor (*n*) for each piece of equipment are listed in Table 4 with the cost then multiplied by the consumer price index (CPI) to adjust for inflation to 2023 USD. The total number of equipment pieces was determined based on the maximum capacity of the equipment and capacity required for the process according to SuperPro Designer or from industrial data. To estimate other DCs, Lang factors for installation to auxiliary facilities were multiplied against each process's EPC. ICs likewise were estimated using the same methodology of multiplying (e.g. prorateable expenses to other cost) Lang factors against the DC. The working capital was assumed to be 5% of the DFC. An annual loan payment (ALP) with an interest rate of 4% and a payback period of 15 years (*t*) was used in each scenario to pay off TFCI costs. See Table 3 for the summary of these calculations for the AOC and TFCI, as well as for the gross and net profits, investment value in NPV (2023), and the production operating

cost (POC), production variable cost (PVC), and the total production cost (TPC) per product, and their location in the MSE-bio/(r)-PET-fibre Ref. tool. Taxes are assumed to be 35%, the NPV<sub>2023</sub> a discount rate (*i*) of 5%.

### 3 Results and discussion

#### 3.1 Economic returns

Beginning with the financial results, the initial findings show that by lowering the production amount and percentage of bio-polyethylene terephthalic (bio-PET) fibre content, compared to the percent amount of recycled polyethylene terephthalic (r-PET) fibres in the plant's polyester fibres (3965 t/year), the overall total fixed capital investment cost (TFCI) and annual operational cost (AOC) reduce. This is because while wheat straw pretreatment, corn stover pretreatment, ethanol (EtOH) production, and isobutene (IBN) production remain at the same scale, less EtOH is needed for ethylene glycol (EG), and less IBN is needed for purified terephthalic acid (PTA) production, decreasing the amount and the size of equipment and machinery to the materials and energy consumed for their conversion. Likewise, with the decrease in bio-PET fibre production, the amount of EtOH and IBN sold for revenue increases, while steam heat sales from bioenergy production remain constant, and some minor by-products such as diethylene glycol (DEG) and triethylene glycol (TEG) decreases. All electricity and low-pressure (LP) steam generated from bioenergy production were used in production for all six blends of polyester fibres manufactured, and

**Table 4** Monte Carlo simulation summary for PET fibres with 0–40% bio-PET content

Bio-PET content	Measure	Scenario 1: net profit	Scenario 1: NPV <sub>2023</sub>	Scenario 2: net profit	Scenario 2: NPV <sub>2023</sub>	Scenario 3: net profit	Scenario 3: NPV <sub>2023</sub>
40.0%	<b>Mean</b>	-7.30E+08	-2.11E+09	9.63E+08	1.28E+08	9.28E+08	1.28E+08
	<b>Std</b>	1.41E+08	1.57E+08	3.22E+08	1.80E+08	1.62E+08	1.63E+08
	<b>Min</b>	-1.06E+09	-2.63E+09	1.43E+08	-4.65E+08	6.52E+08	-1.45E+09
	<b>Max</b>	-2.60E+08	-1.62E+09	2.07E+09	7.02E+08	1.42E+09	3.83E+08
	<b>Risk of loss</b>	<b>100.00%</b>	<b>100.00%</b>	<b>0.20%</b>	<b>23.60%</b>	<b>0.00%</b>	<b>3.50%</b>
20.0%	<b>Mean</b>	-7.04E+08	-2.09E+09	1.03E+09	1.71E+08	9.85E+08	1.70E+08
	<b>Std</b>	1.47E+08	1.63E+08	3.25E+08	1.83E+08	1.73E+08	1.74E+08
	<b>Min</b>	-9.18E+08	-2.59E+09	3.75E+08	-3.31E+08	6.37E+08	-1.45E+09
	<b>Max</b>	-2.14E+08	-1.61E+09	2.07E+09	6.47E+08	1.48E+09	4.37E+08
	<b>Risk of loss</b>	<b>100.00%</b>	<b>100.00%</b>	<b>0.20%</b>	<b>18.10%</b>	<b>0.00%</b>	<b>2.50%</b>
0.0%	<b>Mean</b>	-6.52E+08	-2.05E+09	1.12E+09	2.36E+08	1.08E+09	2.48E+08
	<b>Std</b>	1.61E+08	1.68E+08	3.38E+08	2.01E+08	2.17E+08	2.07E+08
	<b>Min</b>	-7.68E+08	-2.51E+09	6.79E+08	-3.31E+08	8.96E+08	-1.45E+09
	<b>Max</b>	-1.80E+08	-1.52E+09	2.16E+09	8.29E+08	1.60E+09	6.00E+08
	<b>Risk of loss</b>	<b>100.00%</b>	<b>100.00%</b>	<b>0.20%</b>	<b>12.70%</b>	<b>0.00%</b>	<b>2.30%</b>

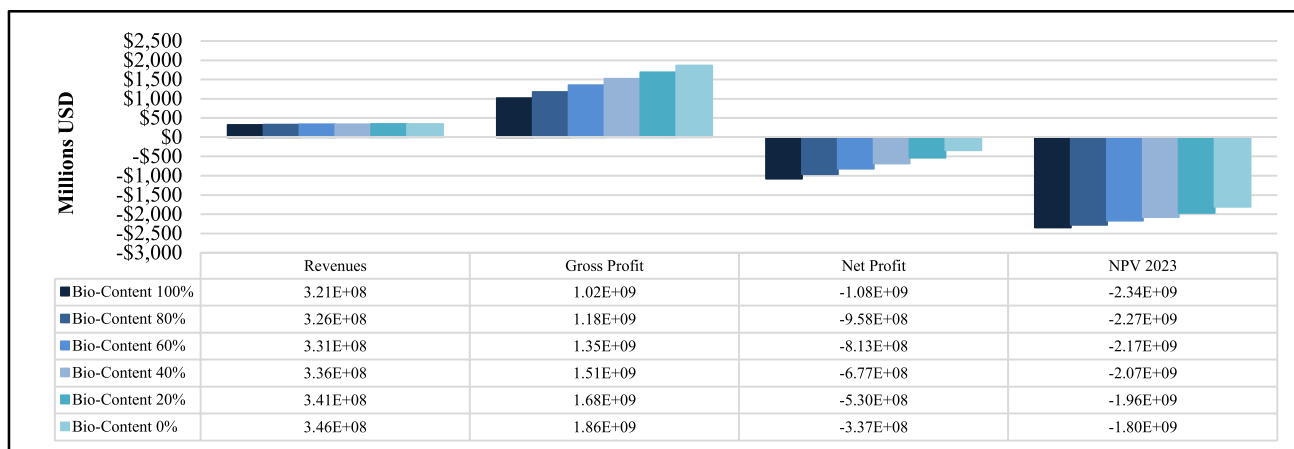


Fig. 3 Financial overview for the mass production of fibres with different percentages of bio-PET content

mid-pressure (MP) and high-pressure (HP) steam were the only revenues generated from energy production. The final financial summary of the revenues, profits, and the NPV<sub>2023</sub> of the PET production and recycling plant over its 18-year operational period are outlined in Fig. 3. On account of the gross profits, the results indicate that the plant’s revenues are sufficient to cover the AOCs, but with decreasing bio-PET production and bio-PET addition in the polyester fibres, the gross profit increases. Naturally, this implies that the production costs of bio-PTA and bio-EG, compared to fossil-PTA and fossil EG from recycled PET, are more expensive to produce. As suspected, the decrease in the production output of bio-PTA and bio-EG, and the percentage of bio-PET content in the polyester fibres, reduces the material and utility costs, or the variable operating costs (VOC), the overall production operating costs (POC), and the total production costs (TPC) in all scenarios (Fig. 4). This is reasonable considering the

number of processes and resources required to produce bio-PTA and bio-EG are greater than recycling fossil-PET fibres for r-PTA and r-EG. Besides the high operational costs associated with bio-PTA and bio-EG production, their TFCI costs are much higher than the enzymatic hydrolysis (EH) recycling process for r-PTA and r-EG, leading to negative net profits and NPV<sub>2023</sub> overall. Thus, considering the high capital costs, specifically related to equipment cost (~27–28% of the TFCI), two other scenarios were evaluated. In scenario 2, it was assumed that a wheat straw pretreatment-to-bio-EtOH plant and a corn stover pretreatment-to-IBN plant and with on-site bioenergy production were already in operation, for several years with their capital costs paid off. In scenario 3, scenario 2 is extended with the assumption that the PET recycling plant line has also been operational and bears no further capital costs. Scenario 1 represents the base results of the newly constructed plant discussed previously. Referencing

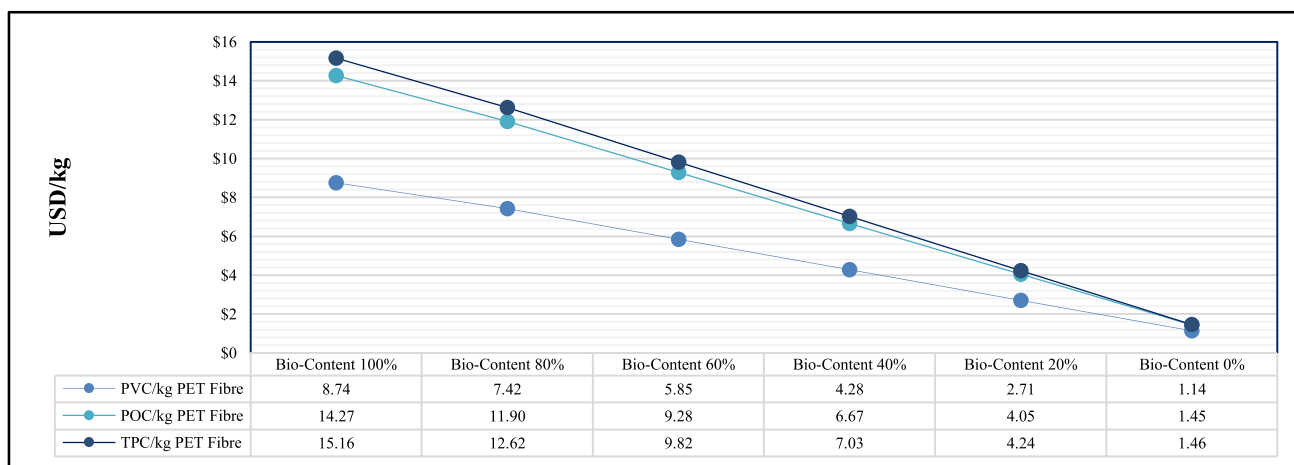
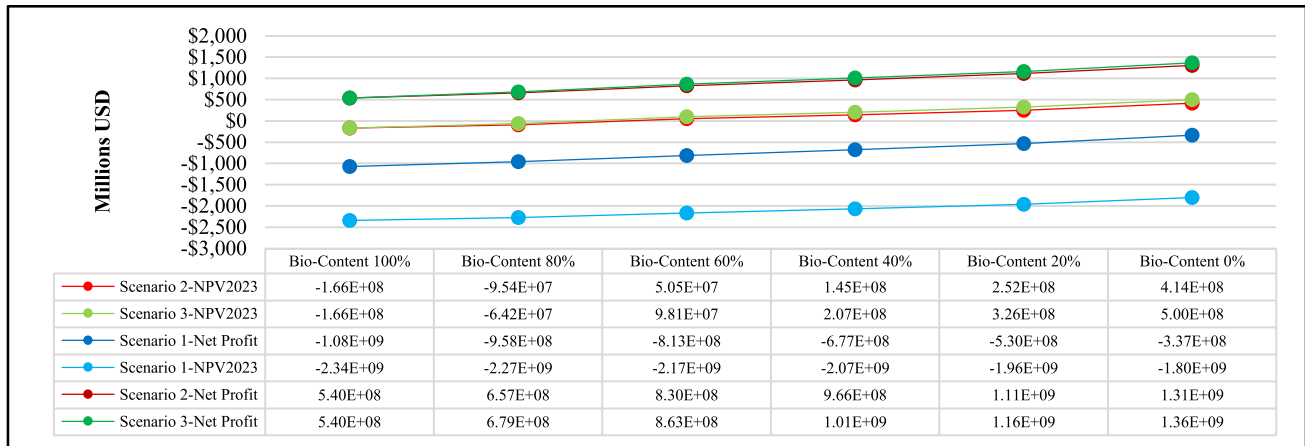


Fig. 4 Production variable cost (PVC), production operating cost (POC), and total production cost (TPC)



**Fig. 5** Net profits and NPV<sub>2023</sub> of scenarios 1, 2, and 3 for the mass production of fibres with different percentages of bio-PET content

Fig. 5, positive profits for scenarios 2 and 3 are possible for all percentages of bio-PET content. In scenarios 2 and 3, a positive NPV<sub>2023</sub> is achievable with  $\leq 60\%$  bio-PET content in the polyester. What can be surmised from these alternative scenarios is that constructing and paying off the capital costs for a brand new wheat straw-EtOH and corn stover-IBN plant lines, with an added waste-bioenergy system would not create enough revenue from surplus EtOH, IBN, or from electricity and steam heat sales, to cover all the facility's costs. While it may seem reasonable to only build the downstream production processes for EtOH conversion to EG and IBN conversion to PTA from a pre-existing bio-ethanol or bio-isobutene plant, respectively, the importance of the EtOH and IBN as the main sources of revenue cannot be understated. Therefore, the best case scenario likely would be to pursue scenarios 2 and 3 and reduce the output of bio-PET fibre content to  $\leq 60\%$  in the polyester.

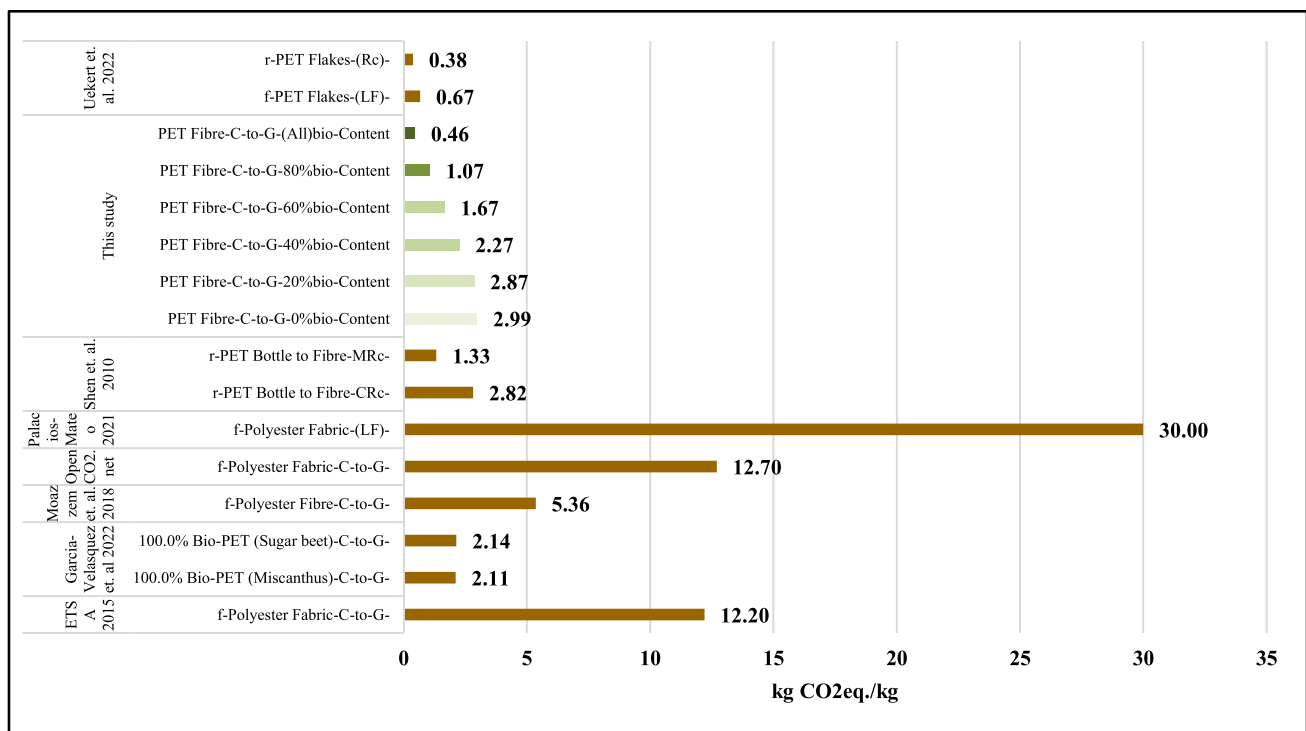
### 3.2 Financial sensitivity and uncertainty analysis

To determine the probability of whether the plant could successfully acquire positive net profits and a positive NPV<sub>2023</sub> for scenarios 2 and scenario 3, and for the production of PET polyester fibres with bio-based content of 0 to 40%, a sensitivity analysis followed by a Monte Carlo simulation was performed. To determine the significance of the revenues and the costs for the 0%, 20%, and 40% bio-PET polyester fibres, each of the revenues and the costs related to the total fixed capital investment (TFCI) and the operational cost (OC) (i.e. the sum of the AOC for 18 years) were first varied by factors of  $\pm 10\%$  from their reference values. In both scenarios, the plant's revenues had the most significance on the profitability and investment value for the bio-PET polyester fibres, followed by TFCI (mostly EPC), and OC (mostly materials). Next, the top five highest revenues,

materials, utilities, and equipment were identified, and the respective prices for each item were varied by factors of  $\pm 2.5\%$ ,  $\pm 5.0$ ,  $\pm 10.0$ ,  $\pm 20.0$ , and  $\pm 40.0\%$  and all possible resulting changes to the net profits and NPV<sub>2023</sub> were collected, and mean ( $\mu$ ) and standard deviation (std.) were calculated (see the MSE-bio/(r)-PET-fibre Ref. tool's Sens. analysis sheet). Upon entering the  $\mu$ , std., and base values for net profit and NPV<sub>2023</sub> per scenario and per PET polyester fibre into the Monte Carlo simulation, the results of 1000 trials and the likelihood of financial success or failure were approximated using normal distribution. The full results can be found in the supplementary file (MSE-bio/(r)-PET-fibre Ref. tool's Monte Carlo sheet), and the summary of the Monte Carlo simulation results for each scenario and per bio-PET content is given in Table 4. It was found that the risk of negative net profits and NPV<sub>2023</sub> is 100.0% certain for scenario 1 for all amounts of bio-PET content. While the predicted results appear varied for scenarios 2 and 3, naturally, scenario 3 had the lowest risk of losses, and each scenario had a lower risk of loss with lower bio-PET content. From these results, it is evident positive financial outcomes are more probable via integration with an existing biorefinery and/or recycling plant lines (scenarios 2 and 3), and with production of mixtures  $\leq 40.0\%$  bio-PET content in the fibres.

### 3.3 Life cycle analysis and carbon emissions

From an environmental perspective, the production of greater additions of bio-PTA and bio-EG content in the PET fibres resulted in a lower carbon footprint, surprisingly. As demonstrated in Fig. 6, when the bio-content rose from 0% bio-PET content to 100% bio-PET content in the PET fibres, the carbon footprint decreased from 2.99 to 0.46 kg CO<sub>2</sub>eq./kg of PET fibre. When comparing these results to other literature examples surveyed, the



**Fig. 6** Comparison of the GWP of different  $\text{kg}_{\text{bio-PET}}/\text{kg}_{\text{PET}}$  content (this study) to other literature examples. Notations: Rc, recycled; MRc, mechanical recycling; CRc, chemical recycling; LF, landfilled; C-to-G, cradle-to-fate; f, fossil

100% bio-PET fibres have a lower carbon footprint (0.46  $\text{kg CO}_2\text{eq./kg}$ ) relative to two other 100% bio-PET fibres made from the conversion of sugar beet and miscanthus into ethylene for bio-EG and bio-PTA via the Diels–Alder reaction [82]. Yet, with the increasing addition of fossil EG and fossil PTA, this study’s PET fibres’ GWP is in a similar range to other recycled fossil PET fibres [65, 83–85]. Likely, the explanation for why the enzymatic hydrolysis (EH) recycling of PET in this study and the other recycling methods of other studies (e.g. mechanical) are higher than new bio-PET fibre production is the fact that the conversion of PET fibres into polyester textile products is a highly energy and material-intensive process. For example, it is quoted that the production of one T-shirt requires as much as 30.53 kWh (203.56 kWh/ $\text{kg}_{\text{T-shirt}}$ ) and roughly 81.62  $\text{kgCO}_2\text{eq./T-shirt}$  (544.13  $\text{kgCO}_2\text{eq./kg}_{\text{T-shirt}}$ ) [10, 86, 87]. This is evident in Fig. 6, as there is a large spike in carbon emissions for PET fabric compared to regular PET fibres. Since the recycled fossil PET fibres also have high carbon emissions associated with the clothing industry’s textile production and consumer use (e.g. from washing), the r-PTA and r-EG carbon impact is higher than bio-PTA and bio-EG. However, for instance, if this study included the conversion of its PET fibres for textiles and their use (i.e. textile manufacturing and washing), it is probable these textiles would have a much higher

carbon footprint. It should be emphasised that the examples of PET chemical and mechanical recycling in Fig. 6 convert PET bottles [64, 65, 85], not textiles, meaning inputting alternative sources of PET waste feedstock likely would have a lower carbon footprint. As it stands, the overall EH recycling process emits much less  $\text{kg CO}_2\text{eq.}$  than the bio-PTA and bio-EG process (Fig. 7), consumes less electricity and steam heat (Fig. 8), and materials (Fig. 9).

## 4 Conclusion

This research study has two primary objectives. The first is to determine how profitability and  $\text{NPV}_{2023}$  and the carbon footprint of polyethylene terephthalate (PET) polyester textile fibres could be enhanced through the smarter application of bio-polyethylene terephthalate (bio-PET) or recycled fossil polyethylene terephthalate (r-PET), or combined mixture. To optimise the application of bio-PET and r-PET in textile fibres, this research study modelled and simulated a wheat ethanol (EtOH) and a corn stover isobutene (IBN) biorefinery and the effects of allocating a portion of EtOH and IBN for ethylene glycol (bio-EG) and purified terephthalic acid (bio-PTA) production, respectively, as well as fossil PET textile enzymatic hydrolysis (EH) recycling into ethylene glycol (r-EG) and purified terephthalic acid (r-PTA), and



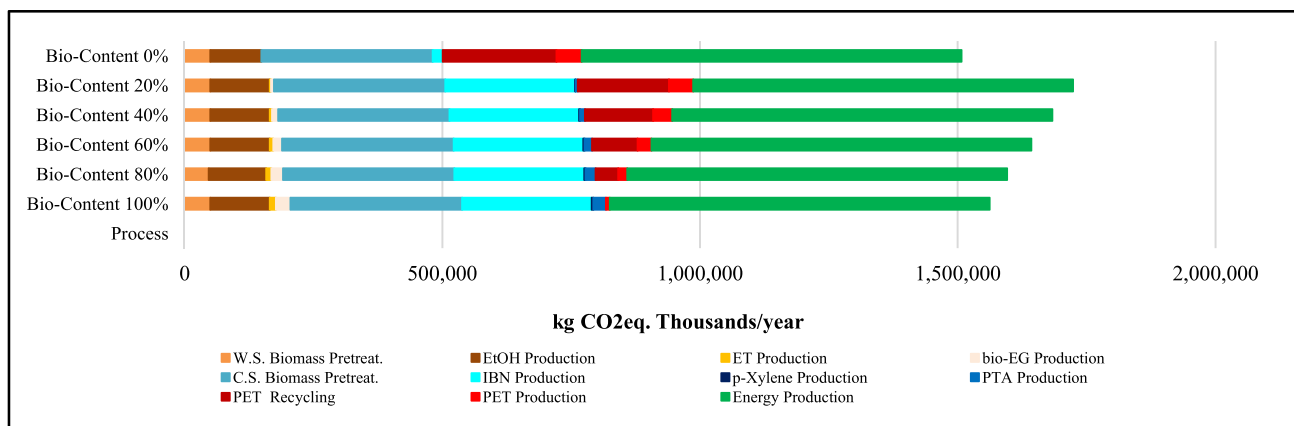


Fig. 7 CO<sub>2</sub> emissions to produce PET fibres with different percentages of bio-PET content

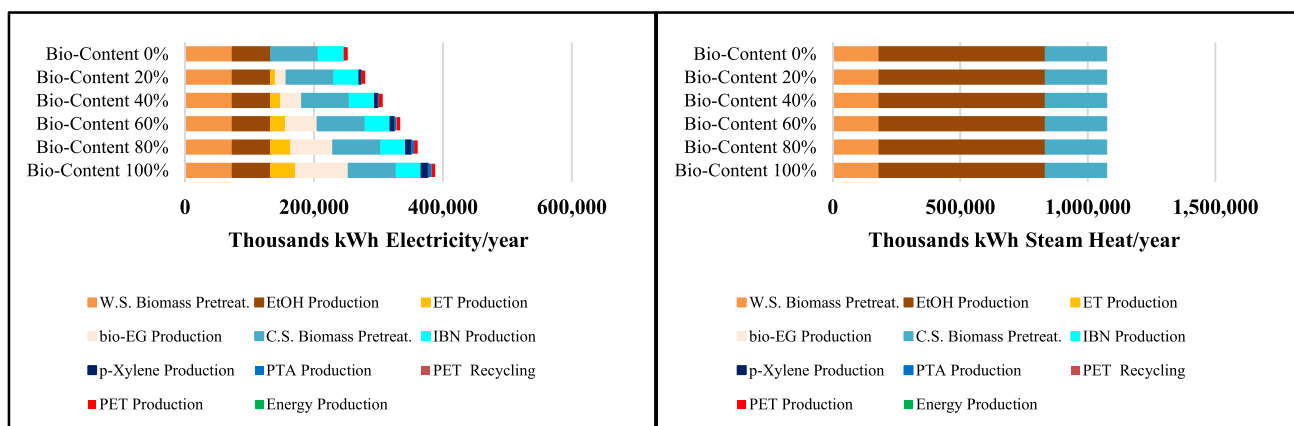
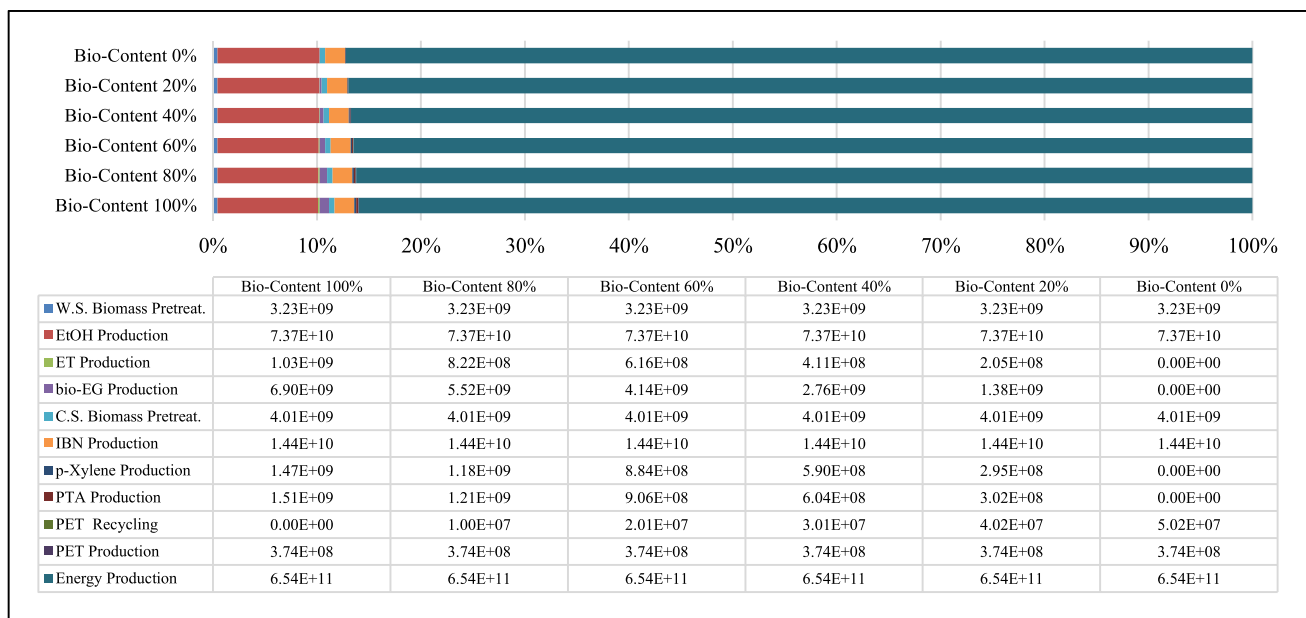


Fig. 8 Energy consumption to produce PET fibres with different percentages of bio-PET content

the production of PET polyester fibres from the acquired EG and TPA. The second goal of this research was to make publicly accessible all the resources, data, and tools utilised in this study for academics to entrepreneurs alike as a reference for the promotion of greater research and development in the direction of more sustainable and affordable bio and circular textiles. Therefore, all energy and material data from the simulation, financial and life cycle analysis (LCA) data, and calculations were compiled into the Microsoft Excel bio/(recycled) PET-fibre Refinery (MSE-bio/(r)-PET-fibre Ref.) tool. In the tool, the financial returns and carbon emissions for six different PET polyester fibres with bio-PET content of 0%, 20%, 40%, 60%, 80% to 100% were estimated for scenario 1 (a newly constructed plant), scenario 2 (newly constructed p-xylene, PTA, ET, EG, PET chemical recycling, and PET production lines only), and scenario 3 (newly constructed p-xylene, PTA, ET, EG, and PET production lines only), with the EtOH and IBN plants in scenarios 2 and 3 already constructed, operational, and with zero capital

expenses. The results concluded that only scenarios 2 and 3 could generate net profits and a positive NPV<sub>2023</sub>. Due to the high dependence on the EtOH and IBN as the main sources of revenue for the plant, only PET fibres with a content of  $\leq 40.0\%$  bio-PET in scenarios 2 and 3 were able to maintain positive net profits and a positive NPV<sub>2023</sub> with reduced risk of loss the lower the bio-PET content. When analysing the carbon impacts, it was found that with greater higher amounts of bio-PET content, from 0 to 100 wt.%, the carbon footprint decreased from 2.99 to 0.46 kg CO<sub>2</sub>eq./kg of PET fibre. However, after reviewing other literature sources, it was discovered that the likely reason why the chemically recycled PET (r-PET) have a higher carbon footprint than new bio-PET fibre production is due to the high energy and material intensity the PET fibres are subjected to when being manufactured into polyester textile products and during their use phase before being recycling. Meaning, if the six textile fibres in this study were converted into finished textile products, used by consumers, and then recycled,



**Fig. 9** Material consumption to produce PET fibres with different percentages of bio-PET content

their CO<sub>2</sub> emissions per kg of fibre may be higher in their second lifecycle than the new virgin bio-PET fibres. More research and analysis should be conducted to ascertain the best ways to reduce resource and waste emissions associated with textile production from bio and recycled PET fibres.

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**Author contribution** Each author declares they contributed to the study's conception, design, and structure from start to finish. Each author agrees they read and approved its contents for its submission and publication. The main material preparation, data collection, and analysis were performed by Nathaniel J. Berger with the advisement, supervision, and assistance of Christoph Pfeifer.

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**Data availability** The authors confirm that all data and materials supporting the findings of this study are freely available within the article and its supplementary files as indicated or as referenced.

## Declarations

**Ethical approval** Not applicable as this work was not for human or animal studies.

**Competing interests** The authors declare no competing interests.

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