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## PEF plastic synthesised from industrial carbon dioxide and biowaste

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### Abstract:

Polyethylene furandicarboxylate (PEF) is considered as a renewable-based solution to its fossil-based counterpart polyethylene terephthalate (PET). However, due to its lengthy and energy intensive production process, PEF has not been established at a commercial scale. Here we present a novel study on PEF produced from industrial carbon dioxide (CO<sub>2</sub>) emissions and non-food derived biomass to provide an alternative for PET. We assess PEF production from an energy consumption, environmental impacts and production cost point of view at an industrial scale using mass and energy balance, life cycle assessment and payback period. The results show that emissions and energy consumption can be reduced up to 40.5% compared to PET. Abiotic Depletion (Fossil) ( $6.90 \times 10^4$  MJ), Global Warming Potential ( $3.75 \times 10^3$  kg CO<sub>2</sub> equivalent) and Human Toxicity Potential ( $2.18 \times 10^3$  kg 1,4 dichlorobenzene equivalent) are the three most significant impacts in producing 1 tonne of PEF. By applying optimal design and mature technology, PEF produced from industrial CO<sub>2</sub> and bio-wastes could be a feasible and competitive substitute to PET and other materials.

**Keywords:** Biomass, Carbon dioxide, Polyethylene furandicarboxylate, Environmental impact, Production cost, Industrial scale

28 Both carbon capture and storage (CCS) and carbon capture and utilisation (CCU) technologies aim to reduce  
29 atmospheric CO<sub>2</sub> emissions<sup>1,2</sup>. The main difference lies in the destination of captured CO<sub>2</sub>—CCS stores CO<sub>2</sub>  
30 (underground or in the form of mineral carbonates) whilst CCU utilises CO<sub>2</sub> directly (as a working fluid in producing  
31 dry ice, refrigeration *etc.*; a solvent for enhanced oil recovery (EOR); or a feedstock for products indirectly converted  
32 from CO<sub>2</sub> *e.g.* feedstocks for urea production)<sup>3-5</sup>. Global Warming Potential (GWP) of CCS is lower than that of CCU  
33 from life cycle perspective, 0.276 tonne CO<sub>2</sub> equivalent·tonne<sup>-1</sup> CO<sub>2</sub> removed compared with 0.495 tonne CO<sub>2</sub>  
34 equivalent·tonne<sup>-1</sup> CO<sub>2</sub> utilised for EOR, for instance<sup>6,7</sup>.

35

### 36 **Status of PEF production pathways**

37 Industrial production plants represent the third largest source of CO<sub>2</sub> emissions in 2014<sup>8</sup>. There is an increasing  
38 interest in shifting raw materials from fossil fuels to bio-based feedstocks, *e.g.* bio-plastics to reduce greenhouse gas  
39 (GHG) emissions<sup>9</sup>. Using biomass and CO<sub>2</sub> as raw materials via carbon fixation for chemicals production is a  
40 technically feasible concept. It has a positive influence on CO<sub>2</sub> reduction and carbon-neutral chemicals production<sup>10,11</sup>.  
41 Among all plastics, polypropylene carbonate (PPC) and polyethylene terephthalate (PET) are petrochemical-based;  
42 polylactic acid (PLA) is bio-based whilst polyethylene (PE) and polyethylene furandicarboxylate (PEF) can be either.  
43 PPC is the first polymer synthesised at a ktonne scale from CO<sub>2</sub> copolymerisation with fossil fuel-based propylene  
44 oxide<sup>12</sup>. Currently, global production of PET bottles can reach up to 15 Megatonne·year<sup>-1</sup>, representing roughly 0.2%  
45 of global primary energy consumption<sup>13</sup>. The main advantage of PEF is its superior performance under severe heat  
46 conditions, gradually replacing PET and resulting in 5.9% of global plastic production<sup>14</sup>. Similar to purified  
47 terephthalic acid (PTA) being an important component of PET production, bio-based 2,5-furandicarboxylic acid  
48 (FDCA) is crucial for PEF production<sup>14</sup>. Various pathways for PEF and FDCA production are shown in Fig. 1<sup>15</sup>. One  
49 conventional PEF production route is converting fructose derived from plants into FDCA in a four-step process  
50 followed by a reaction with ethylene glycol (EG). Currently, Banerjee *et al.*<sup>16</sup> reported that FDCA can also be produced  
51 by reacting 2-furoic acid (FC) with CO<sub>2</sub> in the presence of caesium carbonate. Eerhart *et al.*<sup>14</sup> indicated an  
52 approximately 50% saving in energy and reduction in CO<sub>2</sub> for a combined use of petrochemical and biobased products  
53 and a reduction of 14% for bioplastic products.

54

55

## 56 **Novel PEF production pathway**

57 The novel route of PEF production from industrial CO<sub>2</sub> and bio-waste<sup>17</sup> presented in Fig. 1 consists of four  
58 conversion steps: from xylan to furfural, FC, FDCA, and finally PEF. The first two steps are well-established processes  
59 existed for decades while the last two steps exist only in experimental and pilot plant studies<sup>18,19</sup>. PEF from biowaste  
60 doesn't compete with food sector and the industrial CO<sub>2</sub> could be used as a raw material to achieve carbon mitigation.  
61 While producing the plastic, it could further reduce the amount of waste. Comparably, PEF from 5-  
62 hydroxymethylfurfural (HMF) using sugar and glucose as the raw materials takes the advantages of less energy  
63 consumption and high conversion efficiency whereas food is used to produce HMF which is sensitive to feedstock  
64 cost. This paper aims to assess the novel PEF production pathway at an industrial scale covering CO<sub>2</sub> emissions,  
65 energy consumption, environmental impacts and production costs, which have bridged the knowledge gap for  
66 biowaste and carbon utilisation. A step-by-step process diagram of the PEF production from xylan to furfural, FC,  
67 FDCA and PEF combined with relevant chemical equations is shown in Fig. 2. The processes are detailed in  
68 Supplementary Note 1.

69

## 70 **Results**

71 **GHG emissions and energy consumption.** The mass and energy balance of PEF production process and  
72 inputs/outputs of the combined heat and power (CHP) for steam production are demonstrated in Supplementary Tables  
73 1-3. Based on GWP required from life cycle assessment (LCA) in this study, GHG emissions for PEF using EG from  
74 maize are projected in line with Ref. <sup>20</sup>. Fig. 3 shows that GHG emissions and energy consumption of novel PEF  
75 production pathway are within the range if compared to other bioplastics reported in Ref. <sup>14</sup>. PEF+ is synthesized from  
76 the processes using bio-based FDCA and EG produced from maize. The novel pathway in this study shows an up to  
77 1.86 tonne reduction of GHG emissions per tonne of PEF production, which is close to or lower than those of PET  
78 and other plastics with the exception of PEF, PEF+, and high density polyethylene (HDPE) in Ref. <sup>14</sup>. The excess  
79 CO<sub>2</sub> emissions produced in the latter can be up to 2.2 tonne of CO<sub>2</sub> when compared to the case of PEF+. This is mainly  
80 because PEF processes proposed in Ref. <sup>14</sup> are all in lab scale whilst food (instead of waste as in this study) is used as  
81 the raw material for other plastic products without considering upstream and downstream processes which may cause  
82 a large increment of GHG emissions<sup>21</sup>. As for energy consumptions, the results show that the PEF production pathway  
83 using EG from maize has the lowest energy consumption *i.e.* 46 GJ per tonne of PEF production, indicating the most

84 significant improvement, *i.e.* 40.5% when compared with PTT. Also, the PEF production pathway using EG from  
85 petrochemical has low energy consumption *i.e.* 58 GJ per tonne of PEF production, which is close to or lower than  
86 that of most bioplastics except some materials e.g. PEF<sup>+</sup>. This could be explained by similar reasons for GHG  
87 emissions *i.e.* maturity of production steps and non-food raw material. Besides, GHG emissions reduction is not  
88 proportional to energy consumption. For example, energy consumption of PEF from EG-maize in this paper is reduced  
89 by 37.5% when compared with that of PTT. With regard to GHG emissions, the aforementioned performance is  
90 reduced by 42.3%. The main reasons for that are illustrated as follows: the proposed pathway consumes CO<sub>2</sub> in the  
91 processes and GHG emissions are evaluated in terms of a life-cycle prospective, which are the comprehensive results  
92 after LCA based on mass and energy balance. There is vast potential for the proposed pathway of PEF production to  
93 further reduce GHG emissions using other renewable energy sources e.g. solar, wind, and geothermal energy that  
94 could replace the CHP completely or partially used in this study. The results in Fig. 3 are limited on operating  
95 information in the step 3 of PEF production e.g. pressure, temperature, yield taken from lab-scale experimental results  
96 and the required energy consumption replaced by that of PET polymerisation.

97 **Environmental impacts.** The life cycle impact assessment (LCIA) results and the contribution of individual life cycle  
98 stages towards impact categories assessed in this study are illustrated in Fig. 4(a), showing that Abiotic Depletion  
99 (Fossil), Global Warming Potential, and Human Toxicity Potential (labelled as II, VI and VII respectively) are the  
100 three most significant environmental burdens in producing 1 tonne of PEF, *i.e.*  $6.90 \times 10^4$  MJ,  $3.75 \times 10^3$  kg CO<sub>2</sub>  
101 equivalent and  $2.18 \times 10^3$  kg DCB equivalent respectively. The three impacts are largely attributable to the production  
102 process of natural gas required for operating the PEF plant, the operation and maintenance of the CHP system and the  
103 production process of EG required for producing PEF respectively. Fig. 4(a) also shows that all impact categories are  
104 primarily caused by the operation stage—operating the CHP system is mainly responsible for most impact categories  
105 with the exception of Abiotic Depletion (Fossil) and Global Warming Potential, which are largely caused by the  
106 operation of the PEF production plant, indicating that other life cycle stages are relatively insignificant whilst natural  
107 gas driven CHP is not an ideal option from an environmental perspective despite of its maturity. Besides, compared  
108 to base case, a sensitivity analysis is conducted using 11 scenarios to assess sensitivity of LCIA results as shown Fig.  
109 4(b) which is to investigate life cycle inventory analysis (LCI) quality and assumptions made in the study by  
110 manipulating the magnitude of electricity supplied by CHP, CO<sub>2</sub> reused and natural gas consumption for 1 tonne of  
111 PEF production. Results show that every 10% change in these variables would, respectively, result in approximately

112 17% and approximately 7% of differences respectively in LCIA results of Abiotic Depletion (Fossil) and Global  
113 Warming Potential, which are the two impact categories affected most significantly by these variables. As illustrated  
114 in Fig. 4(c), a similar pattern is also shown by carbon and GHG intensities—the former accounts for carbon emissions  
115 from PEF production only whilst the latter considers GHG involved in all processes. The results indicate that, for the  
116 scenarios assessed in this study, (i) the influences of electricity supply by CHP and natural gas consumption are more  
117 profound than that of CO<sub>2</sub> reused in the process; and (ii) utilising CO<sub>2</sub> generated from the production process can  
118 reduce but not fully offset the environmental impacts of consuming electricity and natural gas during the production  
119 process itself, i.e. fraction of CO<sub>2</sub> that can be utilised is 14.12%. The similarity in the pattern of results shows that the  
120 LCI quality is of a satisfactory level. The sensitivity analysis in 11 additional scenarios present the strength of this  
121 LCA study. The influence of downstream process of EG production cannot be further assessed due to the limitation  
122 of using existing dataset available in GaBi software. The location and the end of life scenario of the production plant  
123 as well as transport and distribution of PEF produce are anticipated to affect the LCIA results; however, their  
124 significance, which could be paramount or trivial, cannot be investigated in this study due to limited data availability  
125 and time constraints.

126 **Economic potential.** As illustrated in Fig. 5(a), scale factor varies from 0.5 to 0.9 with a higher likelihood occurring  
127 between 0.6 and 0.8 indicating a capital investment range of \$237.8–281.8 million. Fig. 5(b) indicates the impact of  
128 PEF prices on payback period for a plant capacity of 50 ktonne·year<sup>-1</sup>. The price is selected based on total capital cost  
129 for PEF production. It is worth noting that the payback period is less than 5 years when market price is higher than  
130 \$4·kg<sup>-1</sup>. As might be expected, the lower the PEF market price is, the longer the payback period becomes. For example,  
131 the payback period is 50 years or more when the PEF market price is lower than \$3·kg<sup>-1</sup>. Within the 0.6-0.8 scale  
132 factor range, the PEF market price cannot be as low as that of PET; otherwise, the payback period will become  
133 unacceptable. This is mainly because the proposed pathway of PEF production is not commercialised with possible  
134 technical barriers e.g. efficient catalyst, cost of material, thermochemical stability and conversion efficiency. If the  
135 barrier could be overcome, a low market price will be achieved. Besides, it is indicated that the PEF market price has  
136 stronger influence over payback period than capex scale factor in this study because the chosen capacity ratio is not  
137 very high.

138 Besides, the payback period can be reduced with plant capacity as shown in Fig. 5(c) where 0.6 is applied as the  
139 capex scale factor. Two relatively low prices *i.e.* \$3 kg<sup>-1</sup> and \$3.4 kg<sup>-1</sup> are used in the analysis since the other price in

140 Fig. 5(b) must result in the lower payback period. It indicates that the payback period will decrease remarkably with  
141 plant capacity at a relatively low PEF price, which proves the feasibility to shorten the payback period with increased  
142 plant capacity. For a higher price, plant capacity has limited influence on the payback period. Thus, both plant capacity  
143 and the selling price are compromised in designing an industrial plant for the novel pathway.

144 Fig. 6 shows PEF production costs under various conditions in which Fig. 6(a) is to compare the costs of this  
145 study and three cases in Ref. <sup>22</sup> at a capacity of 100 ktonne·year<sup>-1</sup>. Negative Y-axis indicates annual revenue of the by-  
146 products and excessive electricity; positive Y-axis represents annual costs of capital recovery, feedstocks, chemicals  
147 (*i.e.* raw materials), Operating and management (O&M) *etc.*; and the red dot presents the production cost of PEF, per  
148 tonne. The cost of PEF production via novel pathway is about \$2435 tonne<sup>-1</sup> which is in the range of \$2370–4879  
149 tonne<sup>-1</sup> reported in Ref. <sup>22</sup>. The production cost of PET is \$1800 tonne<sup>-1</sup> at the expense of 50% additional CO<sub>2</sub> emissions  
150 compared to PEF production via novel pathway proposed in this study.

151 The novel PEF pathway employs CO<sub>2</sub> at 99.5% purity as a raw material. CO<sub>2</sub> can be captured from various  
152 sources including PEF production supply chains and power plants. The main practical obstacles in incorporating a  
153 post-combustion CO<sub>2</sub> capture plant are large energy consumption, high capital cost and operating cost, which depend  
154 on the exhaust gas conditions. The concentration of CO<sub>2</sub> in industrial exhaust gases varies from one to another. For  
155 instance, in descending order, 97%, 77%, 22%, 10–15% and 3–4% volume per volume (v·v<sup>-1</sup>) from ammonia and  
156 ethylene oxide plants, hydrogen production plants, sulphur production plants, coal power plants and gas turbines,  
157 respectively<sup>23</sup>. Thus, CO<sub>2</sub> prices vary with its concentration in the flue gases. The impact of CO<sub>2</sub> prices on the  
158 production cost of PEF is analysed as shown in Fig. 6(b) which ranges \$45–70 tonne<sup>-1</sup> considering CO<sub>2</sub> from natural  
159 gas and coal power plants<sup>24,25</sup>. It is found that PEF production cost increases only by 1.6% from \$2430 tonne<sup>-1</sup> to  
160 \$2475 tonne<sup>-1</sup> when CO<sub>2</sub> price varies up to \$90 tonne<sup>-1</sup>. Results show that CO<sub>2</sub> price has marginal impact on the PEF  
161 production cost. Therefore, CO<sub>2</sub> from various sources including coal and natural gas power plants could be employed.

162 A comparison based on a single bottle can further provide insights into this analysis from the perspective of  
163 consumers or minimising plastic bottle usage. Compared to PET, PEF has (i) better oxygen, CO<sub>2</sub> and H<sub>2</sub>O barriers  
164 (*i.e.* 6, 3 and 2 times more superior, respectively); and (ii) higher resistance to mechanical strain<sup>26,27</sup>. According to  
165 Refs. <sup>28,29</sup>, the wall thickness of a conventional high impact polystyrene (HIPS) cup can be reduced from 0.89 mm to  
166 0.66 mm if impact-modified PLA is used due to the higher stiffness of PLA than that of HIPS. Likewise, a thinner  
167 PEF bottle with reduced mass (and material) can be produced due to its superior properties compared to PET, leading

168 to a corresponding lower PEF bottle selling price. A sensitivity analysis is carried out to determine the maximum mass  
169 of a PEF bottle that can make its selling price more competitive than that of PET. The production cost of a 237 ml  
170 PET bottle is \$0.162<sup>30</sup>, is derived from the total production cost of 1 tonne of PET, *i.e.* \$1800 tonne<sup>-1</sup>. For simplicity  
171 (and assuming that bottle manufacturing costs are mainly material), assuming that the average mass of a 237 ml PET  
172 bottle is 9 g, the production cost of one PEF bottle could be the same as that of a PET bottle when the mass of a PEF  
173 bottle is reduced by 25.9% from 9 g to 6.67 g, as shown in Fig. 6(c). As such, the PEF production cost per bottle could  
174 be the same or lower than that of PET, depending on the mass of a PEF bottle due to its better properties (although  
175 the production cost of 1 tonne of PEF is more expensive than that of PET, as discussed earlier).

176

## 177 **Discussion**

178 A novel PEF pathway employing industrial CO<sub>2</sub> and biowaste is presented which could be a sustainable  
179 alternative for its counterpart, PET. In this study, GHG emissions, energy consumption, environmental impacts and  
180 production cost of novel PEF production pathway at an industrial scale are evaluated based on actual lab-scale  
181 experimental studies and limited by the database of software. The results show that GHG emissions and energy  
182 consumption of the novel pathway are in the same range of other bioplastics. However, it is worth noting that the  
183 proposed alternative does not compete with food sector, which has a large advantage in some countries where primary  
184 food is scarce now or in the future. By using this novel pathway, GHG emissions and energy consumption can be  
185 reduced by up to 40.5% when compared to those of PET production. Whilst all environmental impacts are primarily  
186 caused by the operation stage, the influence of electricity supply and natural gas consumption by the CHP system over  
187 the assessed environmental impacts is more profound than that of industrial CO<sub>2</sub> utilisation. More insights would be  
188 gained from future case studies if transport, treatment and disposal of used lubricating oil, distribution and use of PEF  
189 produce, surplus electricity, and alternative end of life scenarios are assessed in LCA. If renewable energy or carbon  
190 capture is incorporated with natural gas-powered CHP, more potentials of this novel pathway could be further explored.  
191 The process requires CO<sub>2</sub> of high purity which increases its price depending on the sources. Nevertheless, the price of  
192 CO<sub>2</sub> has a marginal impact on the production cost of PEF. The current production cost of PEF is higher than that of  
193 PET. The cost for PEF production can be reduced by optimal design and mature technology. Based on 15 million  
194 tonnes of global PET bottle market per year *i.e.* 1/3 of the global PET production, the novel PEF production pathway  
195 not only offers a viable solution to reuse biomass within an industrial zone but also employs local GHG emissions

196 which will reduce overall carbon foot print in the future. Different technologies for sustainable plastic e.g. bioplastic  
197 development, biorecycling of PET and partially using post-consumer resin PET are gathering the momentum and  
198 could be mutually complemented.

199

## 200 **Methods**

201 The process modelling is carried out by using the chemical engineering process simulation tool, Aspen Plus  
202 version 9. A non-random, two-liquid model (NRTL) property method is used in the modelling<sup>31,32</sup> based on operating  
203 conditions reported in the literature from actual lab-scale experiments and pilot plant studies<sup>33-35</sup>. During the  
204 simulation, processes are up-scaled to determine mass balance and identify the energy demands. Supplementary Figure  
205 1 illustrates the PEF production model where the relevant operating conditions are shown in Supplementary Table 4.  
206 The physical properties of xylan, FC, PDCA and PEF are not available in the standard Aspen Plus properties databases.  
207 As such, these components are defined as conventional solids in Aspen Plus, as summarised in Supplementary Table  
208 5. Information required for conventional solids are heat of formation, density, boiling points, molecular weights and  
209 molecular structures, which are taken from Refs. <sup>36-39</sup>. The heat capacity values of FC, FDCA and PEF are estimated  
210 using the atomic element contribution method of Hurst and Harrison<sup>38,40</sup>.

211 **Combined heat and power.** A CHP system powered by natural gas is considered and simulated in Aspen Plus to  
212 generate the required steam and electricity. The related parameters and conditions are obtained from the simulation  
213 data of Thermoflow. The natural gas driven CHP system consists of a gas turbine with a heat recovery steam generator  
214 (HRSG), and a steam turbine. The gas turbine is a GE LM6000 PC SPRINT selected from the list of commercial  
215 machines available in Thermoflow. The flue gas from the turbines flows into the HRSG where steam is generated to  
216 feed a steam cycle and to the PEF process, as shown in Supplementary Figure 2. Additional steam at 12.7 bar is  
217 produced in the HRSG. The stream mixes with the exhaust steam of the high-pressure steam turbine to provide thermal  
218 energy to the PEF production process.

219 The quantity of CO<sub>2</sub> attributable to steam and electricity is estimated using Equations (1)–(3):

$$E_{\text{steam}} = m_{\text{steam}}[h - h_0 - (T_0 + 273.15)(s - s_0)], \quad (1)$$

$$E_{\text{power}} = P, \quad (2)$$

$$m_{\text{CO}_2, \text{steam}} = [m_{\text{CO}_2, \text{total}}] \frac{E_{\text{steam}}}{E_{\text{steam}} + E_{\text{power}}} \quad (3)$$

220 where  $m_{\text{steam}}$ ,  $h$  and  $s$  are the mass flow rate ( $\text{kg}\cdot\text{s}^{-1}$ ), the enthalpy ( $\text{kJ}\cdot\text{kg}^{-1}$ ) and the entropy of steam ( $\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ );  $h_0$   
221 is the enthalpy input of water at 15 °C under ambient conditions whilst  $s_0$  is the entropy of water ( $\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ ) at  $T_0$ ,  
222 which is the ambient temperature (°C);  $P$  is the power generated by the CHP (kW),  $m_{\text{CO}_2,\text{steam}}$  is the mass flow rate  
223 of CO<sub>2</sub> generated by steam which is consumed during PEF production ( $\text{tonne}\cdot\text{h}^{-1}$ ); and  $m_{\text{CO}_2,\text{total}}$  is the total CO<sub>2</sub>  
224 generated by the CHP ( $\text{tonne}\cdot\text{h}^{-1}$ ).

225 **Life cycle assessment.** PEF production using the proposed novel pathway is then assessed from a LCA perspective  
226 to estimate its environmental impacts covering the four iterative phases of LCA, namely goal and scope definition,  
227 LCI, LCIA and life cycle interpretation in compliance with the Standards established by the International Organisation  
228 for Standardisation (ISO) *i.e.* ISO14040 and 14044<sup>41,42</sup>. The key elements are highlighted here: (1) the product system  
229 of this LCA study is the PEF production plant integrated with the CHP system powered by natural gas; (2) the function  
230 is to produce PEF using EG from petrochemicals for 30 years; (3) the functional unit is 1 tonne of PEF (which is  
231 defined in line with Ref. <sup>14</sup>); (4) the system boundary covers construction, operation and maintenance, and end-of-life  
232 phases of the product system including upstream and downstream processes if relevant data are available in GaBi  
233 Professional Database whilst excluding (i) transport (in line with Ref. <sup>14</sup>); (ii) treatment and disposal of used lubricating  
234 oil during maintenance; (iii) distribution and use of PEF produce as well as surplus electricity generated by the CHP  
235 system; and (iv) co-products of PEF production (*i.e.* furfuryl alcohol and sodium hydrogen sulphate). It is assumed  
236 that (i) the product system will operate following the production profile simulated in Aspen Plus consuming natural  
237 gas at a rate of 9800  $\text{kg}\cdot\text{h}^{-1}$  for 8000  $\text{h}\cdot\text{year}^{-1}$  over 30 years without any defect; (ii) CO<sub>2</sub> produced by the product system  
238 during operation will be utilised in the PEF production process at a rate of 1200  $\text{kg}\cdot\text{h}^{-1}$  (based on Aspen Plus simulation  
239 outcome) as a feedstock; (iii) steel, which is the primary material used in constructing the product system, is 100%  
240 recycled at the end of life; and (iv) the product system is located in Europe. The defined system boundary and the  
241 assumptions present the limitations of this study. Using input and output data gathered from Aspen Plus simulation,  
242 GaBi Database and literature, LCI is carried out, followed by the development of a simplified LCA model using GaBi  
243 software to assess the following impact categories:

- 244 (I) Abiotic Depletion (Elements), kg antimony (Sb) equivalent;
- 245 (II) Abiotic Depletion (Fossil), MJ;
- 246 (III) Acidification Potential, kg sulphur dioxide (SO<sub>2</sub>) equivalent;
- 247 (IV) Eutrophication Potential, kg phosphate equivalent;

- 248 (V) Freshwater Aquatic Ecotoxicity Potential, kg 1,4 dichlorobenzene (DCB) equivalent;  
 249 (VI) Global Warming Potential (100 years), kg CO<sub>2</sub> equivalent;  
 250 (VII) Human Toxicity Potential, kg DCB equivalent;  
 251 (VIII) Photochemical Ozone Creation Potential, kg ethene equivalent;  
 252 (IX) Terrestrial Ecotoxicity Potential, kg DCB equivalent; and  
 253 (X) Odour Potential, kg H<sub>2</sub>S equivalent.

254 The LCIA methodologies available in GaBi *i.e.* CML2016 and “Odour” are applied for the assessment of the  
 255 impact categories (I)–(IX) and (X) respectively. More information about the defined goal and scope, LCI, the  
 256 developed LCA model and the fundamental concept of LCIA methodologies is available in Supplementary Tables 6–  
 257 7 and Supplementary Figures 3–4.

258 **Economic analysis.** Economic analysis of the novel PEF production pathway is carried out by applying a payback  
 259 method in line with mass and energy balance. A process model has been developed for the production capacity of PEF  
 260 estimated from Aspen Plus model *i.e.* 21.4 ktonne·year<sup>-1</sup> from waste. The analysis considers direct, indirect, variable  
 261 operating and fixed costs which may incur during plant construction, operation and maintenance (see Supplementary  
 262 Tables 8–11). The plant capacity of 21.4 ktonne·year<sup>-1</sup> for analysis cannot compete with the PET price of \$1.51 kg<sup>-1</sup>  
 263 at 2017<sup>43</sup>. Considering the pilot plant developed by Avantium and BASF which has a capacity of 50 ktonne PEF·year<sup>-1</sup>,  
 264 the capacity is used for further evaluation<sup>44</sup>. The costs increase with plant capacity, in which the correlation is  
 265 expressed is Equation (4)<sup>45</sup>, as follows:

$$\text{Cost of plant size 2} = \text{Cost of plant size 1} \left( \frac{\text{Plant size 2}}{\text{Plant size 1}} \right)^{\text{scale factor}}, \quad (4)$$

266 where the scale factor for the capex cost is primarily 0.6–0.8<sup>46</sup>. The scale factor depends on plant complexity from  
 267 technical and technological perspectives, novelty and scalability level. It is 0.6 for mature technology and above  
 268 provided novel technology is adopted. Supplementary Tables 12 and 13 present the installation costs of PEF and PET  
 269 production plants. It can be inferred that the installation cost of a PET production plant can be 5–6 times cheaper than  
 270 that of a PEF plant. This is mainly due to the maturity of PET technology where underpinning supply chains are more  
 271 developed and its supporting industry is familiar with the technology. Likewise, it would be expected that the total  
 272 cost of establishing a PEF production plant will decline when PEF production technology becomes mature which is  
 273 related with various factors *e.g.* efficient catalyst, cheap material, good thermal and chemical stability, easy to  
 274 operation and maintenance, etc. After determining a scale factor, annual utilities and raw material costs for a specific

275 plant size, PEF market prices will dictate the operating income which impacts on payback period directly. In this  
276 study, a sensitivity analysis is performed for production capacity of 50 ktonne·year<sup>-1</sup> using bagasse as a raw material.  
277 Total investment cost is extrapolated using Equation (4).

278

#### 279 **Data availability**

280 The data that support the findings of this study are available from the corresponding author upon reasonable request.

281

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370

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372

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376

### 377 **Author contributions**

378 L.J. A.D. J.C. A.M. A.R. and A.S designed the study. L.J. A.D. J.C. provided the analysis. L.J. A.D. J.C. interpreted  
379 the data and wrote the paper. L.J. finalized the writing of the paper.

380

### 381 **Competing interests**

382 The authors declare no competing interests.

383

384 **Figure Caption**

385 Fig. 1. PEF production pathways (adapted from Ref. <sup>15</sup>).

386 Fig. 2. The PEF production pathway from wastes and industrially captured CO<sub>2</sub>.

387 Fig. 3. Comparison of performance of various bioplastics including PEF (a) GHG emissions; (b) energy  
388 consumptions<sup>14</sup> (**Petrochem. PET**: petrochemical PTA and petrochemical EG; **Petrochem. PET+**: petrochemical  
389 PTA and biobased EG from maize; **PEF**: PEF produced from fructose and HFCS; **PEF+**: bio-based FDCA and EG  
390 produced from maize; **HDPE**: petrochemical HDPE; **PHA**: polyhydroxyalkanoates; **PTT**: petrochemical PTA and  
391 bio-based PLA (maize) 1, 3-propanediol; **PLA**: polylactic acid; and **PE**: polyethylene).

392 Fig. 4. The results of (a) LCIA for the base case scenario at different life cycle stages; (b) sensitivity analysis where  
393 11 scenarios (S1–S11) assessing three variables (electricity supply, natural gas consumption and CO<sub>2</sub> reused in  
394 producing 1 tonne of PEF) are compared; and (c) a comparison of carbon intensities for these scenarios.

395 Fig. 5(a) Capital investment versus capex scale factor for a plant capacity of 50 ktonne·year<sup>-1</sup>; (b) The effect of PEF  
396 price on payback period within the range of scale factor from 0.6 to 0.8; (c) Payback period versus plant capacity.

397 Fig. 6. PEF production cost (a) compared with other cases; (b) based on a range of CO<sub>2</sub> prices; (c) based on 237 ml  
398 PET bottle.

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