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### *Second-generation bio-based plastics are becoming a reality - Non-renewable energy and greenhouse gas (GHG) balance of succinic acid-based plastic end products made from lignocellulosic biomass*

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*Published in:*

Biofuels, Bioproducts and Biorefining

*DOI:*

[10.1002/bbb.1849](https://doi.org/10.1002/bbb.1849)

*Publication date:*

2018

*Citation for published version (APA):*

Patel, M. K., Bechu, A., Villegas, J. D., Bergez-lacoste, M., Yeung, K., Murphy, R., Woods, J., Mwabonje, O. N., Ni, Y., Patel, A. D., Gallagher, J., & Bryant, D. (2018). Second-generation bio-based plastics are becoming a reality - Non-renewable energy and greenhouse gas (GHG) balance of succinic acid-based plastic end products made from lignocellulosic biomass: NREU and GHG balance of succinic acid-based PBS products made from lignocellulosic biomass. *Biofuels, Bioproducts and Biorefining*, 12(3), 426-441. <https://doi.org/10.1002/bbb.1849>

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# **Second generation bio-based plastics are becoming a reality – Non-renewable energy and greenhouse gas (GHG) balance of succinic acid-based plastic end products made from lignocellulosic biomass**

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## **ABSTRACT**

Simultaneously bio-based and bio-degradable plastics such as polybutylene succinate (PBS) have the potential to become a sustainable alternative to petrochemical-based plastics. PBS can be produced from bio-based succinic acid and 1,4-butanediol using first-generation (1G) or second-generation (2G) sugars. A cradle-to-grave environmental assessment was performed for PBS products in Europe to investigate the non-renewable energy use (NREU) and greenhouse gas (GHG) impacts. The products investigated are single-use trays and agricultural film, with incineration, industrial composting and degradation on agricultural land as end-of-life scenarios. Both end products manufactured from fully bio-based PBS and from partly bio-based PBS (made from bio-based succinic acid and fossil fuel-based 1,4 butanediol) were analysed. We examine corn (1G) as well as corn stover, wheat straw, miscanthus and hardwood as 2G feedstocks. For the cradle-to-grave system, 1G fully bio-based PBS plastic products were found to have comparable environmental impacts than their petrochemical incumbents, while 2G fully bio-based PBS plastic products allow to reduce NREU and GHG by around one third under the condition of avoidance of concentration of sugars and energy integration of the pre-treatment process with monomer production. Without energy integration and with concentration of sugars (i.e., separate production), the impacts of 2G fully bio-based PBS products are approximately 15-20% lower than those of 1G fully bio-based PBS products. The environmental analysis of PBS products supports the value proposition related to PBS products while also pointing out areas requiring further research and development.

Keywords: Bio-based polybutylene succinate, PBS, second generation feedstocks, energy balance, greenhouse gas emissions, GHG, LCA

## 1 INTRODUCTION

The transition from 1<sup>st</sup> generation bio-based products derived from feedstocks including corn grain, soya, and wheat to 2<sup>nd</sup> generation products derived from lignocellulosic feedstocks, such as agricultural residues and energy crops, has recently become a policy objective. It is the consequence of increased concern about potential issues related to 1<sup>st</sup> generation bio-based products, including potentially accelerated deforestation (direct and indirect land use effects), biodiversity loss, exacerbation of water scarcity and potentially higher food prices resulting in social impacts.<sup>1,2</sup> The priority given to the use of non-food feedstocks is stated in the European Renewable Energy Directive<sup>3</sup> and has been specified in its recent amendment.<sup>4</sup> While major progress has been made in R&D and demonstration of 2<sup>nd</sup> generation bioethanol as transportation fuel,<sup>5-10</sup> it still needs to be demonstrated that advanced bio-based products (typically produced by application of biotechnology or catalytic processes) can be made from non-food feedstocks. Next to “drop-in solutions” (e.g. partially bio-based polyethylene terephthalate/PET, now representing approximately one third of bio-based plastics),<sup>11</sup> this applies also to new, simultaneously bio-based and biodegradable plastics, for example, polylactic acid<sup>12,13</sup> or polybutylene succinate (PBS) which can be derived from succinic acid.

Succinic acid (SA) is one of the twelve high-value bio-based chemicals which, more than a decade ago, was identified by Werpy and Peterson<sup>14</sup> as a compound that has the potential to improve the profitability and productivity of bio-refineries, thereby facilitating the transition from today’s fossil-based industrial chemistry to sustainable bio-based production. This vision, which was reinforced by Bechthold et al.<sup>15</sup> as well as Bozell and Peterson,<sup>16</sup> is about to come to fruition. In 2010, a number of companies began to produce 1<sup>st</sup> generation bio-based SA in various locations across the world,<sup>17,18</sup> with today’s key producers being the companies Reverdia, Bio-Amber, Myriant and Succinity GmbH (BASF+Purac). In line with today’s practice in industrial production, most publications on the environmental assessment of SA and its derivatives evaluate 1<sup>st</sup> generation pathways,<sup>18,19</sup> with only very few exceptions.<sup>20-22</sup> To our knowledge, there are no previous studies on the environmental impacts of end-products made from 2<sup>nd</sup> generation SA-based plastics.

## 2 METHODOLOGY, PROCESS DESCRIPTION, AND INPUT DATA

We apply the principles of environmental life cycle assessment (LCA), which is an internationally standardized methodology for the environmental assessment of products and services,<sup>23,24</sup> consisting of four phases: 1) Goal and scope definition, 2) Inventory analysis, 3) Impact assessment and 4) Interpretation (see below). Recently, a European standard tailored to bio-based products<sup>25</sup> presented the LCA methodology from the perspective of its application to bio-based products, but it does not call for any changes compared to LCA studies conducted prior to its existence. In the following section, we explain the first three phases of our study, while we present the impact assessment in the results section, interpretation in the discussion and provide conclusions in the last section.

## 2.1 Goal and scope definition

The primary goal of this study is to analyse greenhouse gas emissions (GHG) and non-renewable energy use (NREU) for plastic end products made from the 2<sup>nd</sup> generation SA-based polymer polybutylene succinate (PBS). The chosen products are plastic trays used for food packaging (e.g. fruit) and agricultural mulching films. We assume 1 kg of product as the functional units, which represents 53 trays and 67 m<sup>2</sup> of film (see Discussion and Appendix A1 for reasoning). The studied product system covers all steps from cradle to grave, with end-of-life waste management by a) degradation on the field (for film) and b) combustion with energy recovery in a municipal solid waste incineration (MSWI) plant or industrial composting (for trays; Figure 1). PBS products are compared to the current incumbent petrochemical products, i.e. polypropylene and polyethylene terephthalate (PP and PET, for trays) as well as polyethylene (PE, for films), all with MSWI as waste management. PBS trays are expected to compete primarily with PP trays because the two polymers can be used for similar applications in food packaging as a consequence of some similar features (both polymers are opaque, can be coloured, and have similar melting temperatures). However, the molecular structure and polymerisation routes of PBS are more closely related to those of PET (in comparison to PP and PE), which is used as a second incumbent reference material for trays. As a regional scope, we choose Europe, thereby aiming for average conditions in feedstock supply and industrial processing. The main feedstock considered is corn stover, with results for wheat straw, miscanthus and willow being briefly presented (see Discussion). By analogy, PBS is benchmarked against other SA-based polymers (PBST, PBSA and PBAT; see Discussion).

## 2.2 Inventory analysis

The main plastic studied in this paper is (fully or partly) bio-based PBS, a biodegradable polymer which is produced by polymerisation of SA with 1,4-butanediol (BDO). The mass percentages of these two monomers relative to the total feedstock inputs are 57% (SA) and 43% (BDO). We consider 2<sup>nd</sup> generation (2G) SA next to 1<sup>st</sup> generation (1G) SA; as further benchmark we consider petrochemical maleic anhydride and petrochemical SA. For BDO, we distinguish three routes, i.e. production from petrochemicals, hydrogenation of 2G SA<sup>22</sup> and BDO produced by direct fermentation of C6 sugars (Innocenti F, Novamont Group, 2016, pers. comm.).<sup>26</sup> We study fully bio-based (fb) PBS (produced from bio-based SA and BDO) and partly bio-based (pb) PBS (produced from bio-based SA and petrochemical BDO) both with 1<sup>st</sup> generation (1G) and 2<sup>nd</sup> generation (2G) feedstocks (Figure 1). In addition, we study a Best, Reference and Conservative case for fb 2G PBS and a Reference and Conservative case for fb 1G PBS.

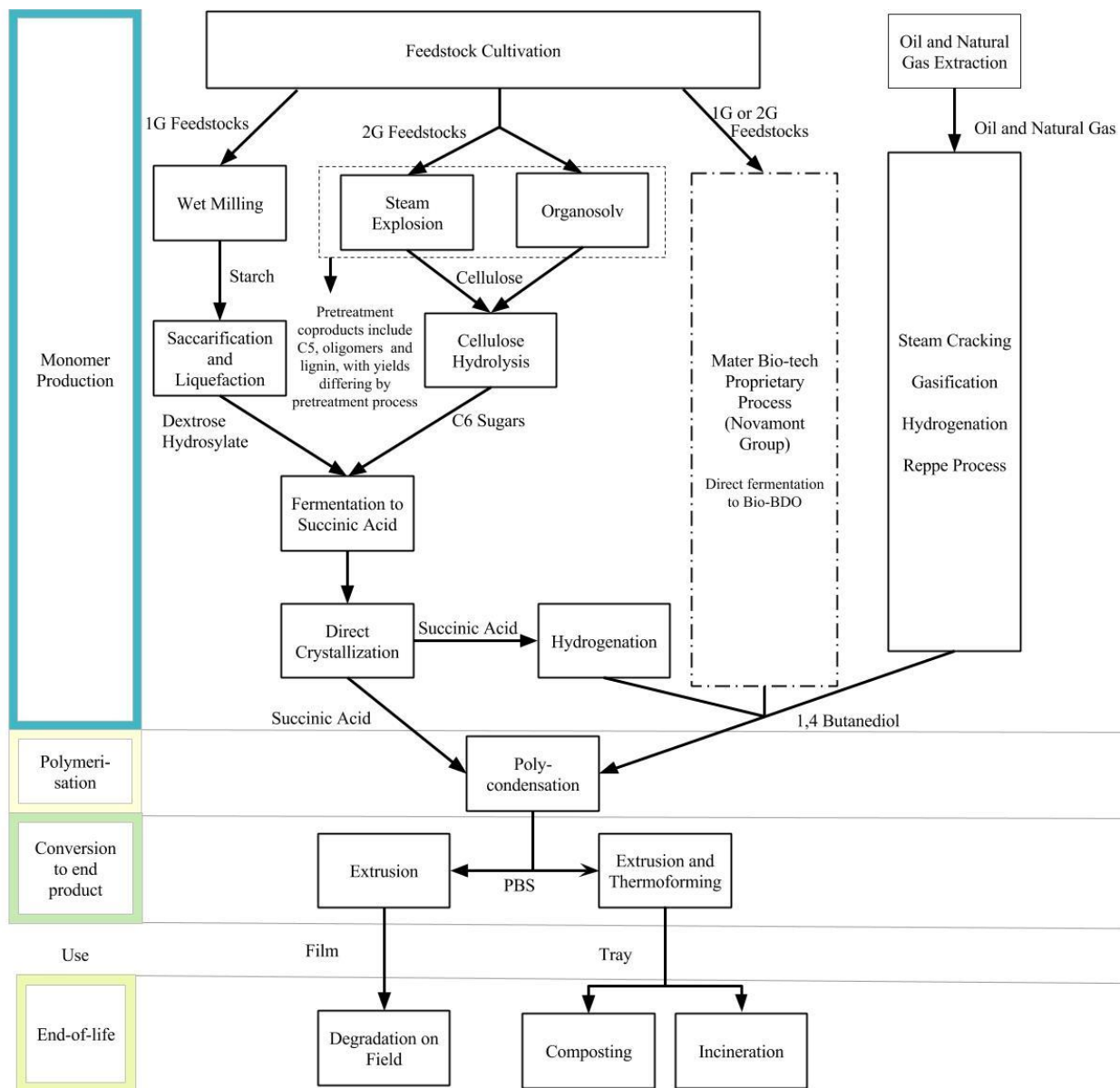


Figure 1: Flowsheet of PBS production (monomer production and polymerisation), conversion to end products, use, and end-of-life waste management options. Labels to the left correspond to contribution analysis (see Figure 5).

Among the wide variety of lignocellulosic feedstocks, we choose corn stover due to its abundance in the northern hemisphere. Its primary constituents are cellulose (37%), hemicellulose (21%) and lignin (18%).<sup>27</sup> We apply economic allocation to assign the impacts of cultivation to corn stover (versus corn<sup>28</sup>; see Appendix A3)\* and pre-treatment processes to fractionate the stover (Villegas et al., forthcoming). We consider here two pre-treatment processes, Steam Explosion (SE; being the most commonly applied process in cellulosic ethanol demonstration plants) and the Organosolv process (OS; Figure 2 and Appendix A2). For SE, we assume a low-severity process (to minimize degradation products) while the OS process uses ethanol as the solvent and sulphuric acid as the catalyst (Table 1; Villegas et al., forthcoming). We also consider an alternative OS process based on wheat straw, which is employed

\*In LCA, there are three predominant allocation methods, i.e. subdivision, system expansion (frequently applied as a credit approach) and economic allocation<sup>23,24,29</sup>

by Compagnie Industrielle de la Matière Végétale (CIMV, Appendix A2).<sup>29</sup> All pretreatment processes produce C6 sugars and C5 sugars, while only the Organosolv processes produce high purity lignin as well (see Figure 2).

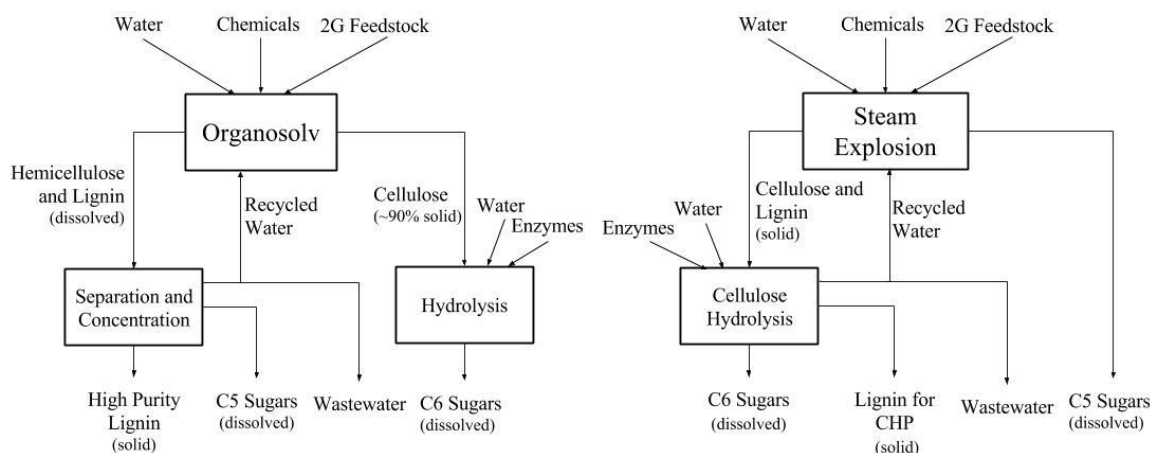


Figure 2: Simplified process scheme for pre-treatment by Organosolv (OS) and Steam Explosion (SE). Dissolved sugars are approximately 20% ds.

For 2G PBS pathways, we assume SA production from C6 sugars by low-pH yeast fermentation with downstream processing by direct crystallisation (this process route co-produces biogas and causes lowest impacts),<sup>18</sup> and account for the latest improvements in SA yields from C6 sugars (Theunissen, L. pers. comm. Reverdia) as well as the latest LCA data for European electricity generation (ENTSO according to Ecoinvent 3<sup>28</sup>; see Table 2; Appendix A4).

As default, the pre-treatment process for converting 2G biomass feedstock to sugars is assumed to be *integrated* with SA production on a single site (Appendix A5). Excess heat available from pre-treatment is used in SA production and the concentration of C6 sugars is avoided (otherwise required before transportation of C6 sugars to a distant SA plant; Table 1, item 1f; Villegas et al., forthcoming). It is assumed that BDO is produced in an *integrated* plant as well. For comparison, the *non-integrated* production of 2G SA and BDO (separate production of C6 sugars and bio-chemicals) is analysed. For both *integrated* and *non-integrated* production, the analysis is performed for a Reference Case and a Conservative Case. Only *integrated* production is considered in a Best Case (Table 1).

As shown in Figure 2, both the SE and OS technology are multi-product processes, yielding C6 sugars from cellulose, C5 sugars from hemicellulose as well as oligomers and lignin. However, only C6 is used to produce SA in all cases. Therefore, allocation (partitioning) or in-house utilization of co-products becomes necessary:

- There is currently no large-scale market for C5 sugars or oligomers of 2G origin, but a potential large-scale usage is 2G biogas production.<sup>30</sup> Therefore, we consider the utilization of C5 sugars and oligomers in biogas production on site using conservative assumptions for biogas yields from corn stover and biowaste, respectively, for all *integrated* and *non-integrated* cases (Appendix A6).<sup>30</sup>
- For both *integrated* and *non-integrated* production, valorisation of biogas and solid waste biomass in CHP facilities is assumed to provide heat and electricity; if required, natural gas is co-combusted together with biogas in the CHP facility. The CHP facilities are modelled with 12-21% electrical and 28%-61% thermal efficiencies (Table 1, item 1e) depending on their fuels and energy needs of each process. Additional electricity demand is purchased from the grid. Excess biogas production, if applicable, is credited to the natural gas grid.
- For lignin produced by SE, we assume lignin valorisation by combined heat and power (CHP) generation on site in the Reference Case and the Best Case (see Table 1). Only OS produces high purity lignin (HPL), for which we assume economic allocation (lignin allocation as by-product of C6 production; Conservative Case, see Table

1, item 1d and Appendix A5). For HPL and C6 we assume market values of 1.00 €/kg HPL and 0.36 €/kg C6 (Villegas et al., forthcoming; Appendix A6).<sup>31</sup>

For comparison, results for 1G PBS based on 1G sugar from corn are presented in two cases; Reference and Conservative\*. To ensure consistency with 2G, we apply economic allocation also to 1G value chain (Appendix A3). As Reference Case, we assume production of 1G sugar in a highly efficient European plant (based on Cok et al.,<sup>18</sup> but updated with latest LCA data for European electricity generation; see Table 2 and Yeung et al., forthcoming) integrated with SA production. Under the Conservative Case we assume a less efficient starch plant, which may be considered as average in Europe (based on EcoInvent 3,<sup>28</sup> see Table 1 and 2) that is not integrated with SA production. To convert the starch to glucose, we assume the impacts of the efficient European process for glucose production and steam-based evaporation for glucose drying (Appendix A7). We assume SA production from 1G sugars and 2G sugars (in both cases in the form of sugar hydrolysate) to be identical.

For 1G BDO, petrochemical BDO, and the incumbent materials, we use the data sources given in Table 2 (see also Yeung et al., forthcoming). The Reference Case for 1G BDO involves estimated data for *non-integrated* production of BDO by fermentation of dextrose (currently operated by Mater-Biotech in Italy; Innocenti F.D, pers. comm. Novamont Group).<sup>32</sup> The Conservative Case for 1G PBS assumes hydrogenation of 1G SA to BDO (Table 2).<sup>22</sup> Similarly, the bio-based BDO used for 2G PBS is divided into three cases (with the best case assuming more energy efficient production of BDO by Mater Bio-Tech, Table 1) with stover as 2G feedstock and *integration* of a 2G pretreatment and BDO facility assumed (see Appendix A8 for 1G to 2G BDO adjustment).

The polymerisation of PBS is traditionally done in two steps; esterification and transesterification.<sup>33</sup> PBS polymerisation is like that of bottle-grade PET<sup>34</sup>, except that PBS polymerisation occurs at lower temperatures and without a solid-state polymerisation step (Theunissen L., Reverdia, 2017, pers. comm.). We therefore estimate the energy of PBS polymerisation by adjusting values from PlasticsEurope for PET bottle-grade to account for the lower temperature of PBS compared to PET and the lack of a solid-state polymerisation step (see Appendix A9).<sup>35</sup> Molar yield for PBS polymerisation from monomers is assumed to be 95%, comparable to 97% for PET (EcoInvent 3).<sup>28</sup>

PET trays from granulates are commercially produced in two steps, i.e. by sheet extrusion followed by thermoforming and calendaring; PP trays are manufactured by Sharpak in a more efficient process, reducing NREU by 19% (Cox M., Sharpak, 2016, pers. comm., see Appendix A9).<sup>36,37</sup> It was assumed that PBS trays were produced in a two-step process much like PET. However, the energy use of this process was adjusted because of the lower melting point of PBS (see Appendix A9). Since the theoretical energy use for PBS extrusion and thermoforming was the average of the energy used for PP and PET, the impacts of making PBS trays was assumed to be the average of the extrusion and thermoforming of PET and PP for all cases. For film production, we assume extrusion for all cases (EcoInvent 3<sup>28</sup> Table 2). The material efficiency for tray and film production is 99% and 97.7% respectively (Cox M., Sharpak, 2016, pers. comm.).<sup>28</sup> Only pure plastic materials were assumed, while commercial production typically uses fillers and additives.

We make the simplifying assumption of 1000 km of transportation by lorry for all bio-based cases, while, for petrochemical polymers, we assume the transportation services are embedded in the reference records (this difference reflects the typically more complex logistic chain of bio-based polymers). The use phases of the products are not considered because their impacts are considered negligible (except for transportation which cancels out across the options). At the end-of-life, PBS trays are incinerated and PBS film is left to decompose on the field (Table 2). As an alternative end-of-life scenario, we also consider the industrial composting of PBS trays. We assume 99% release of stored carbon for incineration and 95% release of stored carbon for biodegradation of films and industrial composting of trays (Yeung et al., forthcoming; see Appendix A10 and A11). In the case of composting, the avoidance of extracting non-renewable moss peat is considered.<sup>38</sup> As for PBS films, biodegradation on the field is assumed, with no credit for avoided moss peat use. Since the incumbents are not biodegradable, MSWI is the only waste management

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\* See discussion section of Yeung et al (forthcoming) for a Best Case regarding 1G PBS production.

option considered (see Appendix A10 for energy credits). We assume the impacts for the removal of PE film from the field (Table 2) and 100km of transit to the incineration facility.

When presenting results for SA or the PBS product (cradle-to-factory gate, see below in Figure 3), we consider temporary storage of atmospheric carbon (negative emissions) as has been suggested and applied for intermediate products (Innocenti F, 2016, pers. comm.).<sup>18,22,39</sup> To ensure consistency, we consider the release of this carbon as positive emissions in the end-of-life stages (see “Embedded CO<sub>2</sub> emissions” in Figure 4).

Table 1: Differing assumptions for the three cases studied (Conservative Case, Reference Case and Best Case)

	<b>Process/Product</b>	<b>Conservative Case</b>	<b>Reference Case</b>	<b>Best Case</b>	
1.) Production of 2G C6 sugar by pre- treatment	1a) Feedstock for 2G SA and 2G BDO	Corn Stover			
	1b) Pretreatment technology <sup>1</sup>	Organosolv (OS)	Steam explosion (SE)		
	1c) Evaluation of C5 sugars and oligomers <sup>2</sup>	Conversion to biogas burnt on-site in CHP or (for <i>non-integrated</i> Reference and Best Case) credited to natural gas grid			
	1d) Evaluation/Allocation of C6 sugars versus lignin	Econ. alloc. based on raw sugar price and high purity lignin (HPL) price	No alloc. needed (C6 is the only output because lignin is burnt on-site in CHP)		
	1e) Total efficiency (%) of CHP (thermal/electrical output)	i) <i>integrated</i> : 73% (0.61/0.12) ii) <i>non-integrated</i> : 74% (0.61/0.13)	i) <i>integrated</i> : 50% (0.32/0.18) ii) <i>non-integrated</i> : 69% (0.59/0.18)	i) <i>integrated</i> : 49% (0.28/0.21)	
	1f) Share of theoretical product concentration energy use assumed to be avoided through <i>integration</i>	80%			100%
2.) Production of 1G C6 sugar by wet milling	1G Dextrose (Corn-based)	Not integrated with SA production; EcoInvent 3 (Maize Starch {DE}, production)	Integrated with SA production; Efficient corn starch mill (Cok et al. <sup>18</sup> )	Integrated with SA production; Efficient corn starch mill (Cok et al. <sup>18</sup> ) <sup>3</sup>	
3.) Production of BioBDO from C6 sugars	3a) 2G BioBDO <sup>4</sup>	Hydrogenation of 2G SA <sup>22</sup>	2G-based Mater-Biotech (estimated current production)	2G-based Mater-Biotech (more efficient/future production)	
	3b) 1G BioBDO	Hydrogenation of 1G SA <sup>22</sup>	1G-based Mater-Biotech (estimated current production)	1G-based Mater-Biotech (estimated current production) <sup>3</sup>	

<sup>1</sup>Each pre-treatment process is explained in Appendix A2 and the chosen allocation process is described in Appendix A4. <sup>2</sup> See flowsheets in Appendix A5. <sup>3</sup> This case is equivalent to 1G Reference Case; an optimistic estimation of 1G impacts is discussed in the ‘best’ case modelled by Yeung et al (forthcoming). <sup>4</sup> See Appendix A8 for adjustment of impacts from 1G BDO to 2G BDO. The estimated current production of BioBDO has not yet been validated by consolidated data because the plant has not been operational for more than a year.



Table 2: Key processes and sources of life cycle inventory data

Process or Material	Case/s	Data Source *	Notes
Corn Stover	All 2G cases	EcoInvent 3 <sup>(28)</sup>	Grain maize, IP, at farm, CH. From cradle to corn stover, economic allocation (Appendix A3)
Corn Grain	All 1G cases	EcoInvent 3 <sup>(28)</sup>	Grain maize, IP, at farm, CH. From cradle to grain, no economic allocation assumed (Appendix A3)
Wheat Straw	2G case in discussion section	Villegas et al., forthcoming	From cradle to straw at pretreatment plant gate, economic allocation (Appendix A3)
Miscanthus	2G case in discussion section	Villegas et al., forthcoming	From cradle to miscanthus at pretreatment plant gate
Willow	2G case in discussion section	Villegas et al., forthcoming	From cradle to willow at pretreatment plant gate
Pre-treatment of Biomass (C6 Production from straw)	All 2G cases	Villegas et al., forthcoming	SE and OS process; adjusted to latest LCA data for European electricity generation (ENTSO), with biogas production from C5 and oligomers (Appendix A2 and A6)
Pre-treatment of Biomass (CIMV)	Alternative OS technology developed by CIMV	Benjelloun-Mlayah, pers. comm.	See Appendix A2.
Biogas Credits	2G non-integrated Reference Case	EcoInvent 3 <sup>(28)</sup>	Credit assumes that impacts of extraction and delivery of natural gas (high pressure, Europe without Switzerland, market for), the embedded NREU and greenhouse gas emissions (0.056 kg CO <sub>2</sub> eq/MJ) are avoided
Wet Milling (Dextrose Production from corn grain)	1G Best and Ref. Case	Cok et al., 2014 <sup>(18,40)</sup>	Economic allocation adjusted from Tsiropoulos et al <sup>29</sup>
	1G Cons. Case	EcoInvent 3 <sup>(28)</sup>	Maize starch production, DE
Succinic Acid Production from Dextrose or C6	All cases	Cok et al., 2014 <sup>(18)</sup>	Adjusted to latest LCA data for European electricity generation (ENTSO) (see electricity record below)
BioBDO Production from SA	Cons. Case	Adom et al., 2014 <sup>(22)</sup>	Used stoichiometric amount of hydrogen (Dunn J, NREL pers. comm.) <sup>21</sup>
BioBDO Production by fermentation of C6 from 1G or 2G Feedstocks	Ref and Best Cases	Novamont Group, pers. comm.	Adjusted for 2G feedstocks in Appendix A8.
PBS Polymerisation	All Cases	PlasticsEurope <sup>(35)</sup>	Adjusted for lower melting temperature and lack of solid state polymerisation step for PBS in Appendix A9.
PP Production	PP	EcoInvent 3 <sup>1(28)</sup>	Granulate, RER
PET Production	PET	EcoInvent 3 <sup>1(28)</sup>	Granulate, amorphous, RER
PE Production	PE	EcoInvent 3 <sup>1(28)</sup>	Low density polyethylene, granulate RER
PP Extrusion and Thermoforming for trays	PP	Sharpak, pers. comm.	Based on PP tray production facility
PET Extrusion and Thermoforming for trays	PET	Sharpak, pers. comm.	Based on PET tray production facility
PBS Extrusion and Thermoforming for trays	All Cases	Sharpak, pers. comm.	PET extrusion and thermoforming adjusted for lower melting point of PBS in Appendix A9. Assume 99% material efficiency with scrap incinerated.
Extrusion for films	All cases	EcoInvent 3 <sup>(28)</sup>	Extrusion, plastic film RER. Assume 97.7% material efficiency with scrap incinerated.
Transportation by Lorry	All cases	EcoInvent 3 <sup>(28)</sup>	Transport, freight, lorry >32 metric tonne, EURO3 RER
Incineration of Plastic <sup>2</sup>	PP	EcoInvent 3 <sup>(28)</sup>	Waste polypropylene CH, treatment of, municipal incineration
	PET	EcoInvent 3 <sup>(28)</sup>	Waste polyethylene terephthalate CH, treatment of, municipal incineration
	PE	EcoInvent 3 <sup>(28)</sup>	Waste polyethylene CH, treatment of, municipal incineration
	PBS	EcoInvent 3 <sup>(28)</sup>	Waste plastic, mixture CH, treatment of, municipal incineration
Collection of Agricultural Film	PE	EcoInvent 3 <sup>(28)</sup>	Baling CH, processing, without plastic wrapping impacts
Incineration of Agricultural Film	PE	Briassoulis et al., 2012 <sup>(41)</sup>	See Appendix A10
Heat Credits for MSWI (avoided heat production)	All cases	EcoInvent 3 <sup>(28)</sup>	Heat, central or small scale, natural gas-fired boiler, Europe without Switzerland, at boiler condensing modulating <100kW
Electricity	All cases	EcoInvent 3 <sup>(28)</sup>	Electricity, medium voltage in Europe, ENTSO. Also used as electricity credit for MSWI
Electricity for Sensitivity Analysis	2G Ref. Case <sup>3</sup>	EcoInvent 3 <sup>(28)</sup>	Electricity, medium voltage in Norway, NO Electricity, medium voltage in Poland, PL Electricity, medium voltage in Italy, IT
Industrial Composting	Alt. to 2G Ref. Case	EcoInvent 3 <sup>(28)</sup>	Biowaste CH, treatment of, composting <sup>4</sup>
Carbon Balance of Industrial Compost	2G Ref. Case	Hermann et al, 2011 <sup>(38)</sup>	In line with Yeung et al., forthcoming and see Appendix A11

Moss Peat Replacement	2G Ref. Case	EcoInvent 3 <sup>(28)</sup>	Peat Moss, RoW, peat moss production, horticultural use
Degradation of Agricultural Film on field	All PBS film cases	Yeung et al., forthcoming	See Appendix A11

\* Reference numbers, when applicable, are in parentheses.<sup>1</sup> EcoInvent 3<sup>28</sup>, instead of PlasticsEurope, was the source of incumbent polymer production data for consistency with Yeung et al., forthcoming. <sup>2</sup>The fossil fuel emissions were changed for these processes to reflect 99% emission of embodied carbon from plastics (Yeung et al., forthcoming)<sup>42</sup> and energy recovery credits acc. to Appendix A10. <sup>3</sup>See discussion for sensitivity analysis. <sup>4</sup>The climate change impacts were changed to reflect long-term carbon storage in compost (in line with Yeung et al., forthcoming, Appendix A11).

### 2.3 Impact assessment

The selected environmental performance indicators are non-renewable energy use (NREU, using indicator “Cumulative Energy Demand V1.09” in SimaPro) and greenhouse gas (GHG) emissions or climate change impact (IPCC 2013 GWP 100a in SimaPro). The early technology development stage of the pre-treatment processes and the resulting lack of data prevent a broader coverage of environmental impacts, which would be needed for a more complete understanding.

### 3 RESULTS

As an important interim result, Figure 3 shows cradle-to-factory gate results for 2G SA and the respective values for 1G SA. If produced in an *integrated* site (integration of pre-treatment with SA production), 2G SA based on the SE process causes 108% lower climate change impacts than 1G SA and requires 46% less NREU. These climate change impacts account for storage of atmospheric carbon in the product (negative emissions); disregarding this storage as applied for cradle-to-grave analyses results in 37% lower GHG for 2G SA compared to 1G SA. The 1G results assume a modern, highly efficient wet mill in Europe, while less efficient starch production increases the impacts of 1G SA (by 58% for GHG and 27% for NREU; see Conservative Case in Figure 3). The impacts for OS are sensitive to the selling price of HPL (1.00 €/kg was assumed), as halving the price would increase impacts of SA by 42% and 11%, while doubling it would decrease SA impacts by 42% and 11%, respectively, for GHG (with accounting of carbon storage) and NREU (see error bars in Figure 3).

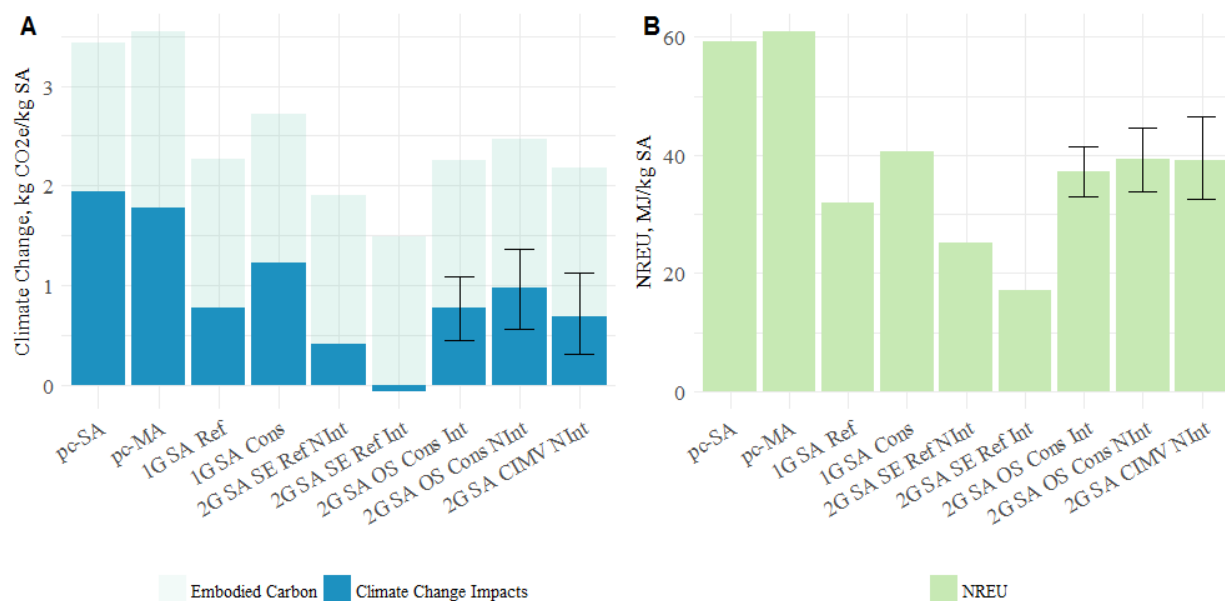


Figure 3: Cradle-to-factory gate climate change impact and NREU of 1G SA Ref (1G Reference Case), 1G SA Cons (1G Conservative Case), 2G SA SE Ref (2G Reference Case), 2G SA OS Cons (2G Conservative Case) and CIMV-based Organosolv (2G SA Cons CIMV) in both *integrated* (Int) and *non-integrated* (NInt) plants for SE and OS. Results for the petrochemical (pc) counterparts maleic anhydride (pc-MA)<sup>18</sup> and petrochemical SA (pc-SA)<sup>18</sup> are also presented.\* For bio-based SA, storage of atmospheric carbon in the product (approx. 1.5 kg CO<sub>2</sub>/kg SA) has been accounted for in the solid blue bars (as negative CO<sub>2</sub> emissions, this storage or embodied carbon is represented as light blue bar sections in Figure 3A and – to ensure comparability – likewise the CO<sub>2</sub> embodied in pc-SA and pc-MA is represented by light blue bar sections)

The *integration* of SE pre-treatment and SA production plants leads to reduced impacts of SA (compared to a *non-integrated* scenario). This is related to the avoidance of concentration of C6 (up to 4.7 MJ NREU/kg C6) and the readily usable excess heat from the pre-treatment process. The heat in the *integrated* facility is provided entirely by biomass and biogas valorisation. For OS, however, the impacts for the *integrated* and *non-integrated* scenarios are comparable. While the *non-integrated* OS and SA plants require more steam and electricity, these utilities are mostly supplied by the two CHPs (with a small amount of electricity from the grid for SA production) while, for the *integrated*

\* Prior to the commercialisation of its bio-based route, succinic acid was exclusively produced from petrochemical sources, albeit in very small volumes. The impacts of petrochemical-based PBS trays are briefly mentioned in Appendix B5 in comparison to fully bio-based PBS. In this section, we do not present petrochemical-based PBS for trays and films because it is not competitive with petrochemical bulk materials.

plant scenario, more electricity is sourced from the grid in relation to the heat demand. Since this electricity is generated at lower efficiency than by CHP, the overall energy use is comparable in the *integrated* and *non-integrated* OS scenarios.

In Figure 4, cradle-to-grave results for the end products (packaging trays and mulching films) are presented assuming the Reference Cases of 1G PBS and 2G *integrated* PBS. For all trays and PE films, the savings of energy and GHG emissions related to MSWI with energy recovery outweigh the impacts for transportation and any handling of the waste, resulting in credits (negative bar sections, Figure 4). The climate change impact of fully bio-based 2G PBS films and trays are smaller (by 34% and 36% respectively) compared to their primary petrochemical counterparts PE films and PP trays. In terms of NREU, fully bio-based 2G PBS films and trays are also smaller than those counterparts (by 36% and 41%, respectively). The GHG and NREU of fully bio-based 1G PBS trays are comparable to one of its petrochemical counterparts, the PET tray. However, 1G PBS trays have a 2% and 7% higher impact than PP trays for climate change and NREU, respectively (Figure 4, see Yeung et al., forthcoming)\*.

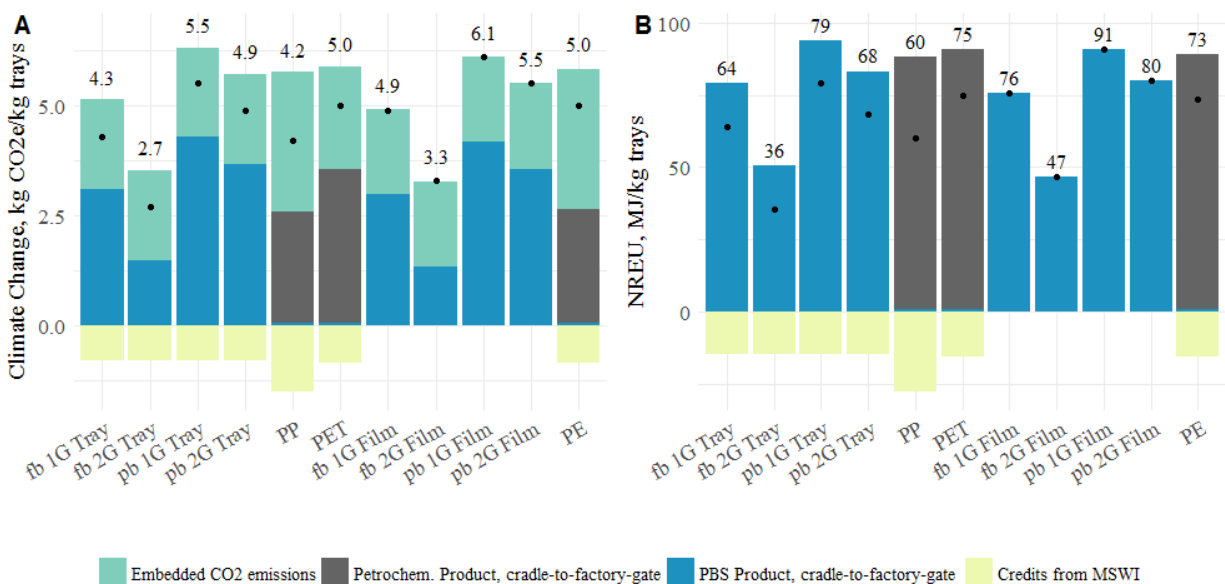


Figure 4: Cradle-to-grave climate change (A) and NREU (B) impacts for plastic trays and mulch films made from 1<sup>st</sup> generation (1G) and 2<sup>nd</sup> generation (2G) PBS, both fully bio-based (= fb) and partly bio-based (= pb) as well as from petrochemical plastics. These results reflect the Reference Case for both 1G PBS and 2G PBS, with corn grain and corn stover as feedstocks, respectively. For 2G PBS, the *integration* of steam explosion and SA production is assumed. End-of-life waste management of trays and PE film by incineration with energy recovery; for PBS films, biodegradation on the field. The points in the bar and labels on top of the bars indicate net climate change (A) or NREU (B) impacts.

In the Reference Case of 2G PBS tray and film production we assume *integration* of pre-treatment and SA fermentation, with both occurring in the same facility (i.e. with a joint CHP and no need for concentration of C6 sugars). With this *integration*, the cradle-to-grave impacts of PBS films and trays decrease by 25-30% for climate change and NREU, respectively compared to *non-integrated* 2G PBS films and trays (see Appendix B1). *Non-integrated* Reference Case 2G PBS trays and films (produced with SE) have lower impacts than 1G PBS products and 1G PBS products have comparable or slightly higher impacts than petrochemical incumbents. *Non-integrated*

\* The conservative case 1G PBS trays has a 10% higher GHG impact and 17% higher NREU impact than PP trays (see Appendix B1). To balance this, there is an optimistic scenario presented in Yeung et al. (forthcoming).

Conservative Case 2G PBS trays and films (produced with OS) have higher NREU and lower GHG than 1G PBS and petrochemical incumbents (see Appendix B1).

As shown in Figure 4, the cradle-to factory gate manufacturing of the PBS product (blue bar section) contributes 28%-100% to the net impacts across the life cycle for 2G and 1G PBS (represented by points). Figure 5 provides a breakdown of impacts by process step for trays. The end of life phase emissions and credits of plastics are divided into three subsections; the emissions involved with only the treatment of plastic in MSWI, the carbon in the material that is released as CO<sub>2</sub>, and credits from the avoided emissions of heat and electricity generation (see End of Life emissions, Embedded carbon and Credits from MSWI in Figure 5). For PBS, the embedded CO<sub>2</sub> emissions are equivalent to the bio-based carbon subtracted from 1,4 BDO and SA in the production stage of these chemicals. In the *integrated* Reference Case of fully bio-based 2G PBS trays, the main contributing factors (from high to low for NREU) are conversion to bio-based BDO, conversion to end-product, succinic acid, and polymerisation, while petrochemical BDO is the most contributing component in the case of partly bio-based PBS (see Yeung et al., forthcoming for 1G PBS contribution analysis).

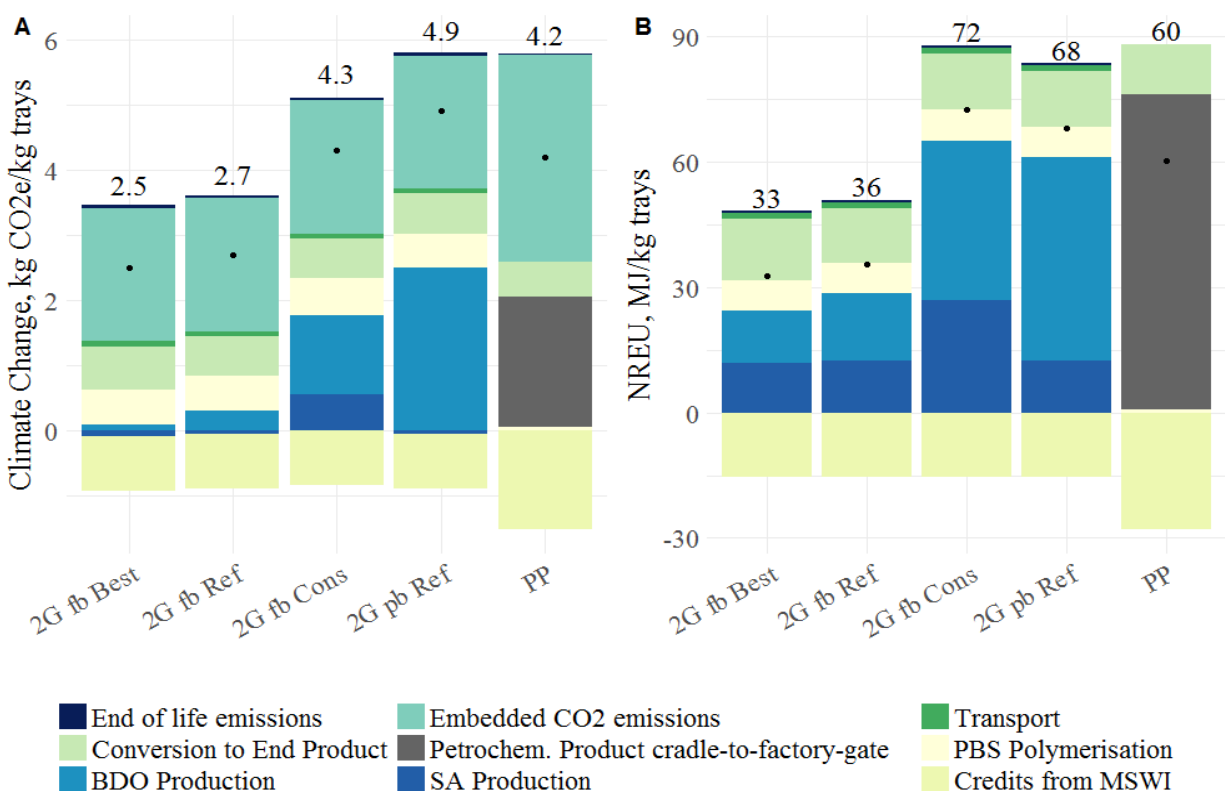


Figure 5: Cradle-to-grave impacts of fb and pb 2G PBS trays and PP trays, with a distinction by Best, Reference (Ref) and Conservative (Cons) Cases, all assuming *integration*, for 2G PBS production for climate change (A) and NREU (B) (see Tables 1 and 2 for scenario descriptions). The points in the bar and labels on top of the bars indicate net climate change (A) or NREU (B) impacts.

Figure 5 demonstrates that, for trays, the 2G Best Case PBS cradle-to-grave climate change impacts and NREU are approximately 40% and 45% lower than the PP tray. For films, the impacts of the Best Case are also almost 40% and 43% lower than those for the PE film (Appendix B1). The conservative cases for both trays and films, however, have higher impacts than their petrochemical incumbents for NREU and slightly lower impacts for climate change (Appendix B1).

As an alternative to incineration of trays (see Figures 4 and 5), it is possible to compost these PBS products. The net climate change impacts of composting (1.5 kg CO<sub>2</sub> eq./kg trays) are larger than those of incineration (1.3 kg CO<sub>2</sub> eq./kg trays) because the credit for incineration (see avoided emissions in Figure 4) is larger than the credit given to compost for avoided moss peat production (not shown). The NREU credits for incineration of PBS trays (15 MJ/kg PBS tray; see credits from MSWI in Figure 4) are higher than those for avoided moss peat production (5 MJ/kg PBS tray) as well. Therefore, incineration is a more favourable end-of-life scenario when considering only climate change and NREU for trays. The incineration of films (not depicted) also has lower impacts (by 8 MJ/kg film and 0.4 kg CO<sub>2</sub> eq./kg film) than the degradation of PBS films on the field (Figure 4).

The release of carbon from fb PBS (2.04 kg CO<sub>2</sub> eq./kg) is marginally lower than for PET (2.28 kg CO<sub>2</sub> eq./kg), and clearly lower than for PE and PP (3.14 kg CO<sub>2</sub> eq./kg). In Figure 4, no distinction is made between carbon dioxide emissions from petrochemical polymers and bio-based PBS since avoided climate impact due to incorporation of atmospheric carbon in the bio-based chemicals has been considered in monomer production (negative emissions). These amounts need to be considered as emissions in the end-of-life stage (equally treated as fossil CO<sub>2</sub>). Therefore, the carbon emitted by incineration of the bio-based products resembles that of petrochemical incumbents.

## 4 DISCUSSION

The chosen functional unit of 1 kg of product can be questioned in view of the different properties of the polymers, typically leading to some differences in the quantities of materials needed to make functionally equivalent products. At the time of writing, there were no prototypes of 2G PBS trays or films that had been fully tested against the incumbents mentioned in this paper. Therefore, we choose one mass unit (1 kg) as functional unit. Alternatively, one could argue in favour of a volume functional unit (e.g. 1 liter), for example if PBS trays were found to be functionally equivalent to PP trays in the case of identical tray design is used (i.e. same shape and thickness). As a consequence of the lower density of PP (PBS is 29% denser), this alternative functional unit choice would lead to different findings compared to those presented above, making PP trays the preferred choice when considering non-integrated 2G PBS scenarios, and yielding comparable results for trays manufactured from PP and PBS from an *integrated* 2G PBS.

The method developed by Ashby et al.<sup>43</sup> allows the quantification of the amount of material to ensure functional equivalence in mechanical terms for a given application (as, for example, implemented by Schrijvers et al.,<sup>44</sup> Hischer et al.,<sup>45</sup> and Broeren et al.<sup>46</sup>). We considered Ashby's methods for PBS trays and films in comparison to the incumbent materials (Appendix A1). For films, the Ashby's method predicts that 1 kg of LDPE film can be replaced by only 0.3 kg PBS, making PBS the preferred choice (Appendix A1). In contrast, around 1.5-2 kg of PBS would be needed to replace 1 kg of PP or PET in trays, making the incumbents the preferred choice in terms of NREU and GHG according to Ashby's method. Interestingly, the PBS tray moulded by Sharpak on PET equipment (i.e. with roughly the same mass input of PBS and PET) showed satisfactory mechanical properties. In order to accurately determine the amount of PBS that is necessary to fulfil the same function as PP (for trays) and PE (for films) further testing of physical properties but also of processibility, transparency, sealing, thermal properties and material migration test would be needed, thereby also considering the usage of various fillers and additives. We conclude that the choice of 1kg of polymer as functional unit is adequate given the current level of knowledge.

Wheat straw, miscanthus, and hardwood were studied as potential feedstocks for trays made from 2G fb PBS. To this end, we used cultivation data and SE pre-treatment conditions modelled by Villegas et al. (forthcoming). Both wheat straw and miscanthus can be processed in the same manner as corn stover (low severity SE), but the pre-treatment of hardwood occurs at higher temperatures and pressures (high Severity SE, Appendix B2). Unlike wheat and corn, the cultivation and harvesting of miscanthus and hardwood do not call for allocation between food-grade products and agricultural residue. Compared to the 2G Reference Case PBS trays based on corn stover, the cradle-to-grave GHG impacts decreased by 31% and 36% for hardwood and miscanthus, but increased by 32% for wheat straw-based products. The NREU decreased by 13% for miscanthus but increased marginally by 2% and 8% for hardwood and

wheat straw-based PBS trays, respectively. The largest reduction in impact for 2G PBS trays was achieved by using miscanthus-based SA and BDO (5 MJ/kg PBS tray and 0.9 kg CO<sub>2</sub> eq/kg PBS trays; see Appendix B2).

As well as variations in feedstock, variations of pre-treatment technologies can be considered. This is especially the case with OS, which can be designed to use different acids as solvents. We therefore compared the OS route to 2G PBS trays, represented by the Conservative Case (*no integration*; 4.6 kg CO<sub>2</sub> and 76 MJ/kg trays, see Table 1) with a real-world example: we considered the OS process developed by Compagnie Industrielle de la Matière Végétale (CIMV) which makes use of formic and acetic acid.<sup>29,47</sup> We assumed CIMV pre-treatment of wheat straw (Benjelloun-Mlayah B, CIMV, 2016, pers. comm.). We found that CIMV's pre-treatment technology scores similarly well as the ethanol/sulphuric acid-based OS process (negligible change in NREU and 8% lower GHG impact compared to OS Conservative Case). The increased yield of C5 sugars and the avoidance of enzymes are advantages of the CIMV process. In addition, CIMV expects their HPL, Biolignin™, to be sold at a contract price of 1.45 €/kg, instead of the 1.00 €/kg price assumed in the Conservative Case.<sup>31</sup> Assuming that all other prices and inputs remain the same, this change in HPL price results in 16% and 7% fewer GHG emissions and NREU for fb 2G PBS trays made with CIMV process compared to the Conservative Case for PBS trays.

It is also possible to sell other products of the pre-treatment process, such as C5 sugars. Using an optimistic market price for C5 derived from the co-fermentation of C5/C6 to bioethanol (Appendix A6), the economic allocation in the *non-integrated* Reference Case C6 was adjusted. When C5 was sold (partitioning) rather than converted to biogas (credit approach), the NREU impacts of C6 increase by 44% and the GHG impacts increase by only 4% , which is due to the higher GHG emission intensity of C6 value chain (including fertilizers) in comparison to the natural gas credits of C5. Another option for the utilization of C5 is the co-fermentation of C5 and C6 sugars to succinic acid and BDO, which has been demonstrated on a lab scale.<sup>32,48</sup> In case of successful development of C5 fermentation routes, further LCA research will become necessary.

It is worthwhile to compare the current results to those published in the context of the BREW study (published in 2006).<sup>21</sup> The impacts of C6 sugar production, as estimated by the BREW report, include significant energy credits due to the burning of waste biomass (Appendix A7), as does this paper in an *integrated* scenario. The pre-treatment system modelled in BREW yielded NREU impacts (-4.4 MJ/kg C6), similar to those of an *integrated* SE pre-treatment (-4 MJ/kg C6) estimated in this paper (Appendix B3). For SA, Patel et al.<sup>21</sup> published in the BREW report an NREU value of 22.0 MJ/kg for SA production from lignocellulosic feedstocks by anaerobic continuous fermentation with a workup via redox and crystallization. For comparison, 2G SA presented in this work has an NREU of 17 and 25 MJ/kg SA (*integrated* and *non-integrated* Reference Case, respectively).

In this study, it was assumed that PBS trays were produced by thermoforming of pre-processed sheets on similar equipment as PET. However, Sharpak has also indicated that it is possible to convert PBS granulates to trays in a one-heat process which avoids the intermediate step of producing and storing plastic sheets before they are thermoformed to the final product. This one-step process is not applicable to PET, but has been implemented for PP due to the high volumes and the properties of PP. Since no technical constraints limit PBS tray production in a one-step process, this could in the longer term decrease the GHG and NREU impacts of tray production from granulates by 14%, assuming the adjustment for impacts due to PBS' lower melting temperature (see Appendix A9).

While the PBS scenarios and inputs used in this paper are representative of Europe, we investigated specific locations of PBS production within Europe (Figure 6, Appendix B4). To this end, the electricity mix throughout the entire process was changed to that of Italy (proximity to Mater Bio-tech), Poland (89% fossil fuel electricity mix) and Norway (96% hydropower mix).

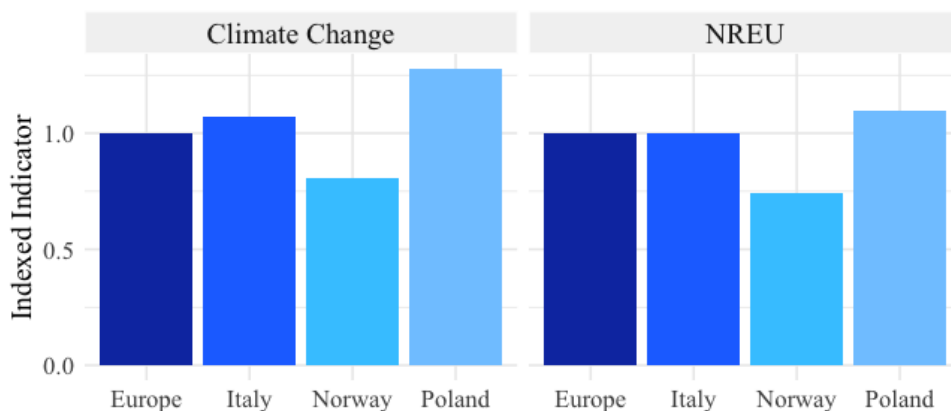


Figure 6: Indexed values of cradle-to-grave climate change and NREU impacts of fb 2G PBS trays (Reference Case, *integrated*) as a function of plant location. It is assumed that BDO production remains in Italy at Mater Biotech plant for each case.

Implementing the Italian electricity mix in comparison to ENTSO does not produce significant differences in the environmental impacts of PBS production (maximum change of 7%). If the process was operated in Norway, the GHG and NREU emissions would decrease by 16% and 26%, respectively. This reflects the low impacts of using hydropower as an electricity source. Electricity generation in Norway has approximately 96% lower impacts than ENTSO electricity for GHG and NREU. The higher impacts of fossil fuel-based power generation in Poland cause a 23% increase in GHG for PBS tray production.

Although incineration of PBS trays has advantages in terms of GHG and NREU, composting of PBS has benefits that are not accounted for by these indicators. Biodegradable PBS trays would avoid the need for industrial composters to sort packaging from food waste. Similarly, degradable agricultural film from PBS would avoid the need for film removal from the field, thereby reducing labour, capital-related and energy costs. In addition, PE film causes soil contamination if it is not completely removed from the fields, which can be detrimental to crop growth.<sup>49,50</sup> The avoided decrease in crop yields was not considered in this LCA because of insufficient data, but may be relevant.

In addition to PBS trays, trays made from other SA-based polymers were analysed (see Appendix B5). These polymers are biodegradable and can be partly bio-based due to the use of SA or BDO monomers. The cradle-to-grave impacts of polybutylene succinate terephthalate (PBST), poly(butylene succinate-co-butylene adipate) (PBSA), and poly(butylene adipate-co-terephthalate) (PBAT) were analysed. The latter has a more established market than PBS and is cheaper. SA and BDO (from the 2G Reference Case, *integrated*) were assumed as monomers for PBST, PBSA and PBAT. Despite the use of these 2G monomers, the impacts of PBAT and PBSA trays are higher than PET or PP trays (by 40-260% compared to PP), which is due to the large NREU and especially CC impacts of petrochemical adipic acid. However, the impacts of 2G PBST tray production are comparable to those of PET and PP trays.

Before concluding, it is necessary to point out that this paper is limited to only two environmental impact indicators. Although bio-based products usually demonstrate lower NREU and GHG impacts in comparison with petrochemical incumbents, the opposite is the case when considering land use or eutrophication as an indicator for sustainability.<sup>51</sup> However, the reduction of soil carbon emissions because of efficient land management has not been considered, which may be especially relevant for the miscanthus and willow-based PBS (Ni et al., forthcoming). The availability of further data on these and other attributes of PBS systems will support extension of this study to include a wider range of indicators.



## 5 CONCLUSIONS

Using moderately optimistic technology assumptions (*integrated* Reference Case) for fully bio-based PBS products derived from 2G SA and BDO, the cradle-to-grave climate change impacts and NREU are 34-36% and 36%-40% lower than those of production from the main petrochemical polymers PP (trays) and PE (films) products, while the impacts of 1G PBS are comparable or slightly higher than production from petrochemical polymers. A key to the lower impacts of 2G SA is to integrate both pre-treatment and monomer acid production on the same site, with excess biomass being valorised by CHP and the avoidance of sugar concentration (as required in *non-integrated* plants). As discussed in this paper, there are some further hitherto unexploited opportunities for reducing NREU and GHG emissions (power supply mix, tray production process). The analysis hence shows the potential for the development of PBS products in the context of an emerging bio-economy. In addition, ongoing research indicates that there are still significant unused potentials for soil carbon management related to other renewable feedstocks such as perennial lignocellulosic biomass crops, thereby allowing further substantial reductions in climate change impact especially for 2<sup>nd</sup> generation chemicals and plastics; this calls for further research.

## 6 ACKNOWLEDGEMENTS

We thank the European Commission's programme Climate-KIC for financial support provided in the context of the project Adaptation and Mitigation through Bio-Succinate Innovation (ADMIT Bio-SuccInnovate). We are also very grateful for the support provided by Lawrence Theunissen and Jo Kockelkoren (both Reverdia), Francesco Degli Innocenti (Novamont), Bouchra Benjelloun-Mlayah (CIMV) and Matthew Cox (Sharpak).

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## APPENDIX

Appendix A: Inventory Data.....	21
Appendix A1: Correcting for material properties according to Ashby .....	21
Appendix A2: Pretreatment technologies .....	22
Appendix A3: Economic allocation for feedstocks .....	23
Appendix A4: Economic allocation for succinic acid process.....	24
Appendix A5: Flowsheet of allocation and integration .....	26
Appendix A6: Allocation for C5, oligomers, lignin, and C6 .....	27
Appendix A7: Conversion of starch to glucose .....	28
Appendix A8: Petrochemical BDO and Bio-based BDO from 2G C6.....	28
Appendix A9: Production of plastic trays.....	29
Appendix A10: Energy recovery credits (MSWI) .....	30
Appendix A11: Composting and Degradation of Field of PBS .....	31
Appendix B: Results and Discussion .....	32
Appendix B1: Results for 2G Reference and Conservative cases for integrated and non-integrated plants....	32
Appendix B2: Results for 2G fb PBS trays from various feedstocks .....	33
Appendix B3: Comparison to BREW Report.....	34
Appendix B4: European electricity supply .....	35
Appendix B5: Comparison to other biodegradable polymers.....	35
Table of references for appendices .....	36

## Appendix A: Inventory Data

### Appendix A1: Correcting for material properties according to Ashby

The functional unit of 1 kg of PBS, PP, PET and PE was chosen for the agricultural film and plastic tray end products. Compared to simply choosing 1 kg, a more accurate definition of the functional unit would account for the material properties of PBS and of the incumbent materials. Such a method was developed by Ashby<sup>1</sup> allowing to calculate the material needed for different types of design objectives and constraints (e.g. twisting of a beam) (Table A1; Equation A1-A3). Such a constraint is described by Equation A1-1 which represents the Material Index (MI) for a light stiff tie, based on stiffness (E) and density ( $\rho$ ), as the material should not deform or break under tensile load<sup>1</sup> (this equation is applied to trays).

$$MI_t = E^{1/3} / \rho \quad \text{Eq. (A1-1)}$$

For agricultural films, the material must not tear; this is described by Equation A1-2, representing a Material Index (MI) based on tensile strength ( $\sigma$ ) and density ( $\rho$ ).<sup>1</sup>

$$MI_a = \sigma / \rho \quad \text{Eq. (A1-2)}$$

The material use for a given application is inversely proportional to the material index MI. The percent change in weight of changing from one material (incumbent material P) to another (new material PBS) can therefore be calculated based on Equation A1-3.

$$\text{Change of weight (\%)} = ((MI [P] / MI [PBS]) - 1) * 100 \quad \text{Eq. (A1-3)}$$

Table A1-1: The material properties of A-PET, PBS and LDPE utilized as inputs in Ashby calculations (PP, A-PET and LDPE from Ashby et al.;<sup>1</sup> PBS from Theunissen<sup>2</sup>)

Material	Parameter	Value	Unit
PP	Density $\rho$	0.9	t/m <sup>3</sup>
	Young's Modulus E	1500	MPa
A-PET *)	Density $\rho$	1.33	t/m <sup>3</sup>
	Young's Modulus E	2600	MPa
PBS	Tensile Strength $\sigma$	46	MPa
	Density $\rho$	1.26	t/m <sup>3</sup>
	Young's Modulus E	575	MPa
LDPE	Tensile Strength $\sigma$	10	MPa
	Density $\rho$	0.92	t/m <sup>3</sup>

\*) A-PET represents amorphous PET.

Table A1-2: Results for trays and film based on the Ashby method. Positive change of weight indicates more PBS is necessary to fulfil the same function.

End Product	Variable	Value	Change of weight
PP Tray	$M_t$	12.72	PP to PBS: 92.7% PET to PBS: 56.7%
PET Tray	$M_t$	10.34	
PBS Tray	$M_t$	6.60	
LDPE Film	$M_a$	10.9	LDPE to PBS: -70.2%
PBS Film	$M_a$	36.5	

Application of the Ashby method using the data given in Table A1-1 indicates that *more* PBS is needed to attain the same stiffness and strength as a PP or PET tray (Table A1-2). While PBS trays are not produced on industrial scale, Sharpak demonstrated that PBS trays can be processed with the same mould as PET (Cox M, Sharpak, 2016, pers.

comm.) and that the mechanical properties were very satisfactory (this would *not* have been expected based on the outcome of the Ashby method). One PBS tray weighed 18.9 grams. The various tests necessary to determine if these trays can be used in similar applications as PP or PET have not been completed. Given the difference in density between PET and PBS, the PBS trays are slightly lighter than the PET trays. To account for the fact that the Ashby method points in the opposite direction and the PBS tray has not yet been fully tested against its incumbents, we chose the conservative assumption that the functional unit is 1 kg of PBS, PP and PET trays.

While in the context of the demonstration project the PBS trays were fabricated on equipment designed for PET trays, PBS trays will have to compete primarily with PP trays, which are processed on different equipment (see Appendix A8; Cox M, Sharpak, 2016, pers. comm.). PBS and PP have some similar properties, such as being slightly opaque and easily coloured. The large density difference between PP and PBS (see Table A1-1) does not necessarily mean that a different number of trays will be produced with the same mass of polymer; as the amount (both mass and volume-wise) of each plastic needed for the same application depends on its properties and equipment processing parameters. These uncertainties make it impossible at this stage in development to determine exactly the amounts of PP and PBS that will fulfil the same function; therefore, we choose the optimistic assumption of equal weights.

To our knowledge, no PBS agricultural mulch film is currently being produced, which would allow to make a comparison with PE products. We therefore assume that the weight of PBS agricultural films is identical to the weight of an LDPE film. To estimate the area of agricultural film, it was assumed that 1 ha of land is covered by 150 kg of LDPE or PBS film.<sup>3</sup> By application of the Ashby method we find that there is the possibility for significant material savings because of the superior tensile strength of PBS (see Table A1-2). Nevertheless, we choose as default the conservative assumption for the functional unit according to which that PBS and PE film have identical weights.

## **Appendix A2: Pretreatment technologies**

For pre-treatment by Steam Explosion (SE), biomass is subjected to pressurized steam for seconds to several minutes, after which the reactor is quickly depressurized. Low and high severity SE use steam at temperatures between 190°C and 230°C and at pressures from 11 atm to 25 atm. After a decrease in pressure, mechanical expansion (resulting in increased reaction surface) and autohydrolysis lead to solubilisation of the hemicellulose sugars. By addition of water and enzymes, the cellulose is hydrolysed into C6 sugars (dissolved) and removed by filtering while the lignin is the remaining solid fraction. The yields of each the three output streams (C6, C5 and lignin, with oligomers present in both C5 and C6 streams) are reported in Table A2-1 (Villegas et al., forthcoming).

Contrary to the SE process, the Organosolv (OS) process uses aqueous organic solvent mixtures to solubilize lignin and hemicellulose; cellulose remains solid and is further processed by enzymatic hydrolysis to produce C6 sugars. The filtrate, containing dissolved hemicellulose and dissolved lignin, is sent to a distillation column, where the solvent is recovered and the lignin precipitates. Apart from the C6 sugars the main products are lignin, C5 sugars and furfural (which is formed from the xylose fraction within the hemicellulose). Lignin from OS processes is purer compared to lignin from other processes and can therefore be used for high quality applications; in contrast, the lignin fraction from other pretreatment technologies is typically combusted (Villegas et al., forthcoming).

It is important to note that there are various types of the Organosolv process depending on the chosen solvent system. The variant considered in this paper uses ethanol in combination with sulphuric acid (based on Eerhart et al.<sup>4</sup> with reaction yields adapted from Kautto et al.<sup>5</sup> and Pan et al.<sup>6</sup>).

The process described in the discussion section is a pre-commercial application of the Organosolv process, developed by CIMV. Much like the Organosolv case presented in the Conservative Case, the feedstock undergoes an extraction step that separates lignin and the C5 sugar stream from the C6 stream (solid). Then, this C6 stream is de-acidified, washed, pressed. Finally, enzymes hydrolyse this stream to glucose. Lignin and the C5 stream are concentrated and the organic acid is removed. Next, the lignin is precipitated and washed. The remaining C5 stream is concentrated and stripped. The concentration of the resulting C5 and C6 streams are 60% ds (dry substance) and 22% ds respectively;

the yields are given in Table A2-1. Solvent is continuously recycled throughout this process, and supplemented with freshly added solvent (Benjelloun-Mlayah B, CIMV, 2016 pers. comm.).<sup>7</sup>

Table A2-1: Yields of pretreatment based on kg of dry output/tonne of biomass input. (Villegas et al., forthcoming, Benjelloun-Mlayah B, CIMV, 2016 pers. comm.)

Pre-treatment	Feedstock	C6 monomers (kg/t biomass)	C5 monomers (kg/t biomass)	Lignin (kg/t biomass)
SE	Corn Stover	354	58	CHP
SE	Wheat	326	57	CHP
OS	Corn Stover	349	53	158
OS	Wheat	323	53	121
OS-CIMV	Wheat	490	220 <sup>1</sup>	269

<sup>1</sup>This stream is not purely C5 sugars, there are also other minor compounds that were present in the biomass

To adjust the global scenario modelled by Villegas et al. (forthcoming) to the European scale, different impacts were utilized for the chemicals and energy necessary. European electricity (ENTSO), sulphuric acid (RER), ethanol (without water, in 95% solution from fermentation RER) impacts from EcoInvent 3<sup>8</sup> and the CHP impacts from Cok et al.<sup>9</sup> replaced the corresponding global impacts assumed by Villegas et al. (forthcoming).

### Appendix A3: Economic allocation for feedstocks

Economic allocation was chosen for the entire supply chain of PBS including the feedstocks. More specifically, allocation was required to determine the environmental impacts of corn stover (versus corn; see main text) as well as of wheat straw (versus wheat straw, see discussion section). This is complicated by the changing prices of both corn and wheat (Figure A3-1).

For corn and corn stover, we assumed are the average prices reported by the USDA<sup>10</sup> and the US Department of Energy,<sup>11</sup> respectively. These prices were chosen because the USA is by far the largest producer of corn and corn stover. As modelled by the Billion Ton Report,<sup>12</sup> the majority of the corn stover currently available is below the price of 60 \$/tonne. This aligns well with the state of technology price reported by the MultiYear Biomass Plan, according to which the grower payment as well as harvesting and storage of stover is 68 USD/tonne.<sup>13</sup>

For wheat and wheat straw we assumed the average prices in Denmark, where there is an extensive market for straw for energy use.<sup>14</sup> This dataset was chosen because similar circumstances can be expected across Europe if wheat straw becomes a valorised resource. However, this price may be an overestimation considering current conditions where straw is used as animal feed.<sup>15</sup>

Given the price changes over time and the choice of only two countries (see Figure A3-1) we apply a simple uniform approach for the two crops, assigning a price of 180 Euro/kg to the crop and 60 Euro/kg to the agricultural residue. However, if prices for corn and wheat continue to decrease and if the stover and straw pieces slightly increase or remain constant (see Figure A3-1), the environmental impacts we assign to stover and straw may be underestimated.

For corn, we assume corn to stover ratio of 1, stover removal rate of 50% and a moisture content of 15% (Villegas et al.; forthcoming). For wheat, we assume that the wheat to straw ratio is 1.3, the straw removal rate is 50%, and the moisture content is 14.5% for both products (Villegas et al.; forthcoming).



Applying economic allocation, 14% of total impacts (main crop and agricultural residue) is assigned to corn stover, while the respective value for wheat straw is 11%. The removal of stover from the field also removes nutrients; the impacts of replacement fertilizer were assigned to corn stover per Villegas et al. (forthcoming).

For consistency with Yeung et al. (forthcoming), the impacts of corn grain were not allocated. Because of the high value and yield of corn (in comparison to stover), this does not significantly impact the results of 1G PBS production. The impacts of 1G PBS trays and films would decrease by less than 2% if economic allocation was applied to corn grain was assumed.

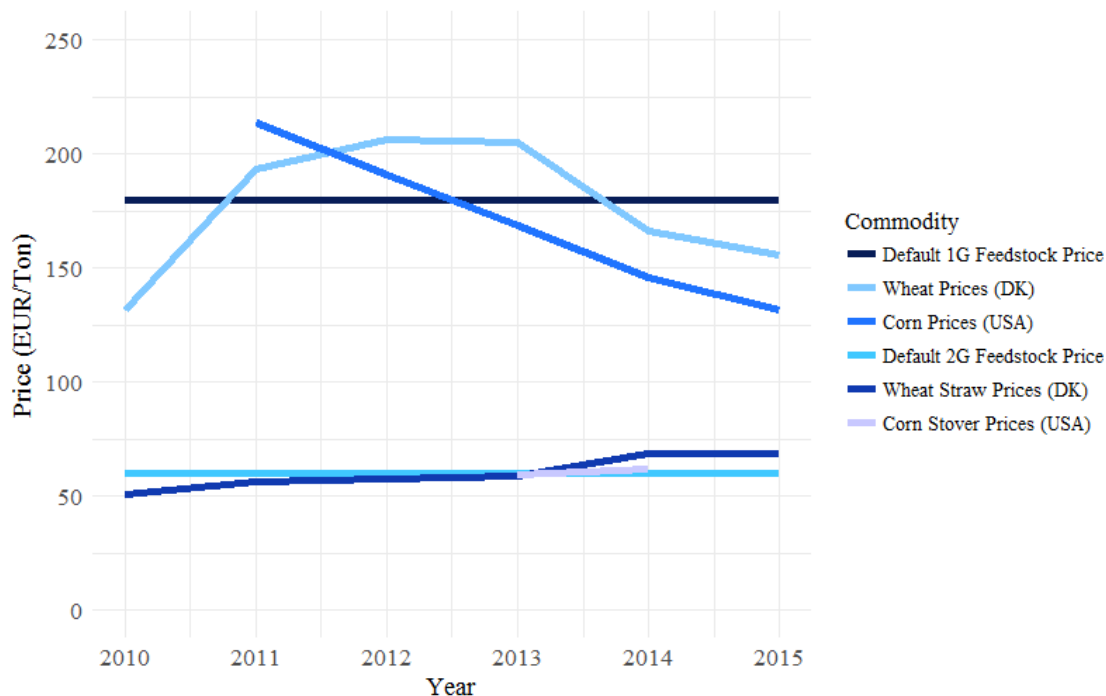


Figure A3-1: Prices of corn, corn stover, wheat and wheat straw<sup>10-15</sup>, in Euro/tonne (conversion using average of 2016 exchange rates<sup>16</sup>)

#### Appendix A4: Economic allocation for succinic acid process

The effect of different allocation methods when calculating the environmental impact of one mass unit of 1G C6 feedstock (dextrose) for bio-succinic acid is described in detail in Tsiropolous et al<sup>17</sup> and Cok et al.<sup>9</sup> As shown in Table A4-1, the differences in allocation methods have a limited effect on the impacts of succinic acid production. The allocation method chosen by Cok et al. as reference case was subdivision while we use for consistency reasons economic allocation (“Black Box economic”) for all analyses related to PBS. We updated Cok et al.’s SA work with the current average European electricity mix (ENTSO from EcoInvent 3<sup>8</sup>) and various dextrose feedstocks (Table 2).<sup>9</sup> In line with the industrial development of succinic acid, the yield of SA from C6 has increased by 20 percentage points (Theunissen, L, pers. comm. Reverdia) since the publication Cok et al.’s study<sup>9</sup>. Therefore, yields of SA from C6 were updated as well.

Table A4-1: NREU and GHG impacts of 1<sup>st</sup> generation succinic acid production from corn, based on different allocation methods (in this paper, the choice of the European electricity mix and updated yields are the only changes applied to the work done by Cok et al. <sup>9</sup>).

Allocation System for 1G Succinic Acid	NREU (MJ/kg SA)	GHG (CO <sub>2</sub> kg eq/kg SA)
Black box mass	31.3	0.71
Black box economic	32.0	0.77
Subdivision	30.3	0.62
Main process	33.1	0.98
System exp. US	33.2	0.83
System exp. Brazil	31.0	0.54
System exp. US/Brazil	32.3	0.71

## Appendix A5: Flowsheet of allocation and integration

Scenarios
a) Non- Integrated Steam Explosion Pretreatment and SA Production
b) Integrated Steam Explosion Pretreatment and SA Production
c) Non- Integrated Organosolv Pretreatment and SA Production
d) Integrated Organosolv Pretreatment and SA Production

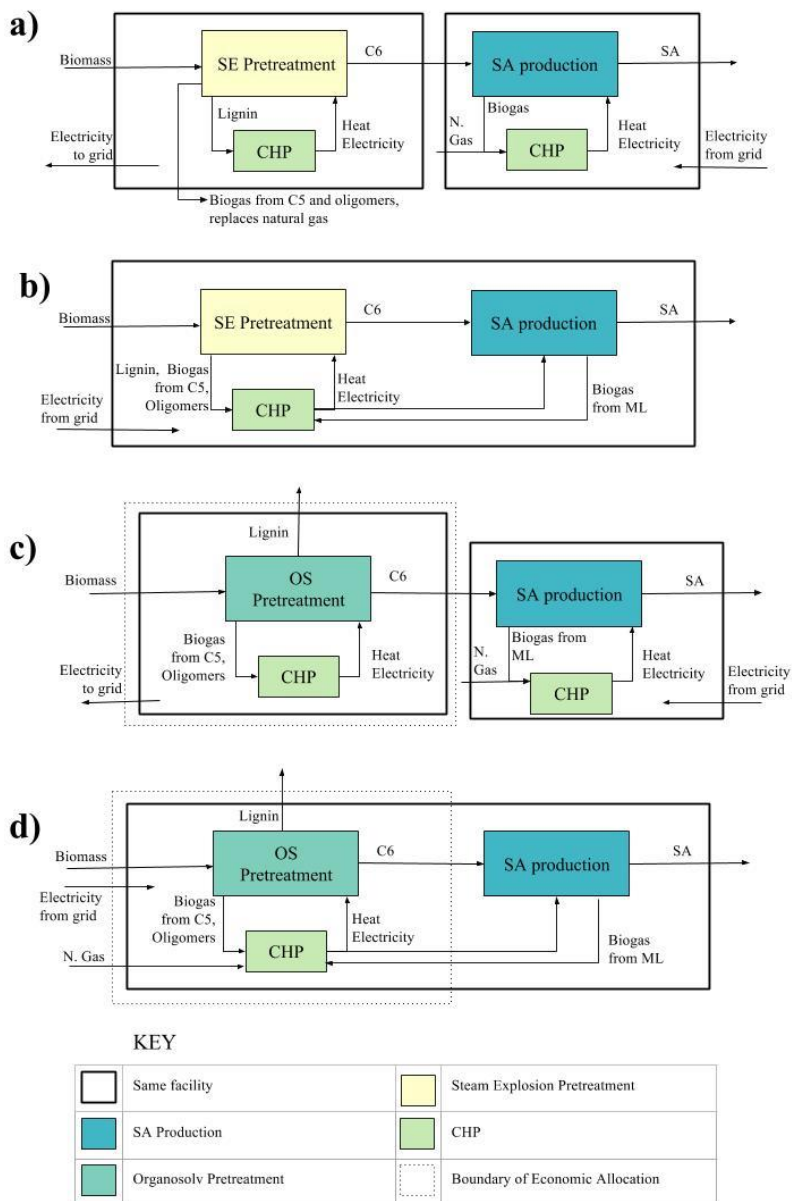


Figure A5-1: Flowsheets of *integrated* (b,d) and *non-integrated* (a,c) production of succinic acid through Steam Explosion (a,b) and Organosolv (c,d) pretreatment. The electricity from the grid represents excess demand of the process not covered by the CHP. The boundaries of economic allocation call for allocation between C6 and lignin for Organosolv (c,d).

Since the *non-integrated* SE pre-treatment and SA production plants (scenario a in Figure A5-1) have only *one* output at each facility (C6 and then SA), there is no need for allocation.

In an *integrated* SE pretreatment and SA facility (case b in Figure A5-1) there is also *one* output, SA, again not requiring allocation. In both SE cases, lignin, hemicellulose and oligomers are valorised internally and provide energy to the facility.

However, in OS processes, lignin is *not* used in the CHP. Therefore, the impacts of C6 and lignin coproduced in the OS process are allocated based on their economic values (case c in Figure A5-1). In the *integrated* scenario (d) it is necessary to first subdivide the facility into OS pretreatment and SA production, resulting in the same approach as case c). After having applied economic allocation to the pretreatment process (C6 and lignin) the impacts of SA production are added (case d in Figure A5-1). It is assumed that all the waste biomass is burned in a CHP plant, supplemented with natural gas, to meet the heat demand first of pretreatment, then SA production. Additional electricity needs are sourced from the grid.

#### **Appendix A6: Allocation for C5, oligomers, lignin, and C6**

For all cases of 2G PBS production, the conversion of oligomers (originating from the pretreatment processes) to biogas was estimated based on the work of Börjesson et al.<sup>18</sup> However, since oligomers are generally more difficult to process than monomers,<sup>19</sup> we assumed that the yield and process energy of oligomer conversion to biogas would be identical to the conversion of manure to biogas.<sup>19</sup> We estimate the calorific value of oligomers based on the equation proposed by Barrio et al.<sup>20</sup> As a result that 28% of the calorific value of oligomers is available in the form of biogas.

Similar to the conversion of oligomers, it was assumed that the C5 hydrolysate is converted to biogas, which is utilized in the CHP (accounted for by means of an energy credit). For the conversion of C5 hydrolysate to biogas the same yield and ratio of process energy to energy in biomass was assumed as for the conversion of maize to biogas<sup>18</sup>. As a result, 42% of the calorific value of the C5 hydrolysate<sup>20</sup> was available in the form of biogas.

For *integrated* cases, this biogas decreases the natural gas demand of the combined pretreatment and succinic acid process. Similarly, biogas replaces natural gas in the *non-integrated* Organosolv process. However, in the *non-integrated* steam explosion process there is no such natural gas demand. Therefore, biogas is credited to the natural gas grid, replacing “natural gas, high pressure, Europe without Switzerland” Ecoinvent 3 record, with biogenic carbon subtracted.

The Organosolv process assumed for the Conservative Case produces both a C6 stream and high purity lignin. We apply economic allocation in order to assign environmental impacts to each product. For the C6 hydrolysate, we use the price of raw sugar from Villegas et al. (forthcoming), converted to Euros using the conversion rates for 2015 (0.9 EUR/1 USD<sup>16</sup>). The assumed price of C6 hydrolysate is therefore 360 EUR/tonne. The assumed price of lignin was 1000 EUR/tonne, which was utilized by Piotrowski et al.,<sup>21</sup> who assumed that the price of lignin would be slightly lower than the price for phenol (1200 EUR/tonne). Lignin is a possible partial replacement for phenol in polyurethanes and resins.<sup>22</sup> Piotrowski et al.<sup>21</sup> also mention the price of HPL from the CIMV process (see discussion section) at 1450 EUR/tonne.

In the discussion section, we assume as alternative option for allocation the use of C5 hydrolysate (from SE and OS pre-treatment) for bioethanol production. In other words, we chose to base the price of C5 on its value contribution to bioethanol, thereby assuming co-fermentation together with C6 hydrolysate. This assumption is based on the conversion of the C5 fraction for cellulosic ethanol production has been demonstrated and may become a commercial reality.<sup>23,24</sup>

The price for ethanol chosen is that for 2015<sup>13</sup>. To estimate the yields of ethanol from both the C5 and C6 fractions, the theoretical yields were calculated from the following stoichiometric equations:<sup>25</sup>





(Eq A6-2)

These theoretical yields were multiplied by the experimentally determined percentage of C5 and C6 conversion to ethanol (75% and 90%) to determine the practical yield.<sup>25,26</sup> On this basis we determine ethanol yield of 0.38 kg ethanol/kg C5 sugar.<sup>26-28</sup> A virtual price can be assigned per kilogram of C5 sugar by multiplying the yield by the price of ethanol (0.67 EUR/kg ethanol). The calculation above assumes a fully developed bio-economy in which the C5 stream is fully valorised for bioethanol production. Under such conditions the value of C5 sugars is clearly higher than today.

## Appendix A7: Conversion of starch to glucose

The inputs for the conversion of starch to glucose were derived from Tsiropoulos et al.<sup>17</sup>. The hydrolysis of starch is carried out with two enzymes,  $\alpha$  – amylase and gluco-amylase<sup>17</sup>. The input of this process is a dilute starch slurry (C6 hydrolysate). We assume a dataset for starch from EcoInvent 3 (Maize starch production, DE<sup>8</sup>), with 14 weight-% of moisture. When adding the conversion impacts to the EcoInvent 3 record,<sup>8</sup> it was assumed that the energy necessary to dissolve the starch is insignificant. We use a conservative assumption regarding the technology applied to dry the glucose slurry; a single-effect evaporator dries the solution (rather than steam supply from mechanical vapour recompression<sup>17</sup>) from 32% ds to 50% ds. To do this, 1.0 kg of water is evaporated for every kg of glucose. We assume that 1.2 kg of steam is needed per kg of water evaporated,<sup>29</sup> and that the impacts of steam are the average of the chemical industry (Steam, in chemical industry, RER).<sup>8</sup>

## Appendix A8: Petrochemical BDO and Bio-based BDO from 2G C6

Petrochemical BDO data was sourced from EcoInvent 3 (butane-1,4-diol production, RER)<sup>8</sup> assuming the production from petrochemical butyne-1,4-diol hydrogenation.

The production of BDO by direct fermentation (currently employed by Mater Bio-Tech) was adjusted to 2G feedstocks using equation A8-1. To this end, the yield of BDO from dextrose or C6 was assumed to be 0.40 g/g or 80% of the theoretical yield;<sup>24</sup> the impacts of 1G Dextrose in the Reference Case were subtracted from the entire BDO production data, and then the impacts of 2G C6 were added.

$$i_{2G\ BDO} = i_{1G\ BDO} - i_{1G\ Dex}/0.4 + i_{2G\ C6}/0.4$$

Equation A8-1

where  $i_{2G\ BDO}$ ,  $i_{1GBDO}$ ,  $i_{1G\ Dex}$ ,  $i_{2G\ C6}$  are the impacts of 2G BDO production, 1G BDO production, 1G Dextrose production, and 2G C6 production, respectively, per kg of chemical produced. To estimate the impacts of BDO production, these savings are heat and electricity credits that replace the gas CHP modelled for non-integrated SA or BDO production (Table A8-1).

Table A8-1 Derivation of 2G BioBDO impacts

Impact (units)	BDO Production Scenario <sup>1</sup>	$i_{1GBDO}$	$i_{1G\ Dex}$	$i_{2G\ C6}$	$i_{2G\ BDO}$
Climate Change (kg CO <sub>2</sub> eq/kg)	Reference	2.37	0.95	0.22	0.54
Climate Change (kg CO <sub>2</sub> eq/kg)	Best	2.05	0.95	0.19	0.16
NREU (MJ/kg)	Reference	61	8.9	-4.0	29
NREU (MJ/kg)	Best	56	8.9	-4.4	23

<sup>1</sup>The impacts of 1G BDO and 1G dextrose are sourced from Novamont Group (Innocenti FD, pers. comm. 2016) and Cok et al.,<sup>9</sup> respectively. The impacts of 1G and 2G BDO have embedded biogenic carbon counted as negative emissions, while dextrose and C6 do not.

## Appendix A9: Polymerisation and production of plastic trays

For lack of available material-specific data, the impacts of the polymerisation of PBS are adjusted from those of the polymerisation of PET. Both polymers are formed by esterification and transesterification of monomers at similar time scales. However, the lower temperature of the PBS process and the lack of a solid-state polymerisation step (compared to PET) cause lower impacts in polymerisation. To quantify this difference, we estimated the difference in heating needs for the two polymers. It was assumed that the polymerisation of PBS occurred at 200°C, while that of PET occurred at 250°C.<sup>30,31</sup> The energy needed to heat the monomers to these temperatures was calculated using the ratio from the following equation:

$$q_{ratio} = \frac{M_{SA}C_{SA}\Delta T_{PBS} + M_{BDO}C_{BDO}\Delta T_{PBS}}{M_{EG}C_{EG}\Delta T_{PET} + M_{TPA}C_{TPA}\Delta T_{PET}}$$

where M is the mass of the monomer, C is its specific heat, and ΔT is the change in temperature (in K) of the monomer as it reaches the polymerisation temperature of PBS or PET from an assumed starting temperature of 293K. The weights of the monomers were assumed to those necessary to produce 1 kg of polymer (note that there are different synthesis efficiencies assumed). The specific heats of the monomers are assumed to be independent of temperature.<sup>32</sup> The above equation yielded a ratio of heat necessary of 0.88, i.e. 12% less energy use needed for PBS than for PET. Using the life cycle inventory of the polymerisation of amorphous PET (EcoInvent<sup>8</sup> and PlasticsEurope<sup>33</sup> assumed to represent a less efficient small scale case), the heating needs of the process were adjusted and new impacts calculated. It was assumed that electricity use and all other impacts remain the same. The heating needs and overall impacts of esterification and transesterification of PET are shown below (see Table A9-1), as well as the estimated impacts of PBS polymerisation. The most recent impacts reported for PET polymerisation<sup>34</sup> are not used to estimate the impacts of PBS polymerisation because of their lack of transparency and the authors' assumption that the large scale and efficiency of PBS polymerisation will not be competitive with that of PET in the near future.

Table A9-1: Summary of impacts of PET polymerisation and estimates of PBS polymerisation. Solid state polymerisation is not assumed for PBS so the impacts of this step for PET are not shown.

Polymer	PET		PBS	
	GHG	NREU	GHG	NREU
Unit	kg CO <sub>2</sub> /kg PET	MJ/kg PET	kg CO <sub>2</sub> /kg PBS	MJ/kg PBS
Heating	0.50	5.8	0.44	5.1
All Impacts	0.60	7.2	0.54	6.5

The plastic trays are commercially produced by sheet extrusion and subsequent thermoforming in two steps from the plastic material received in pellet form. The prototype trays were produced from pre-extruded sheets (Cox M, Sharpak, 2016 pers. comm.). Upon receipt of PBS sheets, Sharpak expected the material to be too flexible for the intended purpose, but the final tray turned out to fulfil all physical property expectations (possibly partly related to the tray design with its ribs). Moreover, its mouldability exceeded that of the PET, being the incumbent material (Cox M, Sharpak, 2016 pers. comm.). The impact and physical properties tested thus far yielded satisfactory results but further trials regarding their application as a food tray are necessary. The equivalent functionality of PBS to petrochemical trays will be dependent on the intended uses of PBS trays (for example a coloured tray that can be frozen), which are not yet known. To determine the intended use of PBS trays, further testing on tray properties is necessary. As explained in the main body of the text, we ignore the small difference in PET and PBS density by choosing 1 kg of trays as functional unit. This simplification is also applied to PP and PBS trays (i.e. 1kg of each is used as a functional unit).

While it is, in principal, possible to produce PBS trays on the same equipment as PP trays, this was not tested due to the small scale of the trials. The mass production of PP trays is performed in a one-step process instead of first extruding plastic sheets which are thermoformed in a separate step (Cox M, Sharpak, 2016 pers. comm.). The one-step process allows to increase in energy efficiency, but this case was not considered for PBS trays which would presumably be produced with the same technology as PET for the time being.

Although the facilities that produce PP and PET trays are in England, the impacts of European electricity mix were assumed for consistency with the remainder of the paper.

To calculate the energy necessary for the extrusion and thermoforming of PBS trays in comparison with PP and PET trays, the melting point and the specific heat of the materials was considered. Although these values depend on the crystallization and melting of the polymers, the energy requirements were estimated by integrating temperature-dependent values of specific heat from 20°C to the melting temperature<sup>35,36,37</sup> and assuming a 70% efficiency of an electric heater. The energy necessary to melt PBS twice (in the same two-step process as PET) was found to be roughly the average of the energy needed to a) melt PP once and b) melt PET twice. This is due to the lower melting temperature of PBS (see Table A9-2). Therefore, we assume the average impacts of PP and PET thermoforming and extrusion to be the impacts of the equivalent PBS process.

Table A9-2: Comparison of physical properties of PBS and incumbent materials under comparable conditions.<sup>38,39</sup>

Physical Property	PBS	PET	PP
Density (g/cm <sup>3</sup> )	1.26	1.37	0.90
Glass Transition Temperature (K)	241	345	260
Melting Temperature (K)	387-389	518-553	450
Estimated energy use for melting 1 kg of polymer (in MJ electricity at plant)	0.85	1.31	0.50

The derived impacts for PP, PET, and (calculated) PBS impacts are less than those presented by EcoInvent for Europe (Figure A9-1) for the thermoforming and extrusion of plastics. However, the energy needs of Sharpak are like other European plants and are specific to tray production (Cox M, Sharpak, 2016 pers. comm.). Therefore, we chose to use adapted impacts of PBS thermoforming and extrusion to trays (derived from Sharpak data) rather than general EcoInvent data.

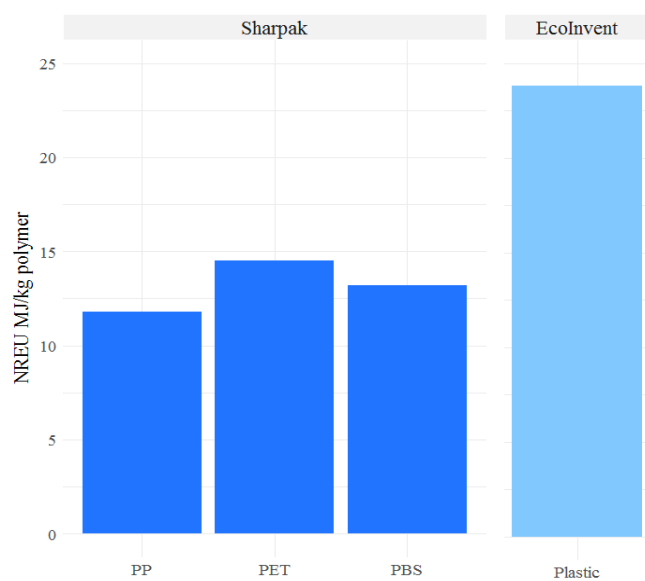


Figure A9-1: Comparison of NREU impacts of thermoforming and extrusion of plastics.

#### Appendix A10: Energy recovery credits (MSWI)

Both heat and electricity credits related to municipal solid waste incineration (MSWI) are specific to Europe. The heat and electricity exported from average MSWI plants was divided by the average calorific value of waste,<sup>40</sup> resulting in yields of 0.12 GJ electricity/GJ heating value of waste and 0.30 GJ heat/GJ heating value of waste. The calorific value of each studied plastic was multiplied by these values to obtain the energy recovered from incineration of plastic waste. The impacts of avoided heat and electricity generation are sourced from EcoInvent 3 (see Table 2).<sup>8</sup>

The authors acknowledge that complete collection and incineration of PE film is an optimistic assumption when considering current practices in Europe. The policies regarding collection of agricultural films varies dramatically by country. Although recycling of the collected film is technically feasible, is it not yet implemented throughout Europe.<sup>41</sup> Alternatively, the landfilling of waste is not desirable, and widespread efforts have been made to limit the landfilling of plastics.<sup>41</sup> Therefore, as a middle ground, we assume incineration with energy recovery as a viable end of life option for agricultural films. It was additionally considered that contaminants from the field (soil, biomass etc.) would decrease the calorific value of the product (see Figure 5 and Table 13 in Briassoulis et al.<sup>42</sup>). This decreased the calorific value of LDPE mulch films by 46% to 24 MJ/kg film.

### **Appendix A11: Composting and Degradation of Field of PBS**

Composting and degradation of PBS is assessed based on the model used by Yeung et al. (forthcoming). We assume that 60% of the embodied carbon in PBS is released at the composting facility<sup>43</sup>, and 35% of the embodied carbon in PBS is released within the hundred years after the application of compost. In other words, 5% of the carbon in PBS is stored in the soil. The final degradation of PBS in compost on the field is estimated based on a data published by Showa Denko<sup>44</sup> and is in line with the empirical work done on PBS degradation in fields.<sup>45,46</sup>

Furthermore, it is assumed that 1 kg of compost (or 2.5 kg of PBS film) replaces 0.79 kg of moss peat<sup>43</sup>. The impacts of moss peat production are sourced from EcoInvent 3 (peat moss production, RER)<sup>8</sup>.



## Appendix B: Results and Discussion

### Appendix B1: Results for 2G Reference and Conservative cases for integrated and non-integrated plants

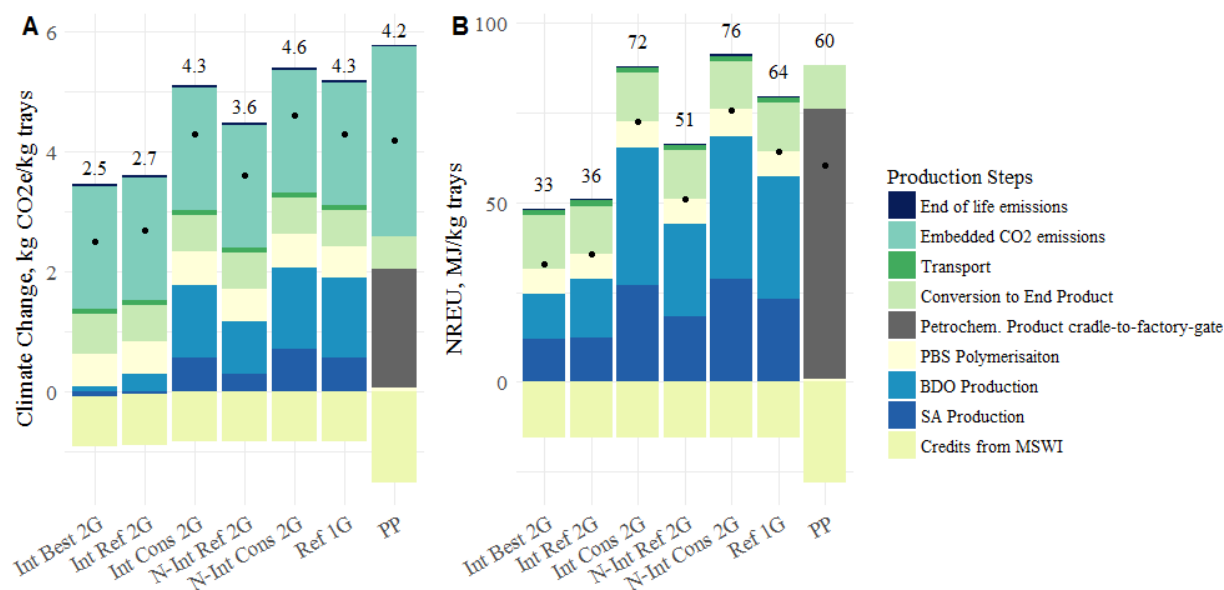


Figure B1-1: Cradle-to-grave Climate change (A) and NREU (B) impacts of 2G PBS trays from corn stover for a) the Best cast b) the Reference case (Ref) and c) the Conservative Case (Cons) with integrated (Int) and non-integrated (N-Int) pretreatment. The points in the bar and labels on top of the bars indicate net climate change (A) or NREU (B) impacts.

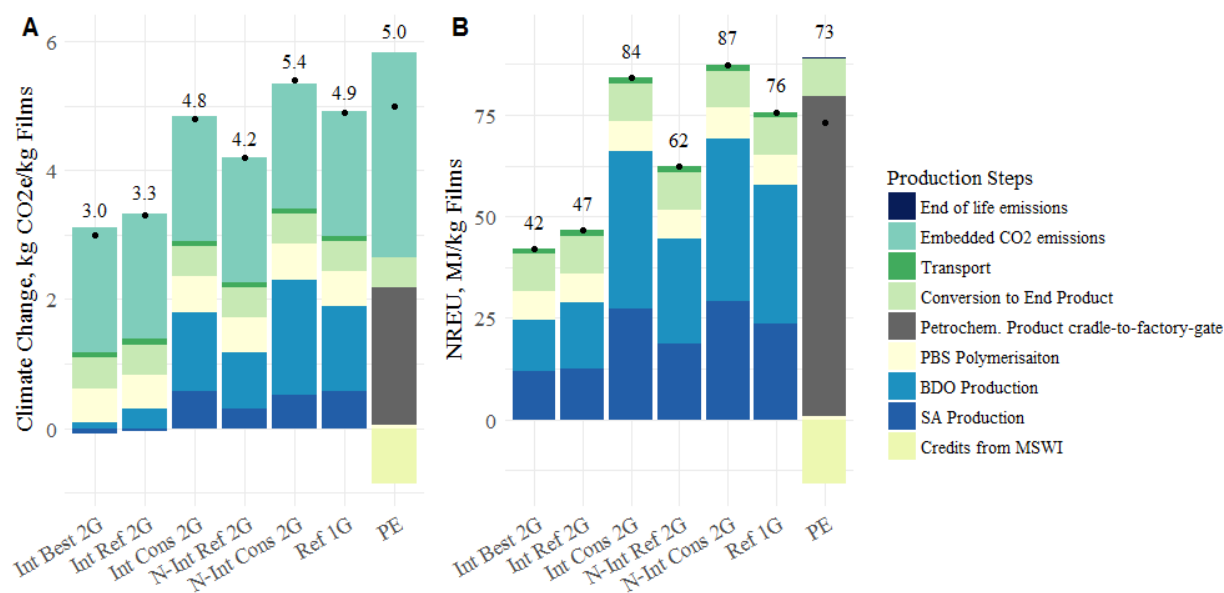


Figure B1-2: Cradle-to-grave Climate change (A) and NREU (B) impacts of 2G PBS films from corn stover for a) the Best Case, b) the Reference case (Ref) and c) the Conservative Case (Cons) with *integrated* (Int) and *non-*

integrated (N-Int) pretreatment. The points in the bar and labels on top of the bars indicate net climate change (A) or NREU (B) impacts.

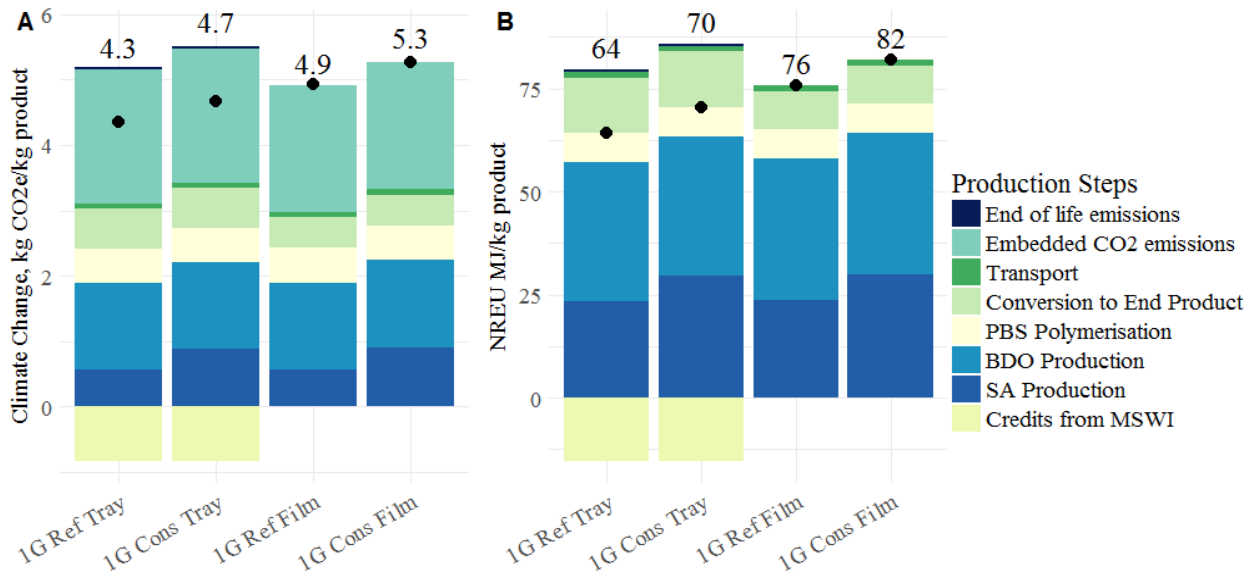


Figure B1-3: Cradle-to-grave climate change (A) and NREU (B) impacts of 1G PBS trays and films from corn grain for a) the Reference case (Ref) and b) the Conservative Case. The points in the bar and labels on top of the bars indicate net climate change (A) or NREU (B) impacts.

### Appendix B2: Results for 2G fb PBS trays from various feedstocks

Both wheat straw and miscanthus can be processed in the same manner as corn stover (low severity SE), but the pretreatment of hardwood occurs at higher temperatures and pressures (high Severity SE). This process involves higher residence times and temperatures (Villegas et al., forthcoming). High pressure steam and a lower concentration of biomass (20% versus 50% solids) are employed (Villegas et al, forthcoming).

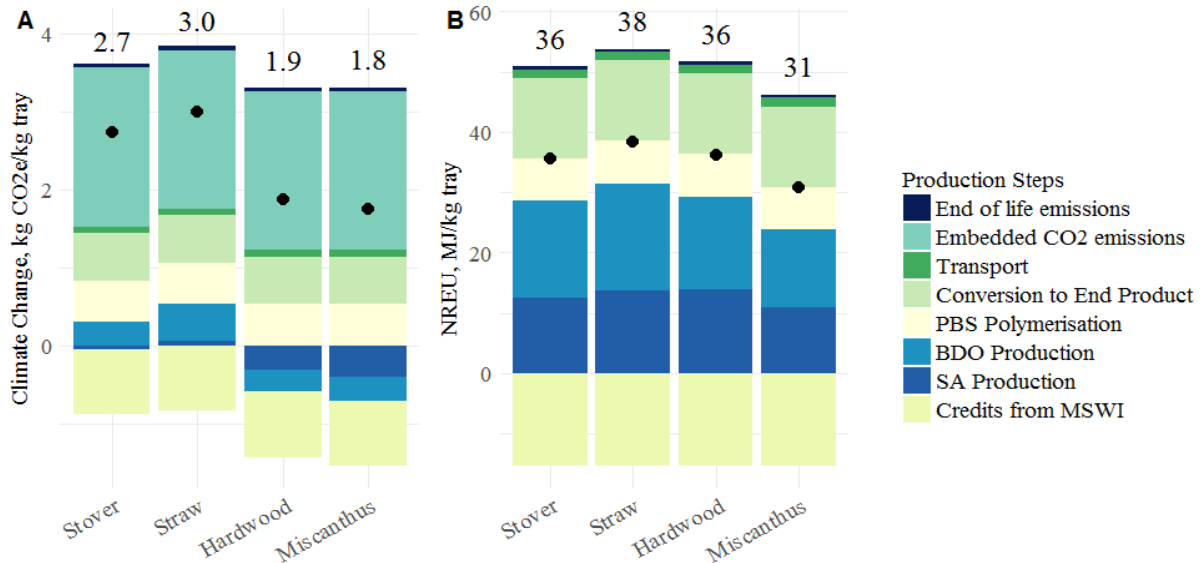


Figure B2-1: Cradle-to-grave climate change (a) and NREU (b) of fb 2G PBS trays based on wheat straw, miscanthus, willow and corn stover from the *integrated* case with pretreatment by steam explosion. Besides feedstock changes, the records are analogous.

### Appendix B3: Comparison to BREW Report

The similar feedstock and concentration of sugars between this work and that of Patel et al.<sup>29</sup> allow for a comparison between the two sources, although functional units and pretreatment processes vary.

Ten years ago, the BREW report outlined the environmental impacts of producing dilute fermentable sugars (C6 and C5, no oligomer production assumed) from corn stover under the simplifying assumption that the both glucose and xylose could be used to produce bio-based chemicals. Today, it is not yet technically feasible to make all C5 and C6 sugars, that are embodied in the feedstock, available for further processing. Instead, we assume that xylose and oligomers can instead be used in biogas production. Therefore, we compare the results for dilute fermentable sugars from BREW to our results regarding dilute C6 sugars because both functional units (and their corresponding impacts) were the assumed as the basis for bio-succinic acid in the respective papers.

In regards to pretreatment, the BREW dataset assumes 1.4-1.5 tonnes of dry matter input of corn stover per tonne of fermentable sugar, a dilute hydrolysate product, and was based on the 2010 design case of the NREL study by Aden et al.<sup>47</sup>. In comparison to BREW, with its more optimistic process design assumptions for Dilute Acid pretreatment of corn stover, we assume as Reference Case pretreatment by low-severity steam explosion (SE, applied to corn stover) adapted from Villegas et al. (forthcoming). It results in a dilute C6 hydrolysate (without need for transportation and storage) and the use of C5 and oligomers which can be converted to biogas. The impacts calculated for C6 sugars account for credits for co-produced energy from the CHP, as is the case for fermentable sugars in BREW.<sup>29</sup>

According to Figure B3-1 (see the data in row E, reproduced from the BREW report<sup>29</sup>), both the NREU and non-renewable greenhouse gas (NRGHG) emissions for producing one tonne of fermentable sugar from corn stover (maize stover) are negative (-4.4 GJ/t sugars and -0.16 t CO<sub>2</sub>/t sugars without subtracting sequestered carbon). This is a consequence of the large credits for co-produced electricity and steam (these credits add up to 9.2 GJ/t) which exceed the process heat and electricity demand of the pretreatment process and the preceding value chains. In comparison, the Reference values of NREU and GHG for low-severity SE in this work amount to -4.0 GJ/t and + 0.22 t CO<sub>2</sub>/t of C6. The NREU value for sugars is similar among the two sources. For GHG impacts, the sign differs (slightly positive vs slightly negative) but both values are close to zero. As a consequence, the results for SA calculated in the BREW report and in the present study are quite similar (see Discussion section in main body of the paper).

All data per tonne of fermentable sugar		1	2	3	4 (=2-3)							
		Total renewable energy REU GJ <sub>HHV</sub> /t	Process energy NREU GJ <sub>HHV</sub> /t	Exported energy = NREU credits GJ <sub>HHV</sub> /t	NREU GJ <sub>HHV</sub> /t	Ranking	NRGHG emissions t CO <sub>2</sub> eq./t	Ranking	Sequestered CO <sub>2</sub> t CO <sub>2</sub> /t	NRGHG minus sequestered CO <sub>2</sub> t CO <sub>2</sub> eq./t	Land use ha/t	Ranking
Dextrose (32%ds) from starch (maize, wet milling) <sup>1)</sup>	A. Default (Detailed mass-based allocation)	17.3	6.2	0.0	6.2	6 <sup>th</sup>	0.40	6 <sup>th</sup>	1.47	-1.07	0.13	3 <sup>rd</sup>
	B. Sensitivity (High energy use for maize)	17.3	10.3	0.0	10.3	7 <sup>th</sup>	0.63	7 <sup>th</sup>	1.47	-0.84	0.13	3 <sup>rd</sup>
Sucrose (59%ds) from sugar cane <sup>2)-6)</sup>	C. Default (Energy credit approach)	41.8	1.7	14.5	-12.8	1 <sup>st</sup>	-0.54	1 <sup>st</sup>	1.54	-2.08	0.13	3 <sup>rd</sup>
	D. Sensitivity (Economic allocation, 20%)	33.4	1.4	--	1.4	5 <sup>th</sup>	0.11	4 <sup>th</sup>	1.54	-1.43	0.10	2 <sup>nd</sup>
C5/C6 sugars (13%ds) from lignocellulosics <sup>7)</sup>	E. Default (maize stover, econ. alloc.)	29.2	4.9	9.2	-4.4	2 <sup>nd</sup>	-0.16	2 <sup>nd</sup>	1.46	-1.62	0.05	1 <sup>st</sup>
	F. Sensitivity (poplar)	35.6	7.6	9.2	-1.7	4 <sup>th</sup>	0.14	5 <sup>th</sup>	1.46	-1.32	0.26	4 <sup>th</sup>
	G. Sensitivity (miscanthus)	34.3	5.2	9.2	-4.0	3 <sup>rd</sup>	-0.04	3 <sup>rd</sup>	1.46	-1.50	0.13	3 <sup>rd</sup>

NR: Non-renewables-sourced; R: Renewables-sourced

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- 2) Sugar cane in Brazil. UU calculations. Average of 2 cases to account for differences in sugar cane composition (Case 1: high sucrose content; Case 2: medium sucrose content).
- 3) Carvalho Macedo, Isaias De (1992): The sugar cane agro-industry -- Its contribution to reducing CO2 emissions in Brazil, Biomass and Bioenergy, Volume 3, Issue 2, pp77-78.
- 4) Carvalho Macedo, Isaias De (1997), Greenhouse gas emissions and avoided emissions in the production and utilization of sugar cane, sugar and ethanol in Brazil:1990-1994, Report for MCT - Coordenacao de Pesquisa em Mudancas Globais, pp5-6.
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- 6) Braunbeck, O., Cortez, L., Walter, A. (1999): Sugar cane resources for sustainable development: A case study in Luena (Zambia). Report for the Stockholm Environment Institute, February, p.11.
- 7) Calculated in BREWtool with NREL data for 2010 design case (Aden et al., 2002), assuming 34% of on-site energy production allocated to pretreatment + hydrolysis.

Figure B3-1: Overview of energy and emission data for sugar feedstocks as used in the BREW model calculations (system boundary: cradle to fermentable sugar), reproduced from Patel et al.<sup>29</sup>

## Appendix B4: European electricity supply

To unify the electricity profiles across the entire value chain, the EcoInvent 3 record “ENTSO” for European grid electricity was assumed<sup>8</sup> (plausible because the records are based on European data).

## Appendix B5: Comparison to other biodegradable polymers

The monomers of PBAT, PBST and PBSA were chosen from lab scale experiments (Table B4-1). Just as for the Reference Case, we assumed the molar efficiency for polymerisation to be 95% and the mass efficiency of conversion of 1 kg of polymer (Table B4-1) to 1 kg of trays to be 95%. The *integrated* Reference Case for tray production, with MSWI as the chosen end of life option, was applied to these polymers (see Table 2). The results are presented graphically in Figure B4-1.

Table B4-1: Monomer amounts of selected polymers.

Monomer/Polymer	PBAT (1kg)	PBST (1kg)	PBSA (1kg)	PBS (1kg)
Succinic Acid(kg)	0	0.44	0.44	0.72
1,4 Butanediol (kg)	0.28	0.33	0.33	0.55
Terephthalic Acid (kg)	0.54	0.61	0	0
Adipic Acid (kg)	0.46	0	0.54	0
Molar mass of polymer (g/mol)	332	392	284	172
Bio-based carbon storage (kg CO <sub>2</sub> /kg polymer)	0.80	1.20	1.20	2.04
Molar efficiency for polymerisation	95%	95%	95%	95%
Source for monomer selection	Schrijvers et al. <sup>3</sup>	Luo et al. <sup>48</sup>	Ahn et al. <sup>49</sup>	Tecchio <sup>50</sup>

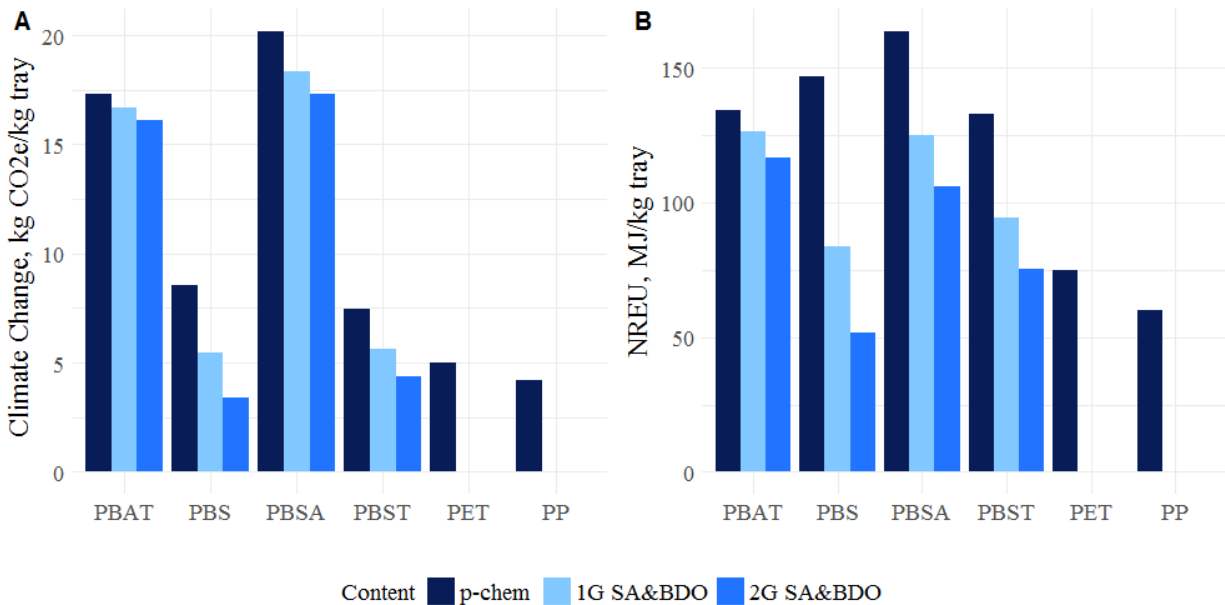


Figure B4-1: Cradle-to-grave climate change impacts (a) and NREU (b) of PBAT, PBST, PBSA, and PBS based on petrochemical BDO and SA (dark blue), 1G SA and BDO (light blue) and 2G SA and BDO (blue). 1G and 2G SA and BDO impacts are based on the Reference case of PBS production. The remaining inputs for the polymers studied are from the *integrated* Reference case of PBS tray production.

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