PEF bottles – a sustainable packaging material

ISO Certified LCA of Avantium's PEF products

conducted by nova-Institute
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1. Introduction

Chemical technology company Avantium partnered with nova-Institut GmbH under the framework of the PEFerence project[1], to perform a full cradle-to-grave Life Cycle Assessment (LCA) for the YXY® Technology, assessing the potential environmental impacts of PEF packaging solutions in comparison to conventional PET alternatives. The LCA is performed according to the ISO 14040/44 standard methodology. A critical peer review of the study, including by experts of incumbent technologies, was conducted in order to verify whether the LCA met the requirements for methodology, data, interpretation, and reporting. In this paper, the main results of this LCA study are summarised.

2. Avantium's YXY® Technology

Avantium is an innovation-driven company dedicated to developing and commercialising breakthrough chemistry technologies for the production of chemicals from renewable feedstock instead of fossil resources. It is proven that the use of renewable carbon feedstocks for the production of plant-based chemicals and plastics has a clear link to reducing the risk of climate change.[2] The carbon absorbed by plants is used to produce chemical materials, which is then released at the end of the product life cycle, with a net neutral impact on the CO_2 concentration in the atmosphere. In contrast to this, fossil-based materials and plastics use fossil carbon, such as petroleum, which was previously stored underground, and release this additional CO_2 into the atmosphere.

Avantium has developed a technology to convert plant-based sugars into FDCA (furandicarboxylic acid), the building block of PEF (polyethylene furanoate): a plant-based, fully recyclable plastic material with superior performance. FDCA is polymerised with plant-based mono-ethylene glycol (MEG) to make a 100% plant-based PEF polymer. Avantium has successfully demonstrated this YXY® Technology in its pilot

[1] PEFerence has received funding from the Bio-Based Industries Joint Undertaking under the European Union's Horizon 2020 research and innovation program under grant agreement no. 744409.
[2] de Jong, E.; Stichnothe, H.; Bell, G.; Jørgensen, H. Bio-Based Chemicals, a 2020 Update. IEA Bioenergy. 2020, ISBN 978-1-910154-69-4.

plant in Geleen, The Netherlands. In December 2021, Avantium has taken a positive investment decision concerning the construction of the world's first FDCA Flagship Plant in Delfzijl (the Netherlands), with construction planned to be completed by the end of 2023 and the aim to be operational in 2024. This will be the world's first commercial FDCA facility and will have a targeted production capacity of 5,000 tonnes per annum. FDCA is the key building block for the 100% plant-based, recyclable polymer PEF (Figure 1). The role of the Flagship Plant will be: to prove the process technology, and to demonstrate the commercial applications of PEF. Ultimately, Avantium intends to sell technology licenses to industrial collaborators who are expected to build production capacities of >100 kt/a based on the knowledge and experience derived from Avantium's operation of the 5 kt/a Flagship Plant.

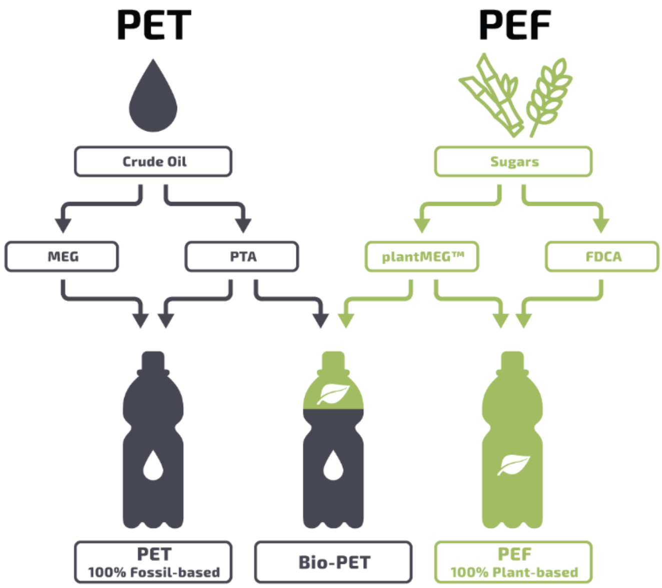

Figure 1: Plant-based PEF bottles

3. PEF: environmental features and functionality

Plant-based

PEF is a 100% plant-based plastic material, made from sugars derived from plants. The sugars (fructose) required to make FDCA can be produced from agricultural crops, such as wheat, corn and sugar beet. When fully technologically developed, PEF can also be produced from cellulose, which is abundant in non-edible biomass, such as agricultural and forestry waste streams. The current process utilises starch from European wheat. The other key building block is commercially available biobased MEG. Avantium opened a demonstration plant for plantMEG™ in 2019 and plans to form a joint venture with the Cosun Beet Company, with the ambition to jointly construct and operate the first commercial plant for the production of plant-based glycols using Avantium's Ray Technology™.

Avantium's Dawn Technology™ converts non-food biomass into industrial sugars and lignin in order to help transition the chemicals and materials industries to non-fossil resources. Avantium runs a pilot biorefinery in Delfzijl, the Netherlands, based on the Dawn Technology™.

Following the development of Avantium's YXY® Technology for FDCA production, the biorefinery Dawn Technology™ for non-food biomass conversion and Ray Technology™ for plantMEG™ have been developed to create a technology ecosystem that supports the sourcing of plant-based feedstock for producing PEF.

Properties

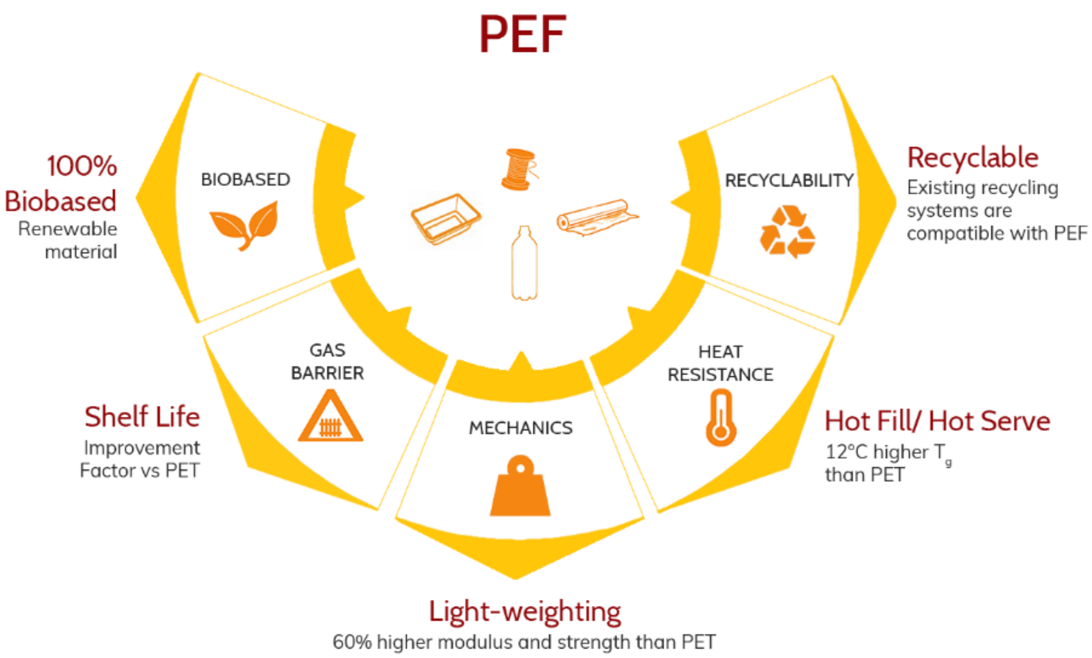

Figure 2: PEF properties

PEF has enhanced barrier, mechanical and thermal properties compared to today's widely used petroleum-based polymers. The barrier properties of PEF, which are ~10x better for O_2, ~15x better for CO_2, and ~2.5x better for water than PET, represent a revolutionary opportunity compared with traditional packaging solutions regarding performance, price, and sustainability when produced at scale. The improved barrier properties lead to a longer shelf life of packaged products. PEF also offers higher mechanical strength, which means that thinner PEF packaging can be produced and fewer resources are required.

In terms of thermal properties, PEF has superior ability to withstand heat and can be processed at lower temperatures. PEF has enhanced mechanical stiffness and allows for increasing shaping possibilities.

Recyclability of PEF

To fully meet the requirements of our time, not only the plant-based source, performance, and cost of PEF are important, but the end-of-life and circularity of PEF are equally important. PEF can be used as a single layer in bottles for soft drinks, beer, and juices, replacing glass bottles, aluminium cans, and multilayer bottles. PEF has proven fit-for-purpose with existing sorting and recycling facilities. PEF can be recycled mechanically and chemically in a similar way using the same equipment used to recycle PET. In addition, PEF can easily be distinguished from PET and other plastics using near-infrared technology, allowing it to be sorted from any PCR or deposit system waste streams.

Multilayer bottles are a valid alternative when the required shelf life cannot be guaranteed by monolayer packaging alone. Currently, many multilayer PET bottles include polyamides (PA), such as MXD6 for barrier properties. However, a common issue for incumbent barrier materials such as PA is their poor compatibility with PET, making it essential to sort out the PA from the PET in the recycling stream. It was demonstrated that PEF has a much lower influence on the quality of the rPET product, making the recycling process with these PEF-based multilayer structures much more robust.

4. Life Cycle Assessment of chosen PEF applications

Goal

A Life Cycle Assessment (LCA) is fundamental to understanding the potential sustainability benefits of Avantium's YXY® Technology and various PEF applications, as well as to identifying opportunities for improvement. LCA is the most recognised method to quantitatively assess potential environmental impacts of products, services, or processes. An LCA can assess the whole value chain of a product, from the extraction or cultivation of raw materials through production, use, and disposal of the product ("cradle-to-grave"). Environmental impacts that are usually evaluated include greenhouse gas (GHG) emissions, impacts on natural resources and on ecosystems.

Therefore, in 2017 Avantium partnered with nova-Institut GmbH under the framework of the PEFerence project, to perform a full cradle-to-grave LCA for the YXY® Technology, assessing the potential environmental impacts of PEF packaging solutions in comparison to conventional PET alternatives. The aim of the LCA is to support technical and capital decisions during the process development of Avantium's YXY® Technology and the commercialisation of PEF-based applications. A benchmark of PEF-based applications against other, non-plastics packaging materials such as aluminium cans or glass bottles was beyond the scope of the study.

This LCA has been conducted compliant with the standards ISO 14040 and 14044. A critical peer review of the study, including experts of LCA methodology and incumbent packaging solutions, was conducted in order to verify whether the LCA met the requirements for methodology, data, interpretation, and reporting.

Products and Functional Unit

The LCA was carried out for a 250 mL monolayer PEF bottle and a 250 mL PET multilayer bottle with 10% PEF, ensuring a minimum of 12 weeks CO_2 shelf life (barrier property) and required mechanical strength for transport and use. The amount of polymer required to fulfil the function of the bottle was calculated based on the gas permeability values of the polymers, assuming that ideal stretch ratios were gained during bottle blowing to ensure the optimal barrier performance of each material. These calculations resulted in bottle masses of 13g for PEF and 24g for the reference PET bottle. Bottle masses were confirmed as being appropriate under the assumptions used by industry experts. However, as different designs can lead to different bottle weights, a comprehensive sensitivity analysis with respect to this parameter was conducted in the LCA.

Table 1: Functional Unit

Aspect	Description
Function	Storing and delivering of beverages (CSD drinks) by means of single-use bottles
How much?	1 bottle with a capacity of 250 mL
Expected level of quality	Mechanical integrity – No breakage during transport Barrier property – CO_2 shelf life of minimum 12 weeks, designed to gain optimal stretching in the bottle walls
Lifetime of the function or service	One time. Single-use, recyclable bottles
Where?	In selected markets: The Netherlands (baseline), Belgium, and Germany

System boundaries: cradle-to-grave

The LCA covered all relevant life cycle stages from cradle-to-grave: from the biomass cultivation (wheat for fructose and sugarcane for bio-MEG feedstocks supply) to the production of PEF-based bottles including their end-of-life options (recycling and incineration). Transport activities are included.

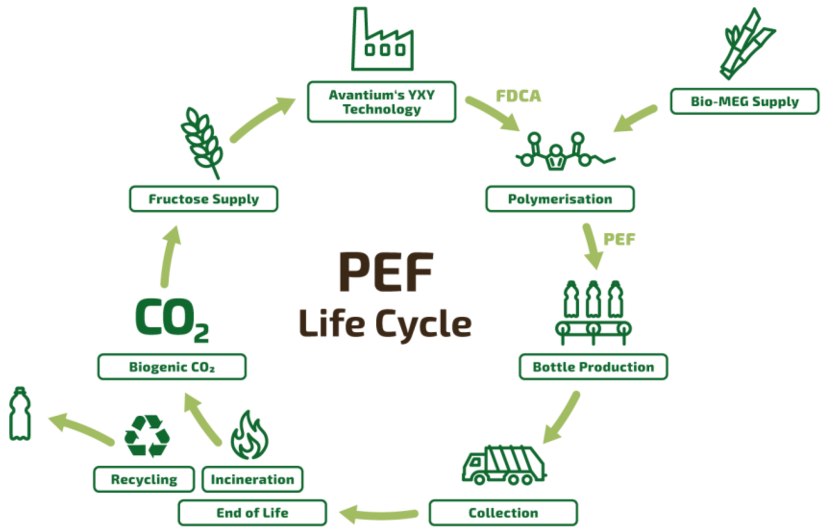

Figure 3: Life cycle stages of monolayer PEF bottles

End-of-Life scenarios: recycling and incineration

It is foreseen that the commercialisation of PEF-based products will initially take place in the Netherlands, Belgium, and Germany. In these countries, the rates for average PET bottle waste collection and recycling are relatively high[3] and landfilling is no longer practiced in these countries.

With regard to the end-of-life scenarios in this LCA, the fate of PET bottles in these countries was considered as being representative for PEF bottles. For instance, a 65%-35% mechanical recycling – incineration ratio was considered for the Netherlands[4].

Allocation rules

Upstream activities (wheat cultivation and milling) produce several co-products (gluten, dietary fibres, oil). In the YXY® Technology, a number of side-products,

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[3] Eunomia 2020: PET Market in Europe: State of Play. Available at https://www.eunomia.co.uk/reports-tools/pet-market-in-europe-state-of-play/.

[4] It was assumed that PEF will initially be mixed and recycled in the PET recycling stream (open-loop recycling) until the market has grown sufficiently to enable an individual material recycling stream.

mainly humins (a polymeric, heterogeneous species with multiple functionalities) are formed. In this LCA, the economic value of the main products FDCA for PEF production and side products such as humins was considered for allocating environmental burdens[5].

Geographical, temporal, and technological representativeness

Avantium's PEF-based products are advanced prototype designs based on model calculations and are substantiated by pilot-scale data, but are not yet commercially available or produced at large scale. The LCA is therefore based on the already-approved engineering data for the first commercialisation phase of Avantium's YXY® Technology (predominantly in the Netherlands, Belgium, and Germany markets) for a plant with a production capacity of 100 kilotonnes FDCA per year. Consumptions and production figures are based on the models for the 5 kt/a Flagship Plant design, scaled-up to 100 kt/a, provided by Avantium and the engineering contractor Worley.

Life Cycle Inventory

The core data used for this LCA were primarily supplied by Avantium, its engineering partner Worley and its feedstock supplier. Secondary data were mostly based on the most recent life cycle models from the Ecoinvent v3.6 database and to a minor extent from other peer-reviewed literature sources. PET bottles were modelled using Ecoinvent data for bottle grade PET production available from most recent Eco-profiles of the European plastics industry. There were no data gaps; data were complete for all impact categories. Altogether, the quality of the data was rated as 'good', which was confirmed by the peer-review panel.

Impact categories

The full LCA evaluated 16 different impact categories, covering a complete set of indicators addressing impacts on ecosystems, human health, and depletion of resources. These were assessed applying the most recent life cycle impact model European Footprint 3.0.

Table 2: Impact categories included in the study

Impact	Unit
Climate change	kg CO_2 eq.
Resource use, fossils	MJ
Resource use, minerals and metals	kg Sb eq.
Particulate matter	Disease incidence
Photochemical ozone formation	kg NMVOC eq.
Ozone depletion	kg CFC-11 eq.

[5] Sensitivity analysis towards economic allocation factors and other allocation procedures are reported in the main study.

Ionising radiation	kBq U-235 eq.
Acidification	mol H^+ eq.
Eutrophication, freshwater	kg P eq.
Eutrophication, marine	kg N eq.
Eutrophication, terrestrial	mol N eq.
Land use	Pt
Water use	m^3 deprivation
Human toxicity, non-cancer[6]	CTUh
Human toxicity, cancer[6]	CTUh
Ecotoxicity, freshwater[6]	CTUe

Carbon storage in plant-based feedstock

One of the inherent advantages of PEF-based products is that they are produced from renewable feedstocks, such as wheat. Since PEF is a 100% plant-based polymer, its production removes CO_2 during feedstock growth. This biogenic carbon is temporarily stored in the plant-based product. At the product's end of life (i.e. when it can no longer be recycled and PEF gets incinerated), the carbon re-enters the natural carbon cycle, thereby closing the carbon cycle.

In this cradle-to-grave LCA, further credits associated with temporary carbon storage or delayed emissions (e.g. through recycling) were not considered.

5. Life Cycle Impact Assessment

Contribution analysis

The potential environmental impacts associated with the 250 mL monolayer PEF bottle and the contribution of the different process stages along the value chain to each impact category are shown in Figure 4.

The LCA found that most of the impacts arise from upstream and downstream processes outside the core YXY Technology. Indeed, in many of the evaluated categories, the feedstock supply becomes an important environmental hotspot. In effect, application of fertilizers and pesticides during agricultural activities, such as wheat and sugarcane cultivation, contribute significantly to many assessed indicators and in particular to acidification, eutrophication, and land and water use potentials.

In the case of climate change and resource use of fossils – categories with high political and societal relevance – the source of impact is well distributed along the PEF bottles value chain – the fructose supply, FDCA production, and the bottle

[6] The characterisation models for these impact categories are considered as not sufficiently robust to be included in external communications according to ILCD levels (EC-JRC 2019:Environmental Footprint version 3.0. Impact assessment method of the European Environmental Footprint).

manufacturing process. The polymerisation step has a minor contribution. The use of minerals and metals is mostly attributed to this step.

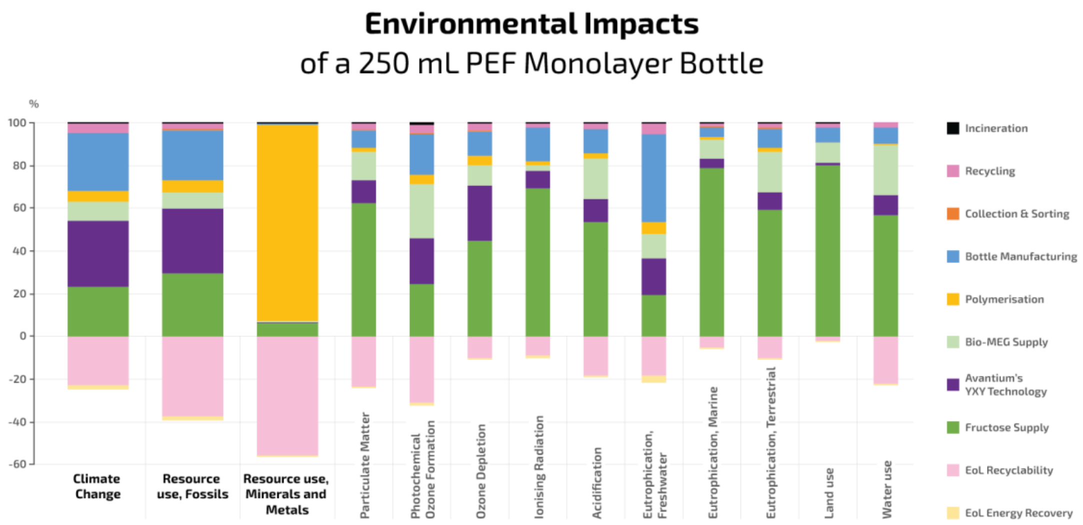

Figure 4: Potential environmental impacts of a 250 mL PEF bottle with contribution analysis

Identification of most relevant impact categories

LCAs generate a broad range of results – different products, scenarios, and figures. The many impact categories lead to a variety of different figures with units that are not intuitively understood by most readers. Normalisation and weighting steps in LCA can help put absolute figures into context and allow the results of different impact categories to be compared in order to assess their relative importance. In this respect, Table 3 shows the most relevant impact categories associated with the 250 mL monolayer PEF bottles obtained after applying the normalisation and weighting factors recommended in the Environmental Footprint 3.0 assessment method.

The most relevant impact categories were found to be predominately the climate change and resource use (mineral and metals and fossils) potentials, which are some of the most relevant impact categories in the current political agenda. On the other hand, typical impact categories linked to agricultural activities (e.g. land and water use) were found to be significantly less relevant and showed a minor contribution to the total environmental impact of PEF bottles.

Table 3: Relevance of impact categories based on normalised and weighted results

Impact	Relevance (%)
Resource use, mineral and metals	40.3

Climate change	15.2
Ecotoxicity, freshwater[7]	11.5
Resource use, fossil	11.0
All other 12 impact categories[8]	22.0

Comparative analysis

The characterised, investigated potential impacts are reported in Table 4 for both 250 mL PEF and PET multilayer bottles. All investigated impacts are mid-point indicators that focus on single environmental issues and are shown without normalisation or weighting.

The comparative analysis after normalisation and weighting is further depicted in Figure 4.

able 4: Impacts of 250 mL monolayer PEF and PET bottles (characterisation)

Impact	PEF bottle	PET bottle	Unit
Climate change	6.2E-02	9.3E-02	kg CO_2 eq.
Resource use, fossils	7.3E-01	1.3E+00	MJ
Resource use, minerals and metals	2.0E-06	3.8E-06	kg Sb eq.
Particulate matter	2.0E-09	1.4E-09	Disease incidence
Photochemical ozone formation	1.2E-04	1.6E-04	kg NMVOC eq.
Ozone depletion	8.7E-09	4.0E-09	kg CFC-11 eq.
Ionising radiation	1.1E-02	4.4E-03	kBq U-235 eq.
Acidification	3.4E-04	2.0E-04	mol H^+ eq.
Eutrophication, freshwater	1.9E-05	2.2E-05	kg P eq.
Eutrophication, marine	2.6E-04	5.5E-05	kg N eq.
Eutrophication, terrestrial	1.3E-03	5.2E-04	mol N eq.
Land use	1.8E+00	2.6E-01	Pt
Water use	3.1E-02	2.1E-02	m^3 deprivation

[7] Characterization model considered as not sufficiently robust to be included in external communications
[8] Individual categories not exceeding the threshed of 5% contribution to the total environmental impact.

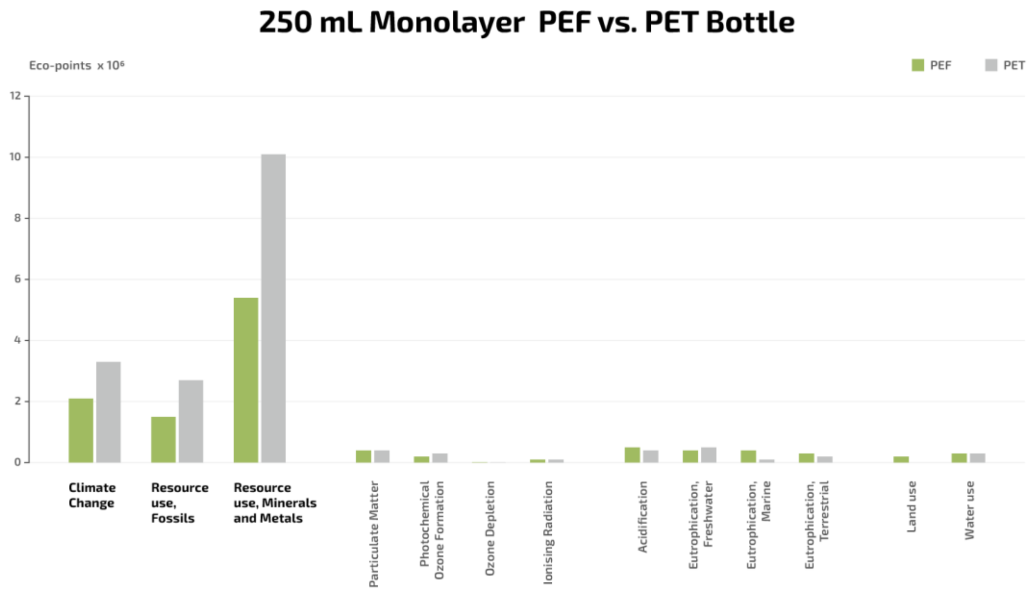

Figure 5: Comparative analysis between a 250 mL PEF and PET bottle

The following conclusions are highlighted from the comparative analysis:

- The use of 100% renewable carbon in PEF instead of fossil carbon in PET for producing 250 mL bottles would result in significant reductions in greenhouse gas emissions (-33%) over the life cycle of the bottles.
- PEF bottles would also contribute to remarkably less finite resource consumption of fossil fuels (-45%) compared to that demanded by PET bottles, due to the mechanical properties of PEF enabling light-weighting.
- These impact potentials are two of the most relevant environmental impact categories in the current political agenda as it is driving the transition from fossil to renewable carbon. This represents a significant benefit because climate change and resource use were found to be the impact categories most heavily influencing the environmental impact of monolayer PEF bottles (see Table 3).
- Significantly, production of PEF reduces the pressure on abiotic resources (minerals and metals) in contrast to PET bottles production.
- The lower environmental footprint of the bio-based alternative can be attributed, to a great extent, to the improved barrier and mechanical properties of PEF, allowing for a substantial reduction of polymer usage in the manufacture of bottles.

- This is also combined with the biogenic nature of the emissions (from renewable carbon) that the bio-based bottle would release upon incineration, which do not contribute additionally to climate change potential.
- The other evaluated impacts were found to be significantly less relevant and contribute to a minor extent to the total environmental impact of PEF bottles.
- Among them, benefits in favour of the PEF bottle was observed in the emission of volatile organic compounds associated with summer smog formation and in the potential of increasing freshwater eutrophication (the process by which an entire body of water, or parts of it, becomes progressively enriched with minerals and nutrients).
- On the contrary, PEF-based bottles would perform worse than the fossil-based PET counterpart in other impact categories mostly linked to agricultural activities (i.e. acidification, terrestrial eutrophication, and land and water use). However, these impact categories were identified to have a minor relevance within the total environmental footprint. These results reflect the fact that the systems compared in this study are based on value chains of vastly different natures (bio vs. fossil-based) which involve different exchanges with the environment.

Multilayer systems

In addition to monolayer PEF bottles, Avantium's PEF is particularly suited for multilayer packaging solutions. Multilayer bottles are a valid alternative when the required shelf life cannot be guaranteed by monolayer packaging alone. Currently, many multilayer PET bottles include polyamides (PA) such as MXD6 to improve their barrier performance. However, a common issue for incumbent barrier materials such as PA is their poor compatibility with PET, making it essential to sort out the PA from the PET in the recycling stream, also resulting in completely taking out multilayer containers by some recyclers to reduce the risk of contamination and rPET performance loss. PEF can be an alternative to barrier materials like polyamides, as PEF offers a good passive barrier for O_2 and CO_2 while not harming the performance of the resulting rPET products at relatively high PEF levels, making the recycling of these multilayer bottles much less dependent on sorting errors. In this respect, PEF could potentially contribute towards reducing the environmental footprint of packaging solutions by increasing the shelf life of products, enabling a reduction in the weight of packaging that is used, and by improving recyclability.

In this LCA, 250 mL PET/PEF multilayer bottles with 10% of PEF were also assessed and compared to reference PET/PA bottles with a typical 7% of PA. The analysis showed that significant reductions of around 37% in GHG emissions could be achieved by replacing the PA layer with PEF, mainly attributed to the recyclability of the PET/PEF system over the non-recyclability of the PA containing system. This replacement would also contribute to a significant reduction of finite resources demand (36% and 52% for fossils and minerals and metals respectively).

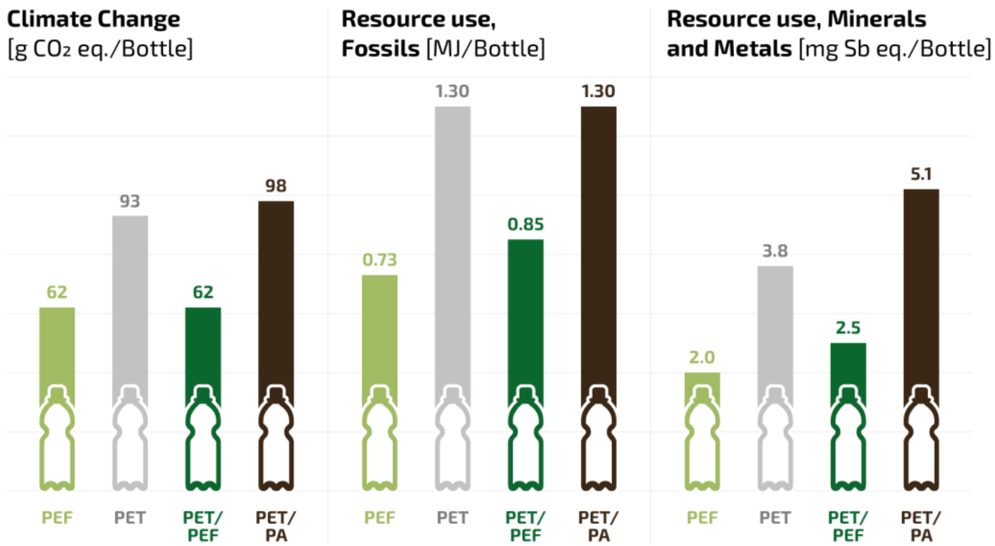

Figure 6: Environmental impacts of 250 mL monolayer and PET/PEF multilayer bottles vs their fossil counterparts

6. Outlook: future scenarios and optimisation possibilities

PEF is a relatively new material and not yet commercially available. PET is a mature product that has been on the market for over 40 years and is produced in a highly established process that runs close to maximum efficiency at a very large scale. It is expected that the commercialisation and growth of the PEF market will lead to substantial economic, technological, and environmental optimisations covering the full value chain. Recent energy optimisation work for an FDCA plant at industrial scale has already shown that energy consumption can significantly be reduced resulting in a further improved LCA. Furthermore, in this LCA, the current energy mix of the Netherlands, which still contains a low percentage of renewable energy, was used. It is foreseen though that in the near future the use of both renewable heat and electricity will become the norm. Considering the fact that the vast majority of GHG emissions in this current version of the LCA of PEF originates from non-renewable power and heat usage in the process (production of FDCA, bottle manufacture, and recycling), this foreseen change will have a very significant effect on the actual impact on the long run. It was assumed that PEF will initially end up in an open-loop recycling stream with relatively low recycling rates. Sufficient growth of the market will enable an individual material recycling stream (close-loop recycling with high efficiencies). Moreover, the PEF process will become much more efficient, both in energy integration and in achieved yields. Therefore, as the PEF technology continues to mature, substantial GHG and other environmental benefits will be achieved when those factors mentioned have come to fruition. In addition, there are various other areas for improvement that may be implemented by Avantium and/or its partners within the PEF upstream or downstream value chains.

Starting with feedstock production, the application of fertilisers and pesticides during wheat and sugarcane cultivation contributes significantly to the impact categories associated with the air- and waterborne release of nitrates, phosphates, nitrogen oxides, and metals above others. As part of Avantium's Sustainability Plan Chain Reaction 2030, Avantium has set the target that by 2030, 100% of the plant-based feedstock used for PEF will come from sustainable sources. In the near future, Avantium will define sustainability standards for the plant-based feedstock and will only work with suppliers to ensure that the used feedstock meets Avantium's sustainability standards. Moreover, the sustainability standards will be incorporated into the licensing agreements for the YXY® Technology.

The impact originated by the plant-based feedstock could be further reduced by a switch to lignocellulosic feedstocks such as originating from second generation biomass. This will be tested at Avantium Renewable Polymers in the framework of the BBI-JU PEFerence project, and should confirm that the YXY® process can use second generation biomass when it becomes available at commercial volumes and pricing.

An update of this LCA is expected once the Flagship Plant in Delfzijl (the Netherlands) is established and fully operational. By then, the opportunities for improvement that influence the LCA results will be better dimensioned and/or implemented into the Flagship Plant design. These might include aspects like better internal integration of heat and power, internal process recycling of secondary raw materials and other process intensification options. In addition, in the framework of the PEFerence project other potential PEF-based applications will be proven and the potential valorisation of side streams (e.g. humins) will be explored.