CASE STUDY ON DETERGENT BOTTLES

An example of weighing sustainability criteria for rigid plastic non-food packaging

A Chemicals Perspective on Designing with Sustainable Plastics: Goals, Considerations and Trade-offs

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Foreword

This case study was developed to provide input to and inform the development of guidance on General Considerations for Design of Sustainable Plastics from a Chemical Perspective. Four case studies were developed as concrete examples to inform these considerations. Two in the plastic packaging sector: biscuit wrapping and detergent bottles; two in the construction sector: flooring and insulation. For this purpose, the case studies start from the premise that plastic material will be used and therefore alternative material selection is not considered. They focus on environmental sustainability aspects related to chemical selection, taking into account health protection across the product life cycle. They do not address cost, performance, and chemical/material availability information, which would need to be considered in an application scenario. They also do not consider a discussion of social and environmental justice impacts.

The examples of material selection within the case studies are developed in the context of the information gathered for the case studies to exemplify the sustainable design process and to highlight key considerations. To make actual decisions about material selection other factors would also need to be considered (as outlined above) and the analysis could be further informed by elements such as life cycle assessment comparing alternatives and a full review of regulatory restrictions.

This document is based on a draft report developed by Partners for Innovation for this project and was reviewed by an OECD expert group supporting this project, which also provided a number of inputs. It was further reviewed by the OECD Working Parties on Risk Management and on Resource Productivity and Waste. Additionally the report was discussed at an OECD workshop on developing the general considerations for design of sustainable plastics from a chemical perspective held in March 2021.

This report is published under the responsibility of the OECD Chemicals and Biotechnology Committee in collaboration with the OECD Environmental Policy Committee.

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List of Acronyms

bioPE	PE made from bio-based feedstock
BPA	Bisphenol A
Cd	Cadmium
ClVOCs	Chlorinated VOCs
CMR	Carcinogenic, mutagenic or toxic to reproduction
Cr	Chromium
Cu	Copper
EBM	Extrusion blow moulding
EDC	Endocrine disrupting chemical
EoU	End-of-Use
ESCR	Environmental stress crack resistance
HDPE	High-density polyethylene
ISBM	Injection stretch blow moulding
IV	Intrinsic Viscosity
Ni	Nickel
NIAS	Non-intentionally added substances
NIR	Near-infra red: used for detecting plastic types in sorting installations
OVOCs	Oxygenated VOCs
PAHs	polycyclic aromatic hydrocarbon
Pb	Lead
PCR	Post-consumer recycled
PE	Polyethylene
PET	Polyethylene terephthalate
PO	Polyolefins
PP	Polypropylene
PVC	Polyvinyl chloride
PVdC	Polyvinylidene dichloride

Rhdpe	Recycled HDPE (High-density polyethylene)
rPET	Recycled PET (Polyethylene terephthalate)
rPP	Recycled PP (Polypropylene)
RSL	Restricted Substances List
SIN list	Substitute It Now List
SSP	Solid state polymerisation
TiOx	Titanium (di)oxide
UV	ultraviolet

Executive Summary

The OECD is conducting a project on the design of sustainable plastics from a chemical perspective, which aims to identify the key considerations regarding environmental sustainability and human health along the product life cycle that should be taken into account when chemicals are selected at the design stage, as well as the potential trade-off between these considerations. Case studies on particular sector/product combinations have been elaborated to inform the development of the general considerations.

In this case study sustainability considerations regarding the polymer selection and chemical composition for single use, rigid plastic bottles for packaging liquid detergent are identified. It builds on the 'Considerations and Criteria for Sustainable Plastics from a Chemicals Perspective' report published by the OECD in 2018 (OECD, 2018a). The case study shows how the principles from the report can be put into practice. An approach is offered for designers of plastic non-food bottles with examples of considerations and trade-offs in the specific case of detergent packaging.

A life cycle approach is used to address all sustainability considerations and demonstrate the complexity of making a profound sustainable chemical selection for plastic detergent bottles. At each stage in the life cycle different considerations regarding sustainability come into play, while decisions in one stage might also affect the impact at others. Considerations are divided in 'polymer considerations', which need to be taken into account to select the main polymer that makes up the bottle, and 'chemical considerations' regarding other chemical substances that might be incorporated in the plastic. In the approach used in this case study, a designer is provided with the information needed to make a preliminary selection for the polymer and to be aware of potential hazards from incorporated substances, so they can communicate with suppliers and make a final decision.

Polymer considerations

Detergent bottles are commonly made from HDPE, PP and PET, these polymers are evaluated in this case study. When selecting a polymer for detergent bottles the most important consideration revolves around closing the material loop of the bottle. Best practices show that bottles can be made with high percentages of recycled content. At end-of-use, these bottles can be collected, sorted and recycled for the production of new detergent bottles, resulting in bottle-to-bottle recycling.

Bottle-to-bottle recycling is most effectively realised for HDPE. For PP, the current general bottle-to-bottle recycling is difficult. However, by using advanced technologies such as the direct blow method, bottle-to-bottle recycling is possible for PP as well as for PE. For rPET bottle-to-bottle recycling competes with the quality and availability of food grade rPET, dependent on the local sorting and recycling infrastructure. When sourcing secondary feedstock, it must be verified that the supplying recycler adheres to all prescribed safety measures.

When designing for a specific detergent, a polymer should be selected which characteristics naturally provide the required (barrier) properties (e.g. UV barrier, resistance against solvents), so that unnecessary use of chemical additives can be avoided.

Collection and recycling rates for high value rigid plastics, such as HDPE and PET, is relatively high. To enable full recovery of the bottle material at end-of-use, a bottle designed for sorting and recycling is a prerequisite. Multiple design guidelines concerning labels, adhesives and closures should be incorporated in the bottle design. Additionally, unnecessary or excessive use of pigments should be prevented to maintain the quality of the plastic recycling streams.

Virgin or bio-based plastics can be used as a carrier of the masterbatch used in the production of bottles from recycled plastic, or to supplement the recycled content for mechanical properties. Bio-based feedstock sources from organic waste streams is the preferred feedstock for this.

Chemical considerations

In general, few chemical additives are used in detergent bottles as these increase costs of the packaging. However, the incorporation of a number of chemical substances in the bottle must be considered. Potential hazards from additives and non-intentionally added substances (NIAS) will in all cases remain a point of attention for the supplier, regardless of the chosen polymer. Therefore, potential hazards need to be investigated in conjunction with the supplier. Special attention should be paid to NIAS for secondary feedstock due to the increased risk of contamination and degradation products.

For packaging UV sensitive substances in PET bottles, a UV barrier is required, e.g. through addition of UV absorbers or blockers, or pigments. UV additives cause yellowing of the recycling stream and pigments result in a grey haze. Therefore, HDPE bottles for UV sensitive detergents are preferred.

To upgrade the rHDPE stream, addition of antioxidants, stabilisers and PP compatibilisers is advised. Carefully select these chemical additives to prevent migration into the detergent and hazards in the end-of-use phase.

It is advised to use as few pigments as possible to colour HDPE bottles. Prefer pigments that are embedded in the polymer matrix and prevent use of pigments associated with human health hazards.

Policy considerations

The life cycle approach has led to recommendations for further research and policy initiatives to address knowledge gaps and overcome systemic obstacles that inhibit sustainable use of detergent bottles.

The use of recycled plastics should be encouraged, for example by demanding a minimum recycled content or offering (positive) monetary incentives such as increasing taxes on virgin feedstock to prevent selection of cheap virgin polymers. Similar measures are required to encourage bottles designed for recycling, for example by reducing taxes for recyclable bottles. As such, a greater amount and a higher quality of recycled plastics will become available.

The use of potentially hazardous substances should be discouraged with bans or financial instruments. Some substances with known or suspected hazards are still used while alternative safe substances exist, because the alternatives are not commercially attractive. Additionally, full transparency on material composition throughout the value chain must be encouraged.

Where these are not already established, mandatory safety standards should be developed for plastic recyclers and waste incinerators based on available practices.

Chapter 1. Introduction

Global plastics production has reached 368 million metric tons and is expected to continue to grow by around 4% annually for the foreseeable future (PlasticEurope, 2020). While plastics deliver many benefits to society, there is an increasing awareness of the potential impact of chemical components of plastics on human health and the environment.

The Organisation for Economic Co-operation and Development (OECD) organised a Global Forum on Environment focused on "Plastics in a Circular Economy: Design of Sustainable Plastics from a Chemicals Perspective" in 2018. The Forum sought to incentivise a shift in sustainable chemistry thinking at the product design stage by identifying good practices, including tools and approaches, as well as a policy framework to reduce the environmental and health impacts of plastics. This resulted in multiple reports on the sustainability of plastics from a chemical perspective.

An outcome to the Global Forum was to work further to develop general considerations for sustainable design of plastics from a chemicals perspective. To help inform the development of the considerations, case studies were developed for particular sector/product combinations. This case study focuses on sustainability considerations at a chemical level for plastic design of detergent bottles. In this case study a life cycle approach is taken for the development of plastics for detergent bottles. Sustainability aspects regarding human health and the environment are considered, resulting in sustainability criteria that support decisions on sustainability for professionals throughout the value chain who are involved in the design of detergent bottles. This enables sustainable designs tailored to the specific life cycle scenario of a detergent bottle.

In the transition to sustainable packaging alternatives such as reusable or refillable packaging, solid detergents and powders have a very high potential to reduce the volume of single use plastic packaging. However, these alternatives are not globally available in high volumes and liquid detergents packed in single-use bottles are still the dominant trend in the market. Thus, efforts in making more sustainable detergent bottles are still highly relevant. Alternative packaging is acknowledged as important, as it offers sustainable product-packaging solutions for detergents, but is regarded as out of scope for this case study focused on detergent bottles.

1.1. Case Study Approach and Structure

1.1.1. Life cycle approach

The sustainability criteria are assessed for the life cycle stages through which a detergent bottle cycles: sourcing of the material, production and filling of the bottle, use of the bottle and detergent and end-of-use at which the bottle is discarded and processed. At each stage in the life cycle different considerations regarding sustainability come into play, and decisions in one stage might also affect the impact in other stages. From a designer's perspective, this journey will start with the use phase. The purpose of the product and the context in which it will be used determine the basic set of technical requirements and constraints for a shortlist of possible materials. Therefore, this case study will consider the use phase first, after which the sourcing of the feedstock, the production of the bottles and its end-of-use phase are discussed. This approach is not to be confused with a Life Cycle Assessment (LCA), a method to determine the overall environmental impact of a specific packaging (or product) throughout its life cycle, while the current study aims to identify and address environment and health considerations in each phase of the life cycle.

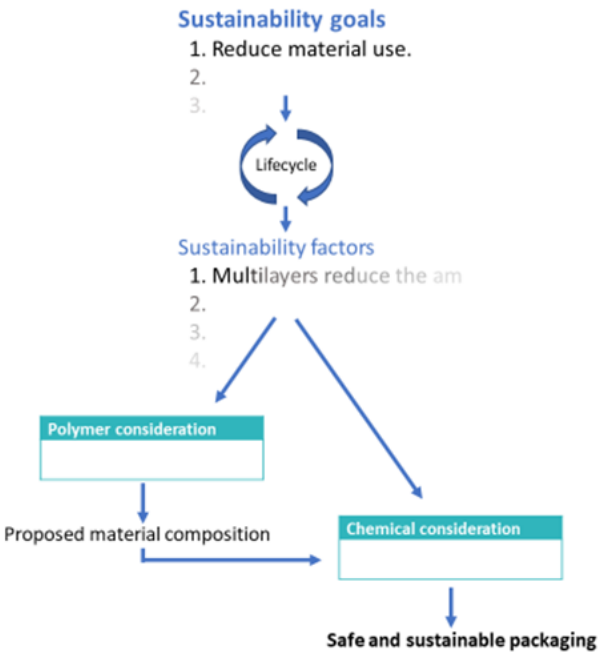
1.1.2. Case study structure

The subsequent chapters discuss the different life cycle stages. A general overview of the life cycle stage is provided in each chapter, describing the different processes and relevant factors that influence sustainability of the packaging. The relevant sustainability factors are identified by keeping a list of Sustainable Design Goals in mind while working through the life cycle stages.

Each sustainability factor leads to key considerations; a decision that needs to be made to select a polymer or a chemical in the production of plastic detergent bottles. Polymer considerations describe what must be taken into account when selecting a polymer. Chemical considerations describe the subsequent choices that must be made with regard to chemical additives used in the production of detergent bottles, once a polymer has been selected.

Once all aspects of the life cycle have been considered, an overview of the key considerations and trade-offs is provided in Chapter 7. Subsequently, the different sustainability criteria emerging from the life cycle stages will be simultaneously assessed in the Material Assessment in Chapter 8.

Figure 1.1. Overview of the approach taken in this case study



1.2. Scope

This case study investigates aspects of environmental sustainability and human health influenced by chemical selection for a rigid plastic packaging for liquid laundry detergents. In the development of a detergent bottle, other aspects related to e.g. financial or social aspects are relevant. However, these are beyond the scope of this case study.

A detergent bottle typically consists of the following elements:

- **Bottle**: Rigid plastic bottle. Some bottles include a handle for extra grip. Transparent bottles and a wide variety of colours can be found on the market.
- **Closure**: A cap or spray dispenser that seals the bottle and can support dosing of the product.
- **Label**: Bottles include labels that communicate necessary information to consumers and support marketing of the product. Usage of wrap sleeves and traditional labels is common.

Figure 1.2. Variation of (laundry) detergent bottles.

Note: Left to right: Representative depictions of HDPE bottle, recycled PET bottle (transparent), PP bottle
Source: © Shutterstock 2021

1.2.1. Scope: Focus on bottles

This case study focuses on rigid plastic detergent bottles. Typically, detergent bottles are made of HDPE, PP or PET. No alternative materials suitable for application in detergent bottles are currently available on the market. The closure and label are only considered when they influence the sustainability of the bottle, e.g. in recycling (Chapter 6). Closures and labels are not considered as separate entities in this case study and are therefore not investigated on a chemical level.

1.2.2. Case study relevance

Additionally, this case study will assess to what extent sustainability criteria from liquid laundry detergent bottles are relevant and applicable to other detergent bottles, such as all-purpose cleaners, shampoo and soap bottles.

1.2.3. Out of scope

The following types of detergent packaging are out of scope:

- **(Refill) packaging multilayer films**: In the detergent aisle, multilayer packaging films are increasingly seen as refill packaging or 'bag-in-box' packaging. In these multilayers different materials are laminated together into a film to obtain the preferred barrier properties. Subsequently, this film is used to produce a pouch. This type of packaging is out of scope as this case study is limited to rigid plastics.
- **Packaging of alternative detergents**: A recent development in the market has been an influx in alternative detergents, such as solid detergents and powders. These products do not necessarily require a bottle for packaging and are therefore regarded as out of scope for this case study.

However, it is worth noting that alternative detergents can play a significant role in offering a more sustainable product-packaging combination.

- **Reusable and refillable packaging**: An influx of reusable and refillable packaging has been seen. However, this case study focuses on single-use packaging, as this is still the dominant packaging in the market. Reusable packaging can play a significant role in offering a more sustainable product-packaging combination.

1.2.4. Packaging requirements

The over-arching requirements set to laundry detergent bottles are:

- Display the detergent at the point of sale in an attractive way;
- Display information about the ingredients and the manufacturer of the detergent;
- Maintain the operational effect of the detergent;
- Make the detergent easy to stack in transport and storage;
- Protect the detergent from leaking during transportation and storage.

1.3. Notable regulations for this case study

Multiple national and international authorities have their own lists of substances that are prohibited or are limited in use for plastics. When performing polymer and chemical selection, local regulations must be adhered to. For an overview of a subset of these regulations please refer to the OECD (2021) publication Guidance on Key Considerations for the Identification and Selection of Safer Chemical Alternatives, Exhibit 5 and to the Regulations and Restrictions page of the OECD Substitution and Alternatives Assessment Toolbox (OECD, 2020). To provide insight in the scope and objectives of such regulations the REACH and CLP regulations of the European Union are briefly described below.

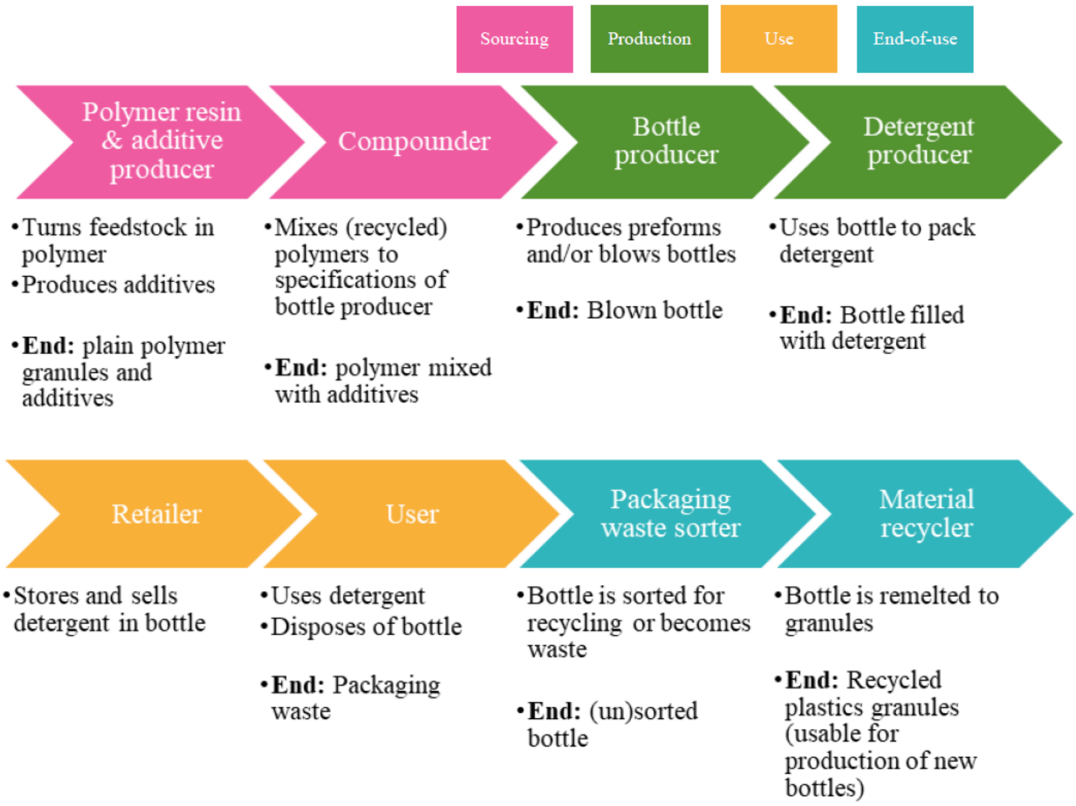
1.3.1. EU: REACH and CLP Regulation

Regulation (EC) No 1907/2006 concerning Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) and Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures (CLP), are regulations in place in Europe to control the health and environmental risks of chemicals. REACH establishes procedures for collecting information provided by industry on the properties and hazards of substances, their uses and exposure potential for human health and the environment, and eventually adopting regulatory measures to control their risks. Whenever a substance poses an unacceptable risk to human health or the environment, restrictions can be adopted to limit or ban the manufacture, placing on the market or use of a substance. For substances of very high concern, as defined in REACH, the use can be subject to authorisation. Currently polymers are not included in REACH.

1.4. Life cycle overview

This section provides a global overview of the life cycle of a detergent bottle. The different stakeholders in the bottle life cycle are visualised in Figure 1.3, indicating their primary activity and end product. Subsequently Table 1.1 provides an overview of the important factors influencing the sustainability of the detergent bottle for each life cycle stage.

Figure 1.3. Visual overview of the life cycle of a detergent bottle.



Note: It is possible that the bottle is not recycled, but incinerated or landfilled.

Table 1.1. Overview of life cycle stages

	Sourcing of Materials	Production	Use phase	End-of-Use
	Production of polymer resin	Production, filling, labelling and closing of detergent bottle	Transportation to user, preservation and dosing of detergent	Disposal, sorting and recycling of detergent bottle
Important sustainability factors	- Polymer options for packaging - Polymer feedstock - Residual substances from polymerisation - Additives used in plastic production	- Production methods - Additives required in production of packaging - Additional chemicals used in production (non-ingredients) - Safety of workers	- Requirements for use (and transport) - Migration of substances into detergent - Waste and pollution generated during product use	- End-of-use scenarios - Recyclability of design - Recyclability of polymers - Recyclability of additives - Safety of workers

Chapter 2. Methodology

2.1. Sustainable design goals

To guide the material and chemical selection, over-arching sustainability goals need to be set. Using secondary feedstock for the production of bottles contributes to closing the material loop, but might require the use of more material and additives. A chemical additive might increase efficiency in the production of the packaging and thus reduce the overall CO_2 emissions in the process, but it could hinder the recycling of the material at the end-of-use. Establishing over-arching sustainability goals from the outset will enable the designer to ensure these kinds of benefits and drawbacks are taken into account when examining material alternatives. Furthermore, the goals will guide the designer in the selection of materials when trade-offs need to be made. The following five sustainable design goals are adopted for the case study of a detergent bottle. Examples of other goals are provided at the end of the section.

1. **Prevent product spoilage**

   The packaging serves to protect the product. Usually the (environmental) impact of the production of the product is higher than that of the packaging's total life cycle. Preventing spoilage of the product before it reaches its intended goal is an important goal in the sustainable design of the packaging.

2. **Reduce material use**

   Packaging is a short-lived product, but amounts to 40% of the world's total use of plastic (PlasticsEurope, 2019). Designers should strive to reduce the use of plastic to the absolute minimum to meet the packaging requirements.

3. **Close material loops**

   Due to the short-lived use of packaging, the used material should be recycled to enable closing the loop. The packaging should be made from secondary feedstock or be recyclable into another product. In an ideal situation a combination of both is made.

4. **Preserve natural capital**

   Humans depend on natural capital for a wide range of ecosystem services. Poorly managed natural capital can destroy productivity and resilience, making it difficult for humans and other species to sustain themselves. Throughout its life cycle the negative effects of the packaging on natural capital should be limited. This includes the chosen feedstock, but also includes effects of production and waste management at the end of life.

5. **Safeguard the health of participants in life cycle**

   From feedstock extraction, through packaging manufacturing and product use, to the eventual end-of-use scenario, the packaging and its subcomponents will interact with humans. The direct negative effects of the packaging and its subcomponents on the health of these people needs to be minimised. The focus with regard to health in this case study will be in three phases of the life cycle:

i. The first is residential human health exposure: hazards for consumers in the use phase through migration of substances into food products or through skin contact with the packaging;

ii. The second is occupational human health exposure during waste management at end-of-use: the hazards for recycling facility employees who get into contact with the chemical substances during treatment of the packaging waste.

iii. The third are hazards for the general population when chemicals enter the environment due to emissions from production and waste treatment.

This focus is applied because it is assumed that the health risks at the plastic producing plants, film manufacturers and product packaging facilities are known and adequate precautions are taken, and that this is not the case for individual consumers, waste management employees and the general public.

2.1.1. Examples of other sustainable design goals

The five goals listed above are selected for this case study. When working on a different packaging or product, other sustainable design goals might come into play, such as:

- Minimise waste
- Improve social conditions throughout the life cycle
- Decouple from fossil resources

2.2. Chemical selection process

During the design process the listed five sustainable design goals must be considered to select the most sustainable plastic(s) to be used in the packaging. During the analysis of the life cycle, it will become apparent that trade-offs must be made. The selection of one material based on one sustainable design goal in one phase of the life cycle can counteract the realisation of another goal in another part of the life cycle. In addition to the selection of the most sustainable polymer for the packaging, the use of chemicals in the production of the polymer and the packaging and their consequences in later stages of the life cycle must be considered.

To select a polymer or a combination of polymers from a list of options, the most important considerations and trade-offs need to be identified. It is not practicable to consider all possible chemical substances and their potential hazards for all the polymers simultaneously. The following selection process is therefore used in this case study and is proposed as a method for safe chemical selection.

1. Based on the over-arching sustainable design goals, identify the sustainability considerations for the packaging throughout the life cycle.
2. List and weigh the sustainability considerations; some will be regarded as key considerations while others have a minor impact on the overall sustainability of the packaging.
3. Collect data on the optional polymers for the plastic bottle.
4. Compare the polymers based on the identified key considerations.
5. Select the polymer that is identified as the best fit (i.e. having minimal or no impact on human health while maintaining the highest level of environmental sustainability) for the detergent packaging.

Subsequently, for the selected polymer only, the relevant chemical considerations should be taken into account. Additives, residual production chemicals, and potential non-intentionally added substances (NIAS) must be investigated on their consequences for environmental sustainability and human health.

6. Demand from all your suppliers that they comply with all applicable regulations.
7. Select a list of hazardous substances or substances of concern to review your packaging with. The selection of the list can depend on the product, previous experience within the design team, or be mandated by company standards. The sources for this list will be discussed in the next section.
8. Check, in collaboration with your material supplier if necessary, whether the found chemical considerations involve any of the substances on the selected list with hazardous substances.
9. If substances on the list are part of a chemical consideration, reconsider the need for using this substance and try to find an alternative substance for the intended goal. Some lists provide overviews of alternative substances. Safe alternatives can be found with the help of ‘positive lists’ such as the Safer Chemical Ingredients List (US Environmental Protection Agency, 2020). For guidance on the selection of alternatives, please refer to OECD (2021).
10. If step 8 cannot be passed, revisit step 5 and select another polymer or polymer combination.
11. If no polymer can be selected without the incorporation of hazardous chemicals, as identified on the list of hazardous substances: Innovate.
    a) Re-evaluate the functional requirements of the packaging (discussed in this case study in Section 3.1): do these enforce unsustainable decisions?
    b) Re-evaluate the shortlist of polymers: is innovation on a material level required?
    c) Re-evaluate the product-packaging combination, can another form of packaging be chosen? This might lead to reusable packaging, packaging-free concepts, or non-plastic materials.

2.2.1. Lists to support the chemical selection process

Hazardous substances or substances of concern can be identified with the aid of a lists of substances. Examples of these lists are the ‘Proposition 65 list’ from the State of California (OEHHA, 2021), the Substitute It Now (SIN) list developed by non-profit organisation ChemSec (ChemSec, 2021) and the Restricted Substances List (RSL) of the Cradle-to-Cradle Products Innovation Institute (Cradle-to-Cradle Products Innovation Institute, 2021).

The Californian list contains substances with known reproductive toxicity or carcinogenic properties. The SIN list consists of chemicals that have been identified by the NGO ChemSec as being Substances of Very High Concern. The SIN list provides information on REACH status, use and function, concerns, production and available alternatives for each chemical. The Restricted Substances List (RSL) is a checklist for materials that are not allowed to be used in Cradle to Cradle certified products. This is a certification for sustainable products and certifies them as safe, responsible, and fit for a circular economy. These lists differ in hazards that are included, how restrictive they are, and whether alternatives are suggested. Besides these three examples, other lists can be used. More lists with hazardous substances are discussed in in the publication *Guidance on Key Considerations for the Identification and Selection of Safer Chemical Alternatives* (OECD, 2021), in the ECHA (2019) publication ‘*Substances of concern: Why and how to substitute?*’, and in the OECD Substitution and Alternatives Assessment Toolbox (OECD, 2020).

Chapter 3. Use phase

In the use phase, the packaging is used for its intended goal: safely transporting the detergent from the producer to the consumer, attracting attention of consumers in shops, providing information to the consumer, preserving the liquid and support its dosing. First, Section 3.1 will elaborate on the functional requirements of a detergent bottle during use. Subsequently, the polymers HDPE, PP and PET are evaluated on the barrier properties required for preserving detergents (Section 3.2) and chemical resistance required for packaging detergents (Section 3.3). Subsequently, additive substances to enhance these properties are discussed.

The use phase touches upon three of the over-arching sustainability goals:

- **Prevent product spoilage**: Preservation of the detergent during transport and use (including shelf life) are essential in preventing detergent from being spoiled or wasted.
- **Safeguard the safety of consumers**: When consumers use the packaging, e.g. when dosing detergent, they should not be exposed to hazardous substances that might be present in the packaging.
- **Preserve natural capital**: Detergents end up in the wastewater system. When substances leach from the packaging material into the detergent, these will end up in the wastewater system and can potentially pose a hazard to the (aquatic) environment and its flora and fauna. Also, users coming into contact with detergents (e.g. while washing clothes) must not be exposed to hazardous substances. Lastly, bottle design influences the amount of transport movements required and associated emissions.

3.1. Functional requirements and bottle design

3.1.1. Transport the detergent to the consumer

Strength and stiffness: One of the primary functions of a detergent bottle is to contain the liquid detergent and transport it safely from the production site to the retailer, then finally to the consumer. A bottle must thus provide sufficient strength and stiffness for transportation. This should be considered in developing a bottle design and selecting a polymer.

An aspect that influences the strength of detergent bottles is the potential reaction between the detergent and the polymer. Detergents contain surfactants[1] which can react with the polymer, causing the bottle to crack. In the past, reactions have partly been prevented by adding more water to detergents formula or developing polymers with an improved environmental stress crack resistance (ESCR). The development of materials with an improved ESCR has led to a trend towards more concentrated products currently seen in the market. ESCR is further addressed in Section 3.3.

3.1.2. Preserve the detergent

Preservation of the detergent is essential. The environmental impact caused by production of the detergent is greater than that caused by the packaging, and thus the primary goal of the packaging is to prevent spoilage of the detergent. A detergent typically has a shelf life of two years. To guarantee this shelf life, the detergent packaging must provide the right barrier properties. For preserving detergents moisture, gas and UV barriers are relevant. Barrier properties of polymers and additives are further explored in Section 3.2.

3.1.3. Use of the detergent bottle

Handles on bottles: For usability purposes, a detergent bottle can include a handle, providing for easier handling and dosing by the consumer. As a rule of thumb, according to the brand owners interviewed, bottles with a volume larger than 2 litres require a handle for usability and dosing. However, at retailers, handles have been found on 1-litre and 1.5-litre bottles. The addition of a handle to the bottle has consequences for the production method of the bottle and therefore influences polymer and chemical selection. See Section 5.1 for further information on production methods.

Box 1. Design considerations

Optimise bottle design for efficient transportation and thus preserve natural capital. This means excessive curves, headspace and 'shoulders' should be avoided. Additionally, it is recommended to only use a handle for bottles with a volume of 2 litres or more.

Box 2. Polymer considerations

Consider which barrier properties are required to preserve the detergent during its shelf life to prevent product spoilage.

3.1.4. Out-of-scope sustainability aspects in the use phase

The following aspects are important in relation to sustainability of the detergent-packaging combination, but are out of scope because they do not influence the chemical selection of polymers.

- **Efficient design**: Another aspect of transportation is the number of transport movements required to transport a certain volume of detergent liquid. When a bottle has a 'space efficient' design, CO2 emissions caused by transportation are minimised, thus preserving natural capital. Factors influencing space efficiency of the bottle are handles, headspace in the bottle, 'shoulders' on bottles, and curved shapes.
- **Dosing of the product**: Avoiding excessive use of detergent is one of the biggest improvements to be made in regard of sustainability. While the reduction of used product would account for the highest reduction of negative sustainability impacts, this would also reduce the impact of the packaging: when the volume of detergent used by the consumer is reduced, the use span of a detergent bottle is expanded, resulting in slower replacement of bottles and thus in a lower volume of plastics.

- **Concentration of detergent**: By increasing the concentration of the detergent, or using detergent powders, more detergent can be transported in a packaging and thus transport is reduced. This contributes to the design goal - preserve natural capital. Additionally, less packaging material is required to provide the same number of washes, thus contributing to the design goal - reduce material use.

3.2. Barrier properties

The required barrier properties for the detergent bottle depend on the composition of the detergent. Typically, moisture, gas and UV barriers are relevant fields for exploration when developing packaging for detergents. Table 3.1 provides an overview of the barrier properties of the different polymers.

3.2.1. Moisture barrier

Over a long period of time, water in the detergent can condensate and migrate through the bottle, causing the detergent to become less liquid or dry out. A moisture barrier is therefore required. Commonly used polymers for detergent bottles (PET2, HDPE and PP) already provide a moisture barrier. This ‘standard’ moisture barrier is more than sufficient to provide detergents with their typical shelf life of 2 years. Therefore, this topic is not further investigated.

3.2.2. Gas barrier

Some detergents contain hydrogen peroxide, which releases oxygen. To prevent build-up of pressure in the bottle, it is essential that the polymer can passively vent the oxygen. The polymer matrix of PET is relatively solid and provides a good gas barrier, which in this case is undesirable as the bottle can deform under the pressure that builds up. HDPE and PP are 30 times more permeable to gas than PET and thus passively vent the oxygen from the bottle (Reynolds, 2010).

3.2.3. UV barrier

The appearance, fragrance or colour of the detergent can change, or ingredients in the detergent might separate or break down when exposed to UV sources. This is especially undesirable when the detergent is packaged in transparent bottles, as this process will be visible to consumers. A UV barrier is therefore required for bottles containing UV-sensitive detergents.

Colour additives as a UV barrier

PET, HDPE and PP polymers are available as transparent material or in opaque colours. Opaque-coloured bottles filter the light and thus provide a UV barrier. The opaque quality of polymers is obtained by adding pigments (colour additives). Adding pigments to HDPE and PP is common practice. Sustainability aspects of these pigments are further addressed in Section 5.3 (production) and Section 6.4 (end-of-use). Adding pigments to PET should be avoided. Opaque PET cannot be fully separated from transparent PET in recycling. Opaque PET in the transparent PET stream will lead to a loss of brightness and transparency, thus reducing the quality, value and applicability of the stream. Additionally, opaque PET cannot be used at the same value but is cascaded to lower-value products such as strapping for palletising.

For transparent bottles, a printed full-body sleeve can provide a UV barrier. However, full-body sleeves might result in difficulties in sorting and recycling; this is further addressed in Section 6.2.

UV barrier in transparent PET bottles

Transparent PET has a very limited light barrier. If UV rays affect the detergent, a barrier needs to be added. This can be done by adding UV absorbers to the resin, which embeds the substance in the polymer matrix. An example of a UV absorber is Tinuvin 234. According to Begley et al. (2004), migration of Tinuvin 234 to the packaged substance is very small and not harmful to human health or the environment. Available information indicates that the usage of UV absorbers do not pose a risk to human health or have an impact on the environment.

From a recycling perspective, addition of UV light blockers is not desirable. It influences reprocessing of the material, and causes a yellowing (discolouration) of the rPET when it is extruded (Schloss, 2017). This then degrades the quality of the recycled material. It is not therefore recommended to add a UV-barrier to transparent PET bottles. When a detergent is sensitive to UV rays, it is recommended to select opaque HDPE or PP.

Table 3.1. Overview of barrier properties of different properties

Polymer	Appearance	Moisture Barrier	Gas barrier	UV-Barrier
HDPE	Translucent*		Passive venting of bottles	
	Opaque		Passive venting of bottles	
PP	Transparent		Passive venting of bottles	
	Opaque		Passive venting of bottles	
PET	Transparent	**	Impermeable	
	Opaque	**	Impermeable	

Note: * *Virgin or natural HDPE is not fully transparent, but partially so. It is therefore indicated here as translucent.*
*** The moisture barrier of PET is inferior to HDPE and PP, but is still adequate for packaging detergents.*
The colour coding is in relation to the barrier property (green: high barrier; red: low barrier) and not in relation to the material suitability.

Box 3. Polymer considerations

Consider which polymer offers the required barrier properties. By selecting a polymer that has the desired characteristics in its standard form, use of coatings and additives can be prevented. This reduces contamination of the polymer and thus promotes closing the material loop. For example, HDPE or PP polymers are to be given preference for UV sensitive detergents.

Box 4. Chemical considerations

When improving the barrier properties of polymers for detergent bottles using additives or coatings, consider the following aspects:

- When using additives or coatings, carefully consider how these behave in the bottle. If not embedded in the polymer matrix these can potentially migrate into the detergent.
- A UV barrier can improve the shelf life of a detergent. A UV barrier can be provided by adding pigments to detergent bottles. Use of pigments is preferred over chemical additives or coatings that provide a UV barrier.
- Use of UV absorbers and blockers in transparent PET is discouraged. When extruded in recycling, these cause yellowing of the material.
- It is recommended to avoid the use of colour additives in PET as this compromises the recyclability of the material.

3.3. Chemical resistance of polymers

The selected polymer for the detergent packaging must be compatible with the (chemical) ingredients of the formula. In laundry detergents, the presence of surfactants is most common. To broaden the relevance and scope of this case study, other chemicals present in (e.g. home care) detergents are also explored. Detergents can contain:

- **Surfactants**: Soaps contain surfactants, which react with polymers. This can lead to bottle cracking. A good environmental stress crack resistance (ESCR) is thus required in selected polymers; this is achieved by optimising the polymerisation process. See the section on ESCR for more details.
- **Solvents**: Used in more aggressive detergents. Highly reactive with most polymers, dependent on the aggressiveness of the solvent. PET is unsuitable for packaging solvents. HDPE can withstand mild solvents (e.g. acetone), but requires fluorination to contain more aggressive variants (e.g. hydrocarbon solvents and aromatic solvents). For packaging detergents, fluorination is not common and should be avoided.
- **Caustics**: Such as caustic soda. These are a very aggressive substances, which can be packaged in HDPE or PP but not in PET. Caustics are not found in laundry detergents, but can be relevant for packaging more aggressive home care detergents.
- **Acids**: These are very aggressive substances. Acids are not found in laundry detergents, but can be relevant for packaging more aggressive home care detergents.

Table 3.2 offers an overview of the chemical resistance of HDPE, PP and PET. HDPE has good chemical resistance against most chemicals and is the preferred polymer for packaging more aggressive detergents. Chemical resistance of polymers can be enhanced by optimising the polymer production process (polymerisation), or by structural enhancement of the bottle design (e.g. adding ribs), chemical treatment (e.g. fluorination of HDPE bottles) or a coating.

Table 3.2. Chemical resistance of different polymers

	Surfactants	Solvents	Caustics	Acids
HDPE		*Can withstand mild solvents*		
PP				
PET				

Note: The colour coding is in relation to the chemical resistance (green: resistant; red: low resistance)
Source: INEOS Olefins & Polymers USA, 2012; RoboWorld, n.d.

3.3.1. Environmental stress crack resistance (ESCR)

Good crack resistance of detergent bottles is essential, to facilitate transport, storage and usability. Stress can be caused by various external factors: e.g. top-load stress during transport, internal pressure or through a reaction with other substances. Detergents contain 'surfactants', which react with polymers and can cause a bottle to crack. ESCR is better in polymers with a high crystallinity – thus HDPE and PP perform worse than PET. For detergents, the following factors influence ESCR:

- **Polymer development**: ESCR resistance of HDPE and PE has drastically improved over the past decades through development of polymers and optimisation of the polymerisation process. Development of these polymers includes altering the catalysts to produce bi-modal HDPE, or by adding a co-monomer (propane) to improve the resin characteristics. This slightly increases the crystallinity of the polymers and thus improves ESCR. Sustainability aspects of the production of polymers are further elaborated upon in Section 4.4.
- **Concentration of detergent**: Highly concentrated detergents contain more surfactants and must therefore be packaged in a bottle made with a polymer with a high ESCR. Recycled plastics have reduced ESCR performance, and packing highly concentrated formulas in 100% PCR bottles is therefore challenging or unfeasible.
- **Bottle geometry**: ESCR can be improved by optimising the bottle geometry, e.g. by using a more organic shape and preventing hard edges.

3.3.2. Migration of substances into the detergent

Migration of the polymer or polymer additives from the packaging to the detergent should be avoided as it can potentially end up in the wastewater or come into contact with users. However, this migration is extremely unlikely. Use of additives is limited for detergent packaging. Additionally, these additives are embedded in the polymer matrix and will not move when evenly distributed because of their size (>1000 Dalton). If migration occurs, risks for natural capital and human health are limited, because detergents are strongly diluted with water resulting in a low number of parts per million (ppm) of the leaked substance. Migration is further elaborated upon in Section 4.4. Polymers are porous and detergent substances can migrate into the absorbing polymer matrix. The consequences of this are further explored in Section 4.3 on recycled feedstock.

3.3.3. Microplastics during use

During use, the detergent bottle is exposed to mechanical stress, caused for example by opening and closing the cap. This mechanical stress can cause degradation of the packaging and release of microplastics. Research on microplastics caused by opening and closing PET water bottles with HDPE caps shows that opening and closing the bottle 100 times results in significant shedding of microplastics (Winkler et al., 2019). This research showed a great difference in cap abrasion between bottles from different brands, which reveals a discrepancy in plastic behaviour. Also, degradation of HDPE appears to be stronger than degradation of PET. A detergent bottle is opened and closed repetitively during its use cycle, and shedding of microplastics can therefore be expected.

In the research by Winkler et al. (2019), a 'squeezing treatment' on PET bottles was also performed, exerting mechanical stress on the bottle wall. This treatment did not significantly increase the amount of microplastics found in the bottled water. Therefore, shedding of microplastics into the detergent due to squeezing is not regarded as likely.

Box 5. Polymer considerations

- Consider which polymer offers the chemical resistance for packaging the detergent. By selecting a polymer that 'naturally' has the desired characteristics, use of coatings and additives can be prevented. This reduces contamination of the polymer and thus promotes closing the material loop.
- Consider shedding of microplastics in the polymer selection. HDPE is expected to shed more microplastics during use compared to PET, but for both the released quantities are small. Also, the shedding can differ based on the polymer composition.

Box 6. Chemical considerations

When using additive substances or coatings on the bottle it is important to carefully consider if these migrate into the detergent. If additives are not embedded in the polymer matrix, migration can take place. If this scenario is likely, safety of the used substances or coating is essential.

Notes

[1] Surface-active-agents. Surfactants are molecules that spontaneously bond with each other to form sealed bubbles. Surfactants lower the surface tension between two liquids, between a liquid and a gas, or between liquids and solids.

[2] The moisture barrier of PET is inferior to that of HDPE and PP. When e.g. laundry detergent is packed in a PET bottle the liquid will dry quicker than when packed in HDPE or PP. A moisture barrier is commonly added in PET bottles for preservation of carbonated drinks. Barriers that are commonly used are for example silicon oxide plasma coating and carbon plasma coatings (European PET Bottle Platform, 2020). As these are not applied in detergent bottles these types of coatings are not investigated further.

Chapter 4. Sourcing of materials

At the stage of sourcing, the material different polymers and polymer feedstocks are considered. This chapter provides guidance in this process. First, Section 4.1 will elaborate on which factors must be considered when selecting a feedstock. Secondary (recycled), bio-based and primary (virgin) feedstock options are investigated. Once sustainability factors are identified, Section 4.2 will evaluate these feedstocks for application in detergent bottles, here a focus on closing the material loop is taken. Subsequently, Section 4.3 explores the chemical aspects of virgin resins; both residual substances from polymerisation and additives in production are considered. As this case study focuses specifically on recycled HDPE and recycled PET, these are further investigated in Section 4.4. Safety issues regarding recycled materials are discussed and additive substances used for improving the quality of the recycled material are evaluated.

The sourcing of materials phase touches upon three of the over-arching sustainability goals:

- **Close material loops**: The selected polymer feedstock is essential in closing material loops. Non-renewable feedstocks inhibit closing material loops, so renewable (recycled and bio-based) materials are preferred as circular options. Additionally, recyclability of the plastic is essential to realise bottle-to-bottle recycling.
- **Preserve natural** resources: The production of plastics might have hazardous emissions to the environment. Additionally, bio-based feedstock might cause deforestation or might be in competition with food supply.
- **Safeguard the health of participants in the life cycle**: In the production of virgin, recycled and bio-based plastics, hazardous substances might be emitted, for example in polymerisation or extrusion, or hazardous additives might be added in the process.

4.1. Feedstock considerations for detergent bottles

This section discusses the overall considerations when selecting a feedstock for detergent bottles. Depending on the polymer(s) chosen for the detergent bottle, there are three main sourcing routes: secondary feedstock, primary renewable resources, or primary non-renewable feedstock.

4.1.1. Secondary feedstock (recycled)

Secondary feedstock, or recycled plastics, can be derived from both renewable and non-renewable resources. The benefit of using secondary feedstock is that recovery of the materials after their primary use generally has a lower environmental and health impact compared to the production of virgin plastics. Using recycled plastics contributes to a circular economy. Additionally, the use of recycled plastic means that this material is not discarded as waste and the impact of incineration or disposal into landfill is prevented. The use of recycled plastic in a new product increases the demand for recycled plastics, which incentivises collection and recycling at end-of-use. Currently, use of recycled plastics in food applications is very limited and only food-grade rPET is widely available. To promote the use of recycled plastics, it is therefore important to apply it wherever food-grade is not required, such as in detergent bottles.

4.1.2. Renewable resources

A resource is considered renewable when the regeneration is able to keep up with the extraction and consumption of the material. Well known examples are fast growing crops such as corn, sugarcane, sugar beet, and wheat. Rapidly renewable resources are selected to decouple feedstock extraction from fossil resources and to preserve natural capital. Using fast growing crops will also reduce the emission of greenhouse gasses (in comparison with fossil-based resources) as the growth of the plants requires them to capture CO2 from the atmosphere. The carbon will be stored in the biomass, be converted to a plastic, and eventually will be released back into the atmosphere again as CO2 or CH4 (methane) when the plastic is incinerated or decomposes at end-of-use.

When selecting a renewable resource as feedstock for the plastic, several sustainability criteria should be considered: land-use change, food scarcity, and agricultural practices. When crops are grown to serve as feedstock for plastic production, arable land is needed. The feedstock is not considered sustainable when it requires the destruction of natural capital, e.g. deforestation of rainforests to gain arable land. The cultivation of crops for plastic production should not compete with food production in areas where arable land or water is scarce or crop yields are unstable. By-products or residues of food production can be selected as feedstock in these cases. Furthermore, if the cultivation of the feedstock heavily depends on fossil-based energy, through petrol for tractors and combines for instance, or on the use of fertilisers, use of hazardous substances such as pesticides, or large amounts of fresh water, the overall environmental impact of the feedstock might be higher than that of fossil-based alternatives.

Not all these factors can readily be taken into account in the selection of a polymer to produce a detergent bottle. When a polymer derived from a renewable resource (a “bioplastic”) is considered, potential suppliers and the origin of the feedstock should be checked on these criteria.

4.1.3. Primary non-renewable feedstock (virgin)

Intuitively, the fossil-based primary feedstock is regarded as the least sustainable. The extraction of the feedstock is polluting and requires the destruction of natural capital. The use of primary (or ‘virgin’) material means that the material cycles will not be fully closed, and continual extraction of the feedstock is needed. However, primary non-renewable feedstock might be required due to unavailability or incompatibility of materials derived from renewable or secondary feedstock. In this case a plastic must be selected that can readily be recycled and the bottle must be designed in a way that enables the highest possible recovery of the material in the existing recycling value chain. In this way, the plastic used in the bottle can be reused in another product, replacing the need for virgin plastics. A polymer from a primary non-renewable feedstock that cannot be readily recycled is an unsustainable material and should not be selected for use in short-lived packaging such as detergent bottles. Requirements for recyclability are discussed in Chapter 6, End-of-Use.

4.2. Feedstock options

Typically, detergent bottles are made of HDPE, PP or PET. Over the last years, it has been observed that PP is less frequently selected and a trend towards PET bottles for detergents can be seen. The latter can be explained by the low price of (virgin) PET and the trend of transparent bottles. In this case study, HDPE, PP and PET are considered, including their recycled and bio-based variants. The previous section laid out the different sustainability considerations for the different available feedstocks. This section will evaluate the different feedstocks for use in detergent bottles. Table 4.3 provides an overview of the different polymer types.

4.2.1. Secondary feedstock (recycled plastic)

Detergent bottles can be produced using recycled plastics. Examples using 100% recycled HDPE or 100% recycled PET are available on the market. It is also possible to combine virgin or bio-based feedstock with recycled feedstock. Some brand owners indicate their use of 50% recycled content sourced from packaging waste for the production of HDPE bottles. However, to maximise sustainability, it is advised to aim for the highest possible percentage of recycled content.

4.2.2. Bottle-to-bottle recycling of rPP requires advanced technology

Production of detergent bottles with recycled PP (rPP) needs advanced technology. Post-consumer rPP consists mostly of injection moulded or thermoformed plastic packaging (PlasticsEurope, 2019). These types of packaging are characterised by a high melt flow index (MFI). However, PP detergent bottles are produced using the extrusion blow moulding (EBM) production technique for which a low MFI is required. rPP is characterised by a high MFI because it is sourced from post-consumer plastics which typically consists of injection moulded or thermoformed plastic packaging. rPP with a low MFI is difficult to source, but availability might improve over time. However, at present, it is difficult to manufacture detergent bottles using rPP with common technology; it requires advanced technology.

4.2.3. Feedstock and availability

Recycled HDPE and PP can be sourced from post-consumer plastic packaging waste. Transparent rPET is sourced from recycled deposit bottles, which is a food-grade source. Using non-food-grade transparent flakes is technically possible for production of the bottles, but supply of these is scarce. When sorting of post-consumer waste improves, supply of non-food rPET might increase; see Section 6.2 for further reflection. Using food-grade rPET for a non-food application means that it is removed from a closed (food-grade) material loop and inhibits future reuse cycles of the material in food-grade applications. rPET is in high demand for food packaging, thus its use for the production of detergent bottles must be carefully considered.

4.2.4. Environmental benefit

CO2 emissions from recycled plastics are generally lower than the emissions caused by virgin plastics (EcoInvent, 2018). Emissions caused by production of virgin polymers are avoided and in general, the emissions caused by plastic recycling are lower. To determine the exact environmental benefit for a detergent bottle, a life cycle assessment (LCA) should be conducted. The impact depends on the specific situation, such as the recycling process, polymer and energy required for the process. According to the EcoInvent database (2018) rHDPE has the lowest footprint with 1,36 CO2/kg compared to 2,11 CO2/kg for rPET. The difference per bottle is expected to be lower, because for the production of PET bottles often less material is required than packaging a similar volume with HDPE.

Table 4.1. Overview of recycled plastics relevant to detergent bottles

Recycled plastic	Common feedstock	Availability	Suitability for bottle production
rPET food grade	Food grade recycled deposit bottles	Commercial scale, in high demand	
rPET non-food grade		Scarce*	
rHDPE	PCR packaging waste	Commercial scale	
rPP	PCR packaging waste	Commercial scale	MFI is too high for EBM

Note: *Availability might improve in the future when sorting installations differentiate between food grade and non-food grade material. See Section 6.2 for more information.
The colour coding is in relation to the adequacy of the attribute (green: adequate; red: inadequate)

4.2.5. Renewable feedstock

Renewable feedstock can be used to complement the use of recycled plastics, when 100% recycled content is not technically feasible. Additionally, renewable feedstock can be used as a carrier in the masterbatch, or the production of closures and labels. Bio-based alternatives are available for PE, PP and PET. However, BioPP is not available at a commercial scale, for HDPE and PET bio-based feedstock is widely available. Table 4.2 provides an overview of these bio-based polymers.

In addition to bio-based polymers with identical functionalities as their fossil counterparts, there are also bio-based biodegradable polymers available, such as PLA or PHA. Under the right circumstances these polymers biodegrade and thus the resources are returned to the earth. However, in practice these biodegradable plastics are often not composted but incinerated, e.g. because most industrial composting installation have a shorter cycle time than required for the full degradation of these plastics. Additionally, it is technically problematic to package detergents in biodegradable plastics. Subsequently, this type of polymer is unsuitable for this case study.

Table 4.2. Overview of bio-based polymers

Polymer	Common feedstock	Availability	Remarks
BioPE	Sugar cane	Commercial scale	Check for competition with food production
BioPP	Waste cooking oils and palm oil	Scarce	Scarce at time of writing, availability is rapidly increasing
BioPET		Commercial scale	Usually a blend with ± 40% bio-based content

Source: Based on Siracusa & Blanco, 2020

4.2.6. Primary non-renewable feedstock

Fossil fuels are not considered to be a sustainable feedstock for the production of detergent bottles. This feedstock is non-renewable and does not contribute to closing the material loop for detergent bottles. Since application of recycled plastic is technically feasible, using primary feedstock in detergent bottles is discouraged.

However, small volumes of virgin polymers may be required, for example as a carrier in the masterbatch and for the production of closures and labels. Additionally, primary feedstock can be used if the technical specifications required for packaging more aggressive detergents cannot be fulfilled using recycled or bio-based polymers. Bio-based polymers should be preferred as much as possible for these purposes.

Table 4.3. Overview of polymers, their renewability and impact on CO_2 Production

Material	Renewability of feedstock	Renewability of material	Impact production CO_2/kg[1]
HDPE	Primary fossil based	Recyclable*	2,17
rHDPE	Secondary fossil based	Recyclable*	1,36[2]
PET	Primary fossil based	Recyclable*	3,30
rPET	Secondary fossil based	Recyclable*	2,11[3]
PETG	Primary fossil based	Non-recyclable	*Unknown*
PP	Primary fossil based	Recyclable*	2,19
BioHDPE	Renewable resource	Recyclable	-0,16[4]
bioPET	Renewable resource	Recyclable*	*Unknown*
bioPP	Renewable resource	Recyclable*	-1,91[5]
rPP	Secondary fossil based	Recyclable*	1,37[6]

Note: * Provided that the bottle design facilitates recycling.

[1] Retrieved from the EcoInvent database 3.5 (2018), unless indicated otherwise

[2 and 3] Calculation of impact based on the impact of virgin material, the impact of the recycling process and substitution of virgin material, considering the allocation factor and the downcycle factor. All factors are retrieved from the EcoInvent database 3.5 (2018).

[4 and 5] Calculation based on values from Chen & Patel (2018) + transport from Brazil to Europe. Land use change can have significant effect, but has currently not been quantified.

[6] Calculation of impact based on the impact of virgin material, the recycling process and substitution of virgin material, considering the allocation factor and the downcycle factor. All factors are retrieved from the EcoInvent database 3.5 (2018).

Box 7. Polymer considerations

When selecting a polymer for detergent bottles, consider the following:

- Prefer recycled (secondary non-renewable) feedstock for the production of detergent bottles. This contributes to a closed material loop and reduces the environmental impact of the packaging. Aim for the highest possible percentage of recycled material.
- Carefully consider using food-grade recycled plastic (e.g. rPET) for the non-food application of detergent bottles, as this limits the availability of food-grade plastics for food-grade applications.
- The production of detergent bottles made of rPP is not technically feasible, because the melt flow index (MFI) of rPP is too high for the commonly practiced extrusion blow moulding (EBM). Therefore, production of PP detergent bottles is not regarded as sustainable.
- Renewable (bio-based) feedstock and primary feedstock can be used to supplement recycled plastics to realise desired mechanical performance, as a carrier of the masterbatch, or the production of closures and labels. Renewable feedstock is preferred over primary feedstock because it is more circular, although it must be certain that the feedstock is not in competition with food production.
- Use of biodegradable plastics is not advised for detergent bottles, because no suitable disposal route is available for packaging of this material.

4.3. Production residues and production additives

Use of virgin plastics (primary non-renewable feedstock) cannot be completely avoided. There is always a masterbatch added to recycled plastics, to improve its performance and the basis for this masterbatch is virgin polymers. Additionally, a combination of virgin and recycled material is used in some bottles. Therefore, this section will consider the sustainability aspects on a chemical level of the production of virgin resin. Virgin plastics are e.g. required as a binder in the masterbatch, but can also be used to upgrade the quality of recycled plastics when this is inadequate.

4.3.1. Production residues

Two main processes are used to produce plastics – polymerisation and polycondensation – and these both require specific catalysts. In a polymerisation reactor, monomers such as ethylene and propylene are linked together to form long polymer chains. Each polymer has its own properties, structure and size depending on the various types of basic monomers used (PlasticsEurope, 2020).

- **Monomers** are the starting molecules, used to form a polymer through polymerisation. Terephthalic acid (TPA) is a monomer used in the production of PET. Migration of residual TPA is regulated in the EU under Regulation (EU)10/2011 on food contact materials with a migration limit of 7.5 mg/kg. Residual monomers are not expected in polyolefins (PE and PP in this case study) as these are very volatile substances that are separated from the polymer pellets produced. A well-known restricted monomer is Bisphenol A (BPA) an endocrine disrupting chemical (EDC) and a migration limit for the substance has been set in EU regulations since 2018, but this is used in the production of polycarbonate (PC).
- **Oligomers** are partially reacted monomers or the result of degradation of polymers. They are mainly found in polyesters (PET and PLA) in food packaging applications, it is unknown if this is different for non-food PET packaging. When modelling migration of oligomers in (r)PET towards water migration levels stay well below the limit of 10 µg·L−1 [1] (Thoden van Velzen et al., 2020). Oligomers can be present in polyolefins as waxes, for instance in very low-density polyethylene

(VLDPEs). It is assumed that oligomers tend to be less hazardous than the starting monomers, but that they are present in higher concentrations in the plastic (Barnes et al., 2007).

- **Catalysts** are chemicals that start or accelerate a chemical reaction. In this case, the polymerisation from monomers to polymers. In the production of PP catalysts can be added that are formed from a 'pre-catalyst mixture' containing, among other substances, phthalates. It forms the catalyst in the reactor in which the polymerisation will take place. Ortho-phthalates such as e.g. Bis(2-ethylhexyl) phthalate (DEHP) have endocrine disrupting properties. These phthalates are usually consumed in the reactions, but traces can be left in the final PP. Most impurities are removed in the purification stage and tests are performed to determine that concentrations are below specified limits so that the material can be used in food-grade substances. Antimony trioxide (Sb2O3) is commonly used as a catalyst in the polymerisation of PET and remains in the material after production, leaching in packed product and to the outside surface. Antimony trioxide is suspected to be carcinogenic and toxic through prolonged or repeated exposure (ECHA, 2020e). Increased leaching of antimony trioxide has been established by higher temperatures above 70°C (Filella, 2020). Concern has been raised over the leaching of antimony trioxide from PET bottles into drinks (Hansen et al., 2010) and the exposure of workers to the substance (Cooper & Harrison, 2009).

4.3.2. Additives in primary feedstock

Additives are used to make plastics easier to process, enhance its mechanical properties (such as impact or stress crack resistance) or give it specific aesthetic qualities. In general, few additives are expected to be used in plastics for detergent bottles. Detergent and bottle producers indicated that only colourants are added, and in some cases additives to provide a UV barrier (PET bottles). Additives require an additional financial investment. Producers therefore try to avoid these where possible, to cut costs.

Although additives may be scarce in detergent bottles, they can be present in some cases. This section will briefly consider additives that can potentially be present in plastic resins for detergent bottles. Table 4.4 provides an overview. A distinction is made between functional additives that alter polymer characteristics, additives used to optimise production processes of e.g. bottles, and additives that are added to alter the appearance of a plastic. Additives for production and aesthetics are discussed in Section 5.3.

Table 4.4. Potentially relevant additives for detergent bottles

Functional additives	Additives used for production*	Additives for aesthetics*
Flame retardants	Antistatic agents	Pigments
Heat and oxidation stabilisers	Slip agents	Fillers**
Biocides	Lubricants	
Plasticisers		
Impact modifiers		

Note: * Further elaborated on in Section 5.3.
** Fillers are not always used for aesthetics only, but this is the relevant functionality for this case study.

Flame retardants reduce the flammability of plastics. They are not added to the resin for the application in detergent bottles. Many flame retardants have been banned due to reproductive toxicity, carcinogenicity and endocrine disruption.

Heat and oxidation stabilisers are used to prevent polymer degradation during extrusion. The amount depends on the chemical structure of the additive and of the plastic polymer (Hahladakis et al., 2018). Examples of antioxidants are 2,6-di-tert-butyl-4-methylphenol (BHT), Cyanox 2246, Irganox 1035, Tinuvin 326, Tinuvin 328, Irganox 1010, and Irganox 1330. BHT and Cyanox 2246 were at higher levels than the specific migration levels in some food simulants(Gao et al., 2011), high migration is especially likely into fatty foods(Barnes et al., 2007). BHT is under assessment for endocrine disrupting properties and is very toxic to aquatic life (ECHA, 2020a), Cyanox 2246 is a reproductive toxicant and is toxic to aquatic life (ECHA, 2020d).

Because detergents might end up in the sewage system, it is advised to avoid the use of antioxidants that have high migration rates and that are highly toxic to aquatic life. The polymer can benefit from the addition of antioxidants, as it prevents degradation of the polymer; this is beneficial when the material is reprocessed during recycling. Adding safe antioxidants is therefore advised.

Clarifying agents or nucleating agents are added to improve the transparency of plastics, and are mainly applied in PP. As PP is semi-crystalline, these nucleating agents are the seeds to start crystallisation. This leads to a product with smaller crystals and gives better optical clarity. No environmental risks are expected with this additive. Potassium benzoate is commonly used as a clarifying agent for this application, and is also used as a food preservative.

Biocides prevent the degradation of plastics from microbiological attacks. It might be used to slow down biodegradation of biodegradable plastics (Groh et al., 2019), and is therefore not relevant to this case study.

Pigments are dispersed within a binder matrix (masterbatch), which is then added during compounding of the granules to imbue it with colour. Coloured plastics pigments are embedded in a matrix and therefore exposure is limited (Cradle to Cradle Products Innovation Institute, 2019). Many detergent bottles are coloured white using the pigment titanium dioxide (TiO_2). Titanium dioxide has suspected carcinogenic properties in powder form (ECHA, 2020g). It is considered safe when used in plastic. Safety and environmental considerations of pigments are further discussed in Section 5.3.

Box 8. Chemical considerations

Chemical additives are added to the virgin plastic to serve specific purposes, but can have consequences for the sustainability of the plastic packaging. They might hamper recyclability or pose a toxicity risk to human health or biodiversity at any point in the life cycle. It should be considered whether the addition of the chemicals to the plastic is indispensable or whether more sustainable alternatives can be chosen.

For detergent bottles antioxidants (processing stabilisers) are the most relevant. Using antioxidants supports the recyclability of the polymer, as it prevents polymer degradation. Avoid using the antioxidants BHT and Cyanox 2246, as these can migrate to the detergent and contaminate the wastewater.

4.4. Secondary feedstock – Recycled plastics

For detergent bottles it is advised to use as much recycled plastic (secondary feedstock) as possible. This section explores additional sustainability aspects for using recycled HDPE or PET for detergent bottles and the additives added to these polymers.

Secondary feedstock is in increasingly high demand. As a consequence, prices increase and are occasionally above the price of their virgin alternatives, which is especially the case for PET. This has led to an influx of 'fake recycled polymers' into the market where virgin polymers that are sold as recycled. Recycled feedstock from suppliers must be scrutinised to prevent such activities.

4.4.1. Recycled HDPE

Colour restrictions of recycled HDPE

rHDPE is not available in a transparent form. The colours that are available are generally less bright compared to virgin material. This is because the pigments of the previous application of the plastics remain in the recycled material. Current colour possibilities are improving due to advanced colour sorting of HDPE flakes.

Smell of recycled HDPE

Polyolefins (PP, PE) have a relatively open structure and when used in (liquid) packaging, substances from the contents can migrate into the polymer matrix[2], causing it to smell. In mechanical recycling of HDPE detergent bottles, the migrated fragrances are partly removed in the washing process and extrusion. However, a slight smell of waste remains. This is often the reason that recycled polymers are rejected for the production of new bottles. However, it is recommended to test rHDPE bottles when filled with the detergent. Because detergents have a strong smell this can cancel out the rHDPE smell. Over time, the fragrance of the detergent will be absorbed in the polymer matrix of rHDPE.

Impurities and safety of rHDPE

The recycled HDPE stream contains contaminations and impurities. For example, surfactants, plasticisers and solvent polymers are found. According to Horodytska et al. (2020) these non-intentionally added substances (NIAS) in HDPE semi-volatile organic compounds (SVOCs) found in the recycled HDPE mainly consists of additive degradation products, e.g. from antioxidants (methyl 3,5-dicyclohexyl-4-hydroxybenzoate) or lubricants (methyl octadecenoate). All degradation products were present in very low quantities. When assessing VOCs in recycled HDPE, it was found that these mainly originate from contaminations from product residues in the packaging waste stream, such as organic waste, cosmetics or detergents (Horodytska et al., 2020). Examples are methyl lactate, hexyl acetate and dimethyl butanedioate. These substances were found in very low quantities. 2-Phenoxyethanol and benzyl acetate (harmful to aquatic life with long lasting effects) were present in the highest concentration and originate from cosmetics.

Recycled HDPE generally contains some PP, for example from the closures used on detergent bottles. For most applications this is not an issue; generally up to 2-3% PP can be allowed, while other sources state that 5% PP contamination is still feasible (Karaagac et al., 2021). When sourcing rHDPE for bottles the maximum PP content should be considered, as it can influence the MFI of the polymer and thus its processability for EBM. Compatibilisers can be used to improve the blend of HDPE and PP. Frequently used compatibilisers are e.g. ethylene propylene elastomer (EPR) and ethylene-propylene-diene copolymer (EPDM). These reduce the modulus and yield stress, while significantly improving elongation at break and impact strength (Karaagac et al., 2021).

Mechanical performance

The environmental stress crack resistance (ESCR) of recycled HDPE is lower than that of virgin polymers. This is caused by the degradation from heating during the recycling process. According to recyclers, the ESCR of rHDPE is sufficient for packaging low-concentrated detergents in bottles made from 100% PCR. However, packaging highly concentrated detergents 100% PCR bottles is very challenging and not always feasible. In these cases, a percentage of virgin feedstock is required. Intensive washing of the packaging waste in the sorting process will reduce degradation due to contamination in the waste stream, and thus supports retaining a good ESCR.

Masterbatch

A masterbatch is added to recycled plastics to improve its performance and appearance. A masterbatch consists of pigments and additives (e.g. antioxidants and compatibilisers), with a virgin polymer base. In general, a masterbatch consists of 5-10% pigments. On average, 3% masterbatch is used in detergent bottles made from rHDPE.

- **Pigments**: safety and environmental aspects of pigments are discussed in Section 5.3.
- **Other additives**: HDPE polymers degrade in quality by heating in the compounding process. This can be countered by adding antioxidants as processing stabilisers. For selection of safe antioxidants, see additives for plastic resin in Section 4.3.

4.4.2. Recycled PET

Discolouration of rPET

rPET is generally food-grade, sourced from recycled deposit bottles. rPET is transparent, but is often characterised by a grey haze and/or yellow discolouration. The former is caused by contaminations in the recycling stream (e.g. coloured PET) and can be worsened by reheat additives and blue colourants that are used to mask yellowing (Alvarado Chacon et al., 2020; Thoden van Velzen et al., 2016). Yellow discolouration is caused by breakdown products in the polymer; e.g. caused by oxidation of diethylene glycol comonomer (resulting in hydroquinone and quinone moieties) (Alvarado Chacon et al., 2020) or from added UV light blockers and oxygen scavengers (Schloss, 2017). In general, the bottles become greyer and yellower with increasing levels of recycled content (Alvarado Chacon et al., 2020).

To prevent a grey haze in the rPET stream, use of coloured and opaque PET should be avoided. Using blue colourants to prevent yellow discolouration must be carefully considered, as this can increase the grey haze of the recycling stream. Some parties offer 'anti-yellowing agents'[3], which are not pigments. The precise nature of these substances is unknown, as is whether they can migrate into the detergent and how they influence the quality of the recycled PET stream. It is preferable to avoid yellowing of the material in the first place. This can be done by refraining from using UV light blockers (e.g. by opting for an opaque HDPE bottle in case of UV-sensitive detergents).

Impurities and migration

rPET can contain impurities, which can potentially migrate into the detergent. Impurities can be degradation products, which are created due to thermal and mechanical degradation in the recycling process. Acetaldehyde is a thermal degradation product from PET (Barnes et al., 2007), is suspected to be carcinogenic and mutagenic and is regulated in the EU with an overall migration limit set at 6 mg/kg. It is a potential hazard for the staff at recycling facilities because it can cause serious eye irritation and is highly flammable (ECHA, 2020b). According to Thoden van Velzen et al. (2020), migrated amounts of acetaldehyde fall within the limits given in the food contact material (FCM) legislation and are therefore also regarded safe in the detergent bottle context.

Contamination of the recycling stream can add NIAS to the secondary material. Thoden van Velzen et al. (2020) found low quantities of benzene in rPET. They attributed the presence of benzene to accidental contamination of the PET recycling with PVC and found that an increase in recycled content increased the levels of benzene. The low concentration of benzene was considered of no concern. However, it was noted that no conclusion could be drawn on the effects of accumulation of the substance over multiple recycling cycles.

Improving mechanical performance

In recycled PET Intrinsic Viscosity (IV) is lower, as rPET breaks down in smaller polymer chains. High IV is desirable as this means the material has better mechanical properties. Through Solid State Polymerization (SSP), the chain lengths are restored, and thus loss of mechanical properties is reduced. SSP is treatment of PET pellets at a high temperature (>210 °C) in a vacuum, which causes a reaction of PET molecules. SSP lowers the concentration of acetaldehyde and ethylene glycol in the rPET pellets and reduces migration during the life cycle (Thoden van Velzen et al., 2020). It is thus advised to always perform SSP.

Box 9. Polymer considerations

- Recycled polymers can contain impurities or non-intentionally added substances (NIAS) (e.g. contaminations or breakdown products). Ensure safety of rPET and rHDPE polymers by evaluating if expected NIAS are below the accepted migration limits.
- Recycled polymers have a reduced ESCR compared to virgin polymers. Therefore, packaging concentrated detergents in bottles made from 100% PCR is challenging or unfeasible. A percentage of virgin bio-based or fossil-based content is required.
- **rPET:** Avoid coloured/opaque PET as this can contaminate the clear rPET stream at end-of-use.

Box 10. Chemical considerations

- **rHDPE:** For improving the rHDPE quality substances are added such as antioxidants, compatibilisers for PP contamination and pigments.
- **rPET:** Do not use UV light blockers as these cause yellowing of the rPET recycling stream.
- **rPET:** Carefully consider using blue colourant as anti-yellowing agents, as these colourants result in a grey haze in the rPET stream.
- **rPET:** Perform SSP of rPET pallets, as this reduces migration of substances during the life cycle.

Notes

[1] 10 $\mu g \cdot L^{-1}$ is the migration limit conventionally applied for non-intentionally added substances (NIAS) not classified as 'carcinogenic', 'mutagenic' or 'toxic to reproduction' (CMR).

[2] The rate of migration follows Ficks law and strongly depends on the molecule size, if smaller then more can migrate.

[3] Such as Ampacet and Sukano

Chapter 5. Production

During production, the detergent bottle is manufactured. Section 5.1 considers the predominant production methods of extrusion blow moulding (EBM), commonly used for HDPE, and injection stretch blow moulding (ISBM), which is used for PET bottles. The impact of production on polymer selection is discussed in further detail in Section 5.2. In production, substances can be added, such as pigments to colour the plastic, or lubricants to enhance mould release in the bottles. The sustainability impacts of these additive substances are elaborated upon in Section 5.3.

The production phase touches upon the following over-arching sustainability goal: reduce material use. The production method in combination with the selected polymer can influence the volume of material used in the manufacturing of the bottle.

5.1. Production methods

This section describes the commonly used production methods for detergent bottles. The production process as indicated in Figure 5.1 is used as an outline.

Figure 5.1. Production and filling process of detergent bottles

Common production methods for detergent bottles are extrusion blow moulding (EBM) and injection stretch blow moulding (ISBM), while other production methods are not common practice for large detergent producers. The two production methods will be briefly explained below; see Table 5.1 for an overview.

5.1.1. Extrusion blow moulding

In extrusion blow moulding (EBM), a parison is extruded, over which a mould is closed. Subsequently, the parison is blown into the mould to shape the bottle. Finally, the trims caused by production are removed. EBM allows the creation of a handle on the bottle, which cannot be achieved using ISBM. EBM requires a low melt flow index (MFI), so HDPE and PP are the most suitable materials for this production process.

In EBM, different layers can be co-extruded. In this way recycled and virgin layers can be combined. This can be desirable for giving the bottle a ‘virgin look’ while simultaneously increasing the recycled content. The same approach can also reduce the need for pigments in a bottle by colouring only the outer layer.

5.1.2. Injection stretch blow moulding

Injection stretch blow moulding (ISBM) consists of two steps: first, a preform is produced using injection moulding, after which this preform is blown into a bottle mould, resulting in a bottle. These two steps can be carried out in one process, or the preform can be purchased externally and reheated before bottle blowing. The latter can prevent emission to the environment due to transporting empty bottles. ISBM is a more expensive process than EBM, but allows for more freedom of form. However, it is not possible to create bottles with handles using the ISBM technique. Generally, ISBM is used to produce PET bottles and sometimes for small HDPE and PP bottles.

Table 5.1. Overview of production methods

Production method	Characteristics
Extrusion blow moulding	- Allows a handle in the bottle design - Less freedom of form - Cheaper than ISBM - Emissions at production of approximately 1,47 CO_2/kg
Injection stretch blow moulding	- Handle on bottle not possible - More accurate, more precise measure tolerance - Expensive compared to EBM - Emissions at production of approximately 1,95 CO_2/kg

5.1.3. Filling

The process of filling a blown bottle with detergent has no further implications for the sustainability of polymer and chemical selection and is thus not further elaborated. However, an aspect that must be considered is the transportation distance between the production facility where the bottles are blown and the location where the bottles are filled. Ideally, bottles are blown and filled at the same location, with a limited distance to the retailers. When bottle blowing and filling is not possible at the same location, it is recommended to consider the environmental impact of transportation of empty bottles versus reheating preforms for ISBM blow moulding.

5.2. Polymer selection

Not all polymers can be used for all bottle blowing production methods. Table 5.2 provides an overview of the suitable production methods for the different polymer feedstocks. As elaborated on in Section 4.2, PP is not considered because EBM is not possible using recycled feedstock[1] (rPP has a high MFI).

5.2.1. HDPE

HDPE bottles can be produced using extrusion blow moulding. EBM of different polymer feedstocks is feasible without the addition of additives or other enabling substances in production. Recycled and bio-based polymers behave differently in production, which requires adjusting of machine settings.

5.2.2. PET

PET detergent bottles are produced using ISBM, which is feasible for PET from different feedstocks without applying additives or other enabling substances for production. Recycled and bio-based polymers will behave differently in production, which requires adjusting of machine settings.

Table 5.2. Overview of polymers and possible production methods for detergent bottles

Polymer	Extrusion blow moulding	Injection stretch blow moulding
(bio)HDPE		Not generally applied
rHDPE		MFI too low
(bio)PET	MFI too high / IV too low	
rPET	MFI too high / IV too low	Bottles made from 100% rPET are on the market

Box 11. Polymer considerations

- EBM is the most commonly used production method for HDPE bottles. Compared to ISBM, it is cheaper, less energy-intensive, and allows for the incorporation of a handle. It does limit the freedom of form in the design.
- For the production of PET bottles, the ISBM process needs to be used. This allows for more freedom of form in the design, but is more expensive, more energy-intensive, and does not allow for the incorporation of a handle.
- By using multiple layers in EBM, the recycled content can be increased by only using virgin material in the outer layer. The need for pigments can be also reduced as these are only required in the outer layer of the bottle.

5.3. Additives used in production

This section describes the additives used in the production of the bottles, such as pigments and lubricants that support the production process.

5.3.1. Pigments

Pigments are coloured, insoluble chemical compounds with the ability to give colour to another material. In plastics, pigments are dispersed within a binder matrix (masterbatch), which is then added during compounding of the granules to imbue it with colour. In general, a masterbatch consists of 5-10% of pigments, the remainder being virgin polymers or other additives. The use of pigments in PET is not advisable. Opaque PET is recycled into low-value products such as strapping. Transparent blue bottles can contaminate the food-grade PET stream. This section thus focuses on pigment use in HDPE. On average, more pigments are needed to colour recycled bottles compared to virgin bottles. In a virgin bottle, approximately 2% masterbatch is required, compared to around 3% in rHDPE bottles.

Dyes, soluble colourants, are not discussed in this case study as these are not commonly used in the production of detergent bottles.

5.3.2. Safety of pigments

Pigments can be divided into two groups (Cradle to Cradle Products Innovation Institute, 2019):

- **Inorganic pigments**: Inorganic pigments, often metal oxides or metal sulphides, usually show high light fastness and temperature stability, but often limited brilliance. The major inorganic pigments include titanium dioxide, iron oxide, zinc oxide, zinc sulphide, barium sulphate, chromium (III) oxide, cobalt blue, lead oxide, cinnabar and cadmium yellow.
- **Organic pigments**: Similar to dyestuff molecules, organic pigments can be classified according to their chemical structure. Classes of organic pigments include: Azo pigments, Disazo pigments, Polycyclic pigments, Anthraquinone pigment, Dioxazine pigments, Triarylcarbonium pigments and Quinophthalone pigments. Azo pigments are the most commercially important group of organic pigments.

According to the Cradle to Cradle Products Innovation Institute (2019) "…very few pigments are hazardous. The main reason for this is that most pigments are poorly water soluble and predominantly chemically inert, and as a consequence are not bioavailable. Being not bioavailable means that it is not absorbed in a living organism. In coloured plastics pigments are embedded in a matrix and therefore exposure is limited." However, safety of added pigments should be carefully considered[2]. For pigments used at a concentration of >100ppm in detergent bottles, the following rules apply (Cradle to Cradle Products Innovation Institute, 2019):

- **Organohalogens**: pigment containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.
- **Toxic elements**: Pigments containing lead, cadmium, mercury, vanadium, chromium (VI), cobalt, nickel, arsenic, antimony or selenium should be avoided. For example, mercury may damage fertility or cause harm to the unborn child (ECHA, 2020f).
- **Reductively cleavable aromatic amines** such as azo pigments containing one or more carcinogenic aromatic amines should be avoided. Carcinogenic amines are also on the REACH restricted substances list (ECHA, 2020c).

Note that if a pigment is assessed according to the stringent Cradle to Cradle criteria, the pigment is not automatically suitable for usage in detergent bottles. The Carbon black pigment, for example, is C2C bronze-certified. However, as described in Section 6.2, use of carbon black inhibits correct sorting of the packaging and thus prevents its recycling.

5.3.3. Lubricants

In the production of bottles, lubricants can be used to release bottles, making processing easier and reducing cycle times. Lubricants are only required for complex geometries, while bottle producers indicate they are rarely used for detergent bottles. Commonly used lubricants are paraffin waxes and glycerol stearates. Currently, these present no cause of concern during production, use, or reprocessing at end-of-life. However, little research has been done into the impurities (Bradley & Coulier, 2007) and migration (Wagner, 2012) of these substances. In HDPE, metal salts of stearates can be used as an internal lubricant; these types of products are in the positive list, EU no. 10/2011.

According to Thoden van Velzen et al. (2020), acetone, butanone and furan are detected as migrants from rPET. These are expected to be residues from solvents used to clean and protect moulds at small-scale production facilities. Their concentrations in the mineral water simulants were well below the limit of 10 $\mu g \cdot L^{-1}$[3] and are thus not of concern for detergent bottle applications.

Box 12. Chemical considerations

- Most pigments do not have health consequences because they are embedded in the polymer matrix and exposure is therefore limited.
- Avoid using halogen-containing pigments because the combustion products in case of incineration are toxic. Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.
- Pigments containing toxic elements such as lead, cadmium, mercury, vanadium, chromium (VI), cobalt, nickel, arsenic, antimony or selenium should be avoided.
- Azo pigments containing one or more carcinogenic aromatic amines as defined in European regulation 76/769/EEC should be avoided.
- Carefully consider the necessity of using lubricants to release bottles from the mould.

Notes

[1] rPP has a high MFI, whereas EBM requires a low MFI.

[2] This can be done by checking whether a pigment is REACH-compliant or present on the *Restricted Substances List* issued by the *Cradle to Cradle Institute.* However, additional steps can be taken to ensure the safety and sustainability of pigments, by following *Colorants (Textile Dyestuffs and Pigments) Assessment Methodology* required for Cradle to Cradle certification. An assessment will then be made whether a pigment is chemically stable or whether it has the potential to form products with a hazardous reaction.

[3] 10 $\mu g \cdot L^{-1}$ is a migration limit conventionally applied for non-intentionally added substances (NIAS) not classified as 'carcinogenic', 'mutagenic' or 'toxic to reproduction' (CMR).

Chapter 6. End-of-Use

This phase includes disposal of the packaging by the user, collection and sorting of the packaging and recycling of the materials. Collection methods of plastic waste vary from sorted collection to no collection at all, with the impacts of these different waste collection methods discussed in Section 6.1. A collected detergent bottle must be sorted into a mono-material stream in order to be recycled effectively. Common sorting methods are discussed in Section 6.2, in which their implications on the bottle design are also evaluated. Once sorted into a mono-stream, the bottle can be mechanically recycled. The recyclability of the different polymers and the sustainability impacts of the recycling process are considered in Sections 6.3 and 6.4, which focus on the influence of additive substances on recycling. Chemical recycling is not deemed an effective end-of-use scenario for detergent bottles, although Section 6.5 briefly discusses its implications. Unfortunately, not all detergent bottles are currently recycled, therefore incineration and disposal in landfill are discussed in Section 6.6.

This phase touches upon three of the over-arching sustainability goals:

- **Close material loops:** Closing the material loop on detergent bottles is feasible, therefore bottle-to-bottle recycling should be aimed for.
- **Preserve natural capital:** Melting (recycling) and burning (incineration) of plastics releases hazardous fumes into the environment. Therefore, safety precautions should be taken to preserve natural capital. Additionally, landfilling and littering of the packaging should be prevented at all times as this will result in microplastics and can be harmful to aquatic and terrestrial animal life.
- **Safeguard the health of participants in the life cycle:** The End-of-Use (EoU) stage should be safe for all parties involved. This includes safe disposal by the user and safe recycling processes for workers, without exposure to unsafe or toxic substances.

In the chemical selection for plastic packaging, it should be taken into account how the packaging will most likely be processed at end-of-use. The available waste infrastructure determines the choices that need to be made: the design of the packaging must fit the most sustainable option for processing at end-of-use. This includes the fact that collection and sorting of the packaging is required before any of the aforementioned processes. In case of recycling, the material must be recoverable in the best possible quality to be reused in a new product or packaging. In all scenarios, exposure of waste management workers to hazardous chemicals or emissions of hazardous substances to the environment must be prevented. Emissions of greenhouse gases should be limited.

There are two end-of-use scenarios to be considered for detergent bottles: mechanical recycling or incineration and landfilling. Both scenarios start with disposal of the detergent bottle; this is elaborated in Section 6.1 on waste collection.

The following EoU scenarios are regarded as out-of-scope:

- **Composting**: The composting of a plastic packaging requires the packaging to be made of a biodegradable polymer. As discussed in Section 4.2, this feedstock is not considered for detergent bottles.

- **Littering**: Littering of plastic packaging has detrimental effects on the environment but is not considered as an EoU scenario in this case study. Detergent bottles are not commonly littered by consumers as they serve a clear indoor purpose and are subsequently disposed of in household waste streams.

6.1. Waste collection

When discarded properly by the consumer, detergent bottles can be collected via three main routes: residual waste, separated plastic packaging waste, and post-separation. Which route the packaging follows depends mostly on local availability of the collection system and consumer behaviour. Note that in some countries informal waste collection methods provide input for recycling.

6.1.1. Residual waste

Most plastic packaging is currently disposed of with the municipal waste collection of residual household waste. This means that the detergent bottles are mixed with food scraps and other unsorted materials. It might be sorted out for recycling in a ‘post-separation plant’, sometimes also known as a ‘post-collection separation plant’. However, in most countries, this is not common practice. Unsorted residual waste is either incinerated or disposed of in landfill.

6.1.2. Separated plastic packaging waste

If available, the detergent bottle can be discarded by the consumer through the separate collection of plastic packaging waste, pre-sorted from the residual waste by the consumer at home. Rigid plastic bottles are easily recyclable, and in most OECD countries, a collection system is in place. How this system is organised varies a great deal between countries; from collection at consumers’ homes to central collection points where consumers can take their pre-sorted packaging. After collection, the plastic stream is sorted into mono-material streams, see Section 6.2.

6.1.3. Post-separation

Recent technological developments allow for the separation of plastic packaging waste from mixed residual waste in post-(collection-)separation facilities. Availability of these sorting facilities is not widespread at the time of writing (late 2020). After sorting, the separated plastic will be transferred to a sorting installation.

6.1.4. Plastic recycling rates

The rates of plastic recycling vary significantly by country, by waste stream, and by polymer type. For example, recycling rates for PET and HDPE are typically higher than recycling rates of PP. PET and HDPE are used in large quantities for (food) packaging which is better recycled in general compared to other applications. Volumes of rigid PP packaging are relatively low and are therefore not generally recycled. This motivates the use of PET or HDPE polymers in detergent bottles, as recycling at end-of-use is better developed for these polymer types.

Recycling rates for clean, high-value plastics found in rigid packaging are generally higher than e.g. film packaging. The plastics can be more easily repurposed and are interesting from an economic perspective. Therefore, it is expected that recycling rates for plastic detergent bottles are higher than the average rate for plastics in general.

Box 13. Polymer considerations

In the selection of a polymer the end-of-use scenarios should be considered. Determine which disposal routes are available for the packaging and to which EoU scenarios this will lead to: mechanical recycling or incineration and disposal into landfill.

a) When mechanical recycling is available, make sure a polymer is selected that is mechanically recycled in the region and optimise the packaging for recycling.
b) When mechanical recycling is unavailable, the material loop cannot be closed. Reconsider the use of single use plastic packaging and explore use of reusable packaging or other alternatives. Focus on reducing the environmental footprint of the packaging as much as possible, to preserve natural capital.

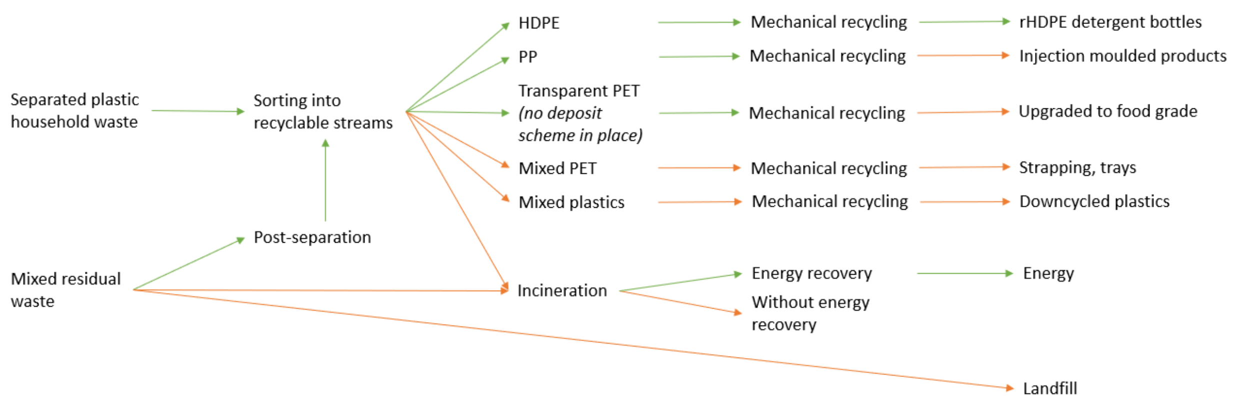
6.2. Sorting – Recyclability of packaging design

Plastics that are either pre-separated in households or separated from the residual waste after collection are sorted in a few main polymer 'streams', which vary by country. Figure 6.1 shows commonly seen recycling routes and sorted plastic streams. Rigid PET, HPDE and sometimes PP are usually sorted as individual streams.

6.2.1. Sorting of non-food PET bottles

When a deposit bottle scheme is in place, PET bottles are sorted in the mixed PET stream. This material is reused in low-value products. When no such scheme is in place (e.g. in the United Kingdom, France and Belgium), transparent PET bottles used in non-food applications are sorted into the transparent PET stream. This stream is reused in food grade applications. To allow for food-grade use, only 5% of non-food packaging is allowed in this stream. When too many non-food products are packaged in PET, the value of this stream drastically decreases. In conclusion, currently no EoU scenario is available in which PET detergent bottles are optimally recycled. When sorting techniques improve and allow differentiation between food and non-food packaging, the EoU scenario for PET detergent bottles will improve. Additionally, non-food PET might be sorted and recycled for reuse in non-food packaging. However, these effects of advanced sorting remain speculative.

Figure 6.1. Different disposal routes and recycled plastic streams



6.2.2. Design for sorting

To enable the correct sorting of a detergent bottle, the complete packaging design, including closures, labels and adhesives, must facilitate the common sorting process in place. This section explains the sorting process, evaluates the complete design of the detergent packaging and highlights which design considerations influence sorting of the plastic bottle in each sorting step. These aspects are described separately for HDPE and PET bottles as these have different requirements.

6.2.3. Overview of the sorting process

To create clean mono-streams sorting of the packaging and polymers, (a combination of) several techniques can be adopted. Which technique is applied depends on the technological advancement of the sorting/recycling facility. Often, plastic streams are sorted multiple times to create a high-quality mono-stream. The sorting process is broadly as follows:

1. **Sorting packaging in mono-streams:**
   a) Near-infrared (NIR): NIR scanners positioned above the conveyor belts detect the polymer type of a packaging using the infrared technique. Based on the identification, the packaging is sorted in a mono-stream, for rigid plastics usually rigid PET and HDPE, sometimes PP.

   b) Advanced sorting (HolyGrail project): Recent developments of digital watermarks and chemical tracing have the potential to drastically improve sorting of packaging waste, e.g. sorting food grade packaging from non-food-grade packaging. This can potentially create a food-grade feedstock for rHDPE and rPP. Digital watermarks can be printed on the label or physically incorporated into the plastic itself. The watermark is read and the system can extract information on packaging sorting from a database.

   Chemical or fluorescent tracers can be added to packaging labels and detected using a UV lamp; this allows sorting of food and non-food packaging. Both types of advanced sorting are currently tested and evaluated (New Plastics Economy, n.d.).

2. **Shredding packaging into flakes**

3. **Washing of flakes:** The flakes are washed to remove contaminations from the stream, for example organic waste and product residues, and to remove labels, adhesives and ink. The washing step is essential in creating a clean polymer stream. The water temperature and detergents used depend on the recycling facility and material stream. It usually ends with rinsing the flakes to remove all detergents.

4. **Flake sorting:** So far, the packaging is sorted into mono-streams. However, the stream is still contaminated by other polymers, for example caused by closures that were attached to the detergent bottle at disposal. Flake sorting varies by polymer stream:

   a) Sink float for PET: The density of PET is higher than that of PP and PE; in water, PET will sink, whereas PP and PE will float. This principle is used to sort PET flakes.

   b) NIR flake sorting for HDPE

6.2.4. Sorting packaging in mono-streams – Correct use of labels

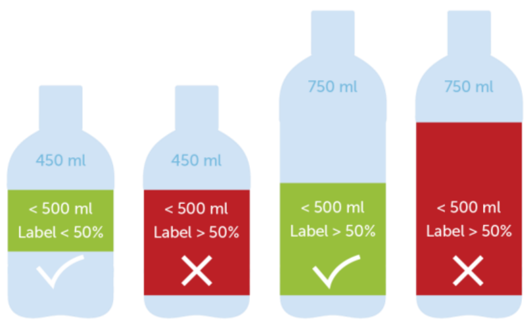
Incorrect usage of labels inhibits correct sorting of the bottle using NIR technology1. When the surface area of the label is too large the NIR will sort the bottle based on the material of the label rather than the bottle material. When these are not made of the same material, the bottle will end up in the wrong recycling stream. This problem is well-known when using full body sleeves2. In the table below, guidelines for correct usage of labels can be found for HDPE and PET bottles. Additionally, it must be noted that PVC labels must be avoided. PVC results in impurities in the recycling stream, potentially causing health risks.

Table 6.1. Label guidelines for HDPE and PET bottles

Bottle material	Label material	Label size*	Sortable with NIR	Recyclability of bottle-label combination
HDPE	PE	Not relevant because same polymer as bottle	Yes	Yes
	Paper	Not relevant because paper interferes with PE recycling	No	No
	PP or PET	<50% for <500ml <70% for ≥500ml	Yes	Yes
		>50% for <500ml >70% for ≥500ml	No	No
PET	PET	Not relevant because same polymer as bottle	Yes	No**
	Paper, PE, PP	<50% for <500ml <70% for ≥500ml	Yes	Yes
		>50% for <500ml, >70% for ≥500ml	No	No

Note:
* See Figure 6.2 for and illustration of the label sizes.
** PET labels (films) pollute the recycling of rigid PET. This is predominantly because the labels are heavily printed, and the inks influence the colour and transparency of the rPET.
Source: Based on KIDV (2021) and RecyClass (2020a, 2020b)

Figure 6.2. Guidelines for Label Sizes



Source: KIDV (2021)

6.2.5. Sorting packaging in mono-streams – Pigments

To create dark coloured bottles, carbon black is often used as a pigment. However, the use of carbon black in plastic packaging inhibits detection of its material by NIR scanners. Carbon black strongly absorbs infrared radiation as well as visible light, so the NIR light is not reflected into the detectors. Packaging containing carbon black pigments are therefore not sorted into mono-streams and end up in the mix-stream or are incinerated.

6.2.6. Shredding process – Metals in packaging

When the bottles are sorted into HDPE and PET mono-streams, the packaging is shredded into flakes. As a general guideline, metals must be avoided in packaging, as they can damage the recycling installation (RecyClass, 2020a). Metals are often applied in closures, such as springs in spray dispensers. As closures are often attached to the bottle at disposal, these will end up in the mono-streams. Therefore, metal caps, springs or other components should be avoided.

6.2.7. Washing process – Label adhesives

Once the detergent bottle is sorted in the HDPE or PET mono-stream, the bottle is shredded into flakes and washed to remove residues of the product, organic waste, labels and adhesives. Adhesives are used to secure labels to the detergent bottles. The adhesive must dissolve to release the label from the bottle. When the adhesive is not selected correctly, it can pollute the recycling process, for example by giving the recycled material a yellow hue or by creating gels that obstruct the process. In particular, hotmelts and pressure-sensitive adhesives cause problems in recycling. The adhesive should be selected so that it is washed off during the sorting process. This depends on the water temperature and detergents used in the washing process. The table below shows the guidelines for selecting adhesives.

Table 6.2. Adhesive guidelines for HDPE and PET bottles

Bottle material	Adhesive soluble or releasable in:	Washing temperature
HDPE	Water	<40°C
PET	Alkali / Water	60-80°C

Source: RecyClass 2020b, 2020a

6.2.8. Flake sorting – Closure design

In the aforementioned steps, the packaging is sorted into mono-streams, shredded and washed. A mono-stream can be contaminated by other polymers, for example caused by the closures used on bottles[3]. When these are attached to the bottle upon disposal, these will end up in the bottle polymer mono-stream. Closures on HDPE and PET bottles are often made from PP, which thus contaminates the HDPE or PET stream. To increase the purity of a mono-stream, additional sorting steps can be applied, such as sink-float for PET streams and NIR flake sorting for HDPE streams.

- **Sink-float of PET stream**: This sorting method is based on the principle that the density of PET is higher than that of PP and PE. This means that PET will sink in water, whereas PP and PE will float. To ensure a pure PET stream, it is important that no fillers are used in PP or PE closures, because this alters the density of the polymer[4]. If the addition of fillers increases the density of PP or PE above 1g/cm3, the polymer will sink along with the PET, polluting the stream.
- **NIR flake sorting of HDPE stream**: Closures are generally made from PP. HDPE and PP have a similar density and can thus not be separated from each other using sink-float sorting. This means PP can potentially end up in the HDPE stream. Innovative recyclers have introduced a NIR flake sorter in the sorting process. This means that PP from closures can be separated from the HDPE stream to minimise PP content in PE.

Box 14. Design considerations

When a bottle is mechanically recycled, investigate the local sorting and recycling process. In general, when mechanical recycling is considered, the following design rules need to be adhered to, to allow sorting of the plastics in a bottle in clean mono-streams:

- Labels: Avoid the use of full body sleeves and PVC labels.
- Labels: Select the material and size of the label to enable correct sorting of the bottle.
- Closures: Avoid fillers in PP and HDPE closures that increase the density above 1g/cm3, to enable the closure material to be separated from the plastic bottle. Use of fillers in PP and PE can increase the density of the polymer, causing it to sink rather than float. The recycling process is based on the floating properties of PP and PE.
- Adhesives: Select adhesives for the label that are soluble or can be released in the washing process.
- Apply a digital watermark or fluorescent tracer to the label or bottle to allow sorting of the packaging as part of the HolyGrail project. Follow developments on this project and design accordingly.

Box 15. Polymer considerations

Only source recycled polymers from certified recycling facilities that take the prescribed safety measures. As such, exposure of hazardous substances to workers and residents nearby is avoided.

Box 16. Chemical considerations

When mechanical recycling is considered, the following rules need to be adhered to:

- HDPE and PP: Ensure the density of HDPE and PP used in bottles is not above 1g/cm3. Otherwise, the plastic will not be sorted for recycling. Therefore, use a mono-material and avoid fillers.
- Pigments: Avoid using carbon black as a pigment, because it prevents correct sorting of detergent bottles and thus inhibits recycling.

6.3. Mechanical recycling – Recyclability of plastics

The previous section elaborated on how detergent bottles are sorted, shredded and washed, resulting in mono-stream materials, in this case PET and HDPE streams. This section reflects on the recyclability of the resulting polymer streams in the compounding process. First, a brief overview of the process of mechanical recycling is given.

6.3.1. Quality degradation of polymers in recycling

In mechanical recycling, polymers are melted and reworked to regranulate. This process results in degradation of the quality of the polymers, as they break down at high temperatures in an extruder. This is on a microscopic scale and is often not detected on a macroscopic scale in standard polymer tests. However, this effect will be stronger after several recycling cycles. Maintaining the quality of recycled polymers over time depends on the stabilisation of polymers at recycling. Stabilisation is conducted by mixing in virgin polymers or additives at the compounding stage of recycling. Currently, this is inherent in the recycling process, because a lot of plastic packaging material is still made from virgin polymers. This results in a high percentage of virgin material in each recycling batch.

6.3.2. Recyclability of plastics

As described in Section 4.2, detergent bottles are highly suitable for applying large quantities of recycled polymers. In the transition to a circular economy, bottle-to-bottle recycling is desirable: recycling polymers from used detergent bottles and using these for the production of new bottles[5]. This strategy is preferred over cascading the recycled polymers to other, lower-value applications. The next sections will evaluate the feasibility of bottle-to-bottle recycling for HDPE, PP and PET detergent bottles.

6.3.3. Bottle-to-bottle recycling

- **HDPE flakes** from detergent bottles are highly recyclable. rHDPE typically has a low melt flow index (MFI) because the recycling stream predominantly consists of bottles made using extrusion blow moulding (EBM). This makes rHDPE suitable for extrusion blow moulding (EBM) of new detergent bottles, and thus bottle-to-bottle recycling can be realised.

  Application of rHDPE beyond EBM is limited because it cannot be applied in food applications[6] and is generally unsuitable for injection blow moulding (IBM). This could be an argument to promote the uptake of rHDPE in detergent bottles, as it stimulates demand.
- **PP flakes** from detergent bottles are highly recyclable. However, the PP stream is unsuitable for production of detergent bottles. The PP stream predominantly consists of thermoformed and injection moulded packaging, EBM bottles only make up a small percentage of this stream. The MFI is therefore high and the stream is unsuitable for EBM of detergent bottles. ISBM of PP bottles for detergents is not practised. Bottle-to-bottle recycling can thus not be carried out.
- **PET flakes** from detergent bottles are highly recyclable. However, recycling of transparent PET is focused on food-grade quality, but detergent bottles are not food-grade and would thus contaminate this stream. The quality of the flakes allows the production of new bottles, but the recycling system does not facilitate this at the moment. When the HolyGrail project is more developed, this is expected to improve.

Table 6.3. Overview of bottle-to-bottle recycling of plastics

	Recyclability	Used in the production of new detergent bottles	Other applications of recycled plastic
HDPE			Building plumbing
PP		Properties of rPP are not fit for EBM and thus bottle-to-bottle recycling cannot be achieved.	Injection blow moulding products
PET		This is technically possible, but not executed in practice. rPET for detergent bottles is generally sourced from a food-grade stream.	Applied in strapping for e.g. pallets (cascading). rPET from detergent bottles cannot be used for food applications.

Box 17. Polymer considerations

For detergent bottles, the aim should be bottle-to-bottle recycling. Evaluate the recyclability of the selected polymer and whether the recycled polymer can be used as a feedstock for the production of new detergent bottles.

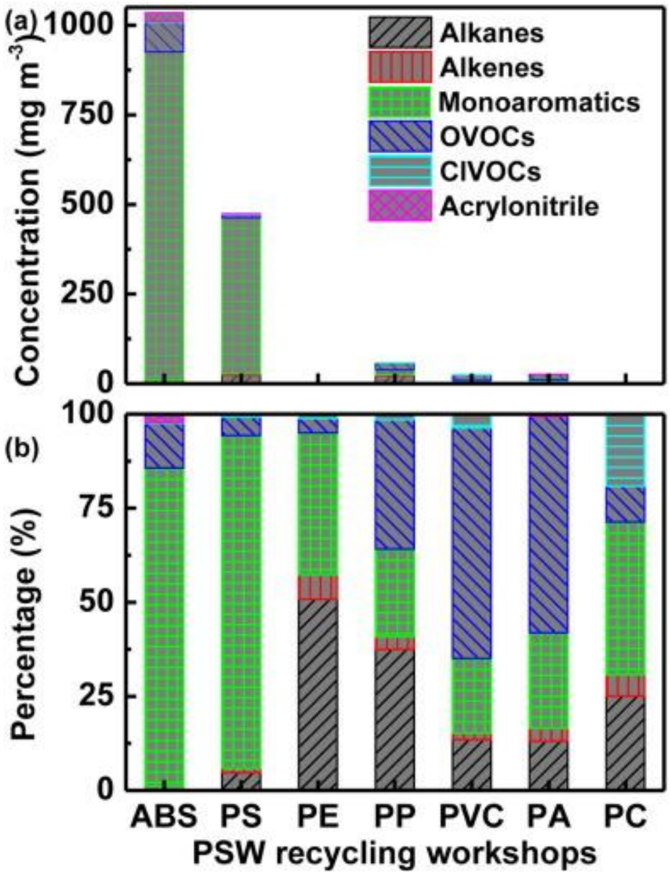
- HDPE: Bottle-to-bottle recycling is possible for HDPE. HDPE detergent bottles are collected and mechanically recycled, and the recycled plastic is suitable for the production of new bottles.
- PP: Because the MFI of rPP is too high for extrusion blow moulding of new bottles, bottle-to-bottle recycling cannot be carried out for this polymer.
- PET: Bottle-to-bottle recycling is technically feasible for PET, but currently not executed in practice due to restrictions in the sorting and recycling system. However, developments are expected to enable bottle-to-bottle recycling for PET in the future.

6.3.4. Safety issues in plastic recycling

The melting of plastic creates fumes, also called Volatile Organic Compounds (VOC), which are often polymer degradation products. Other causes are additives or food residues attached to the plastic waste (Yamashita et al., 2007).

VOCs pose a serious threat to human health: the immediate effects are severe irritation to the eyes, nose and lungs. Prolonged exposure to fumes of any synthetic plastic with no safety precautions can lead to cancer, birth defects and illnesses (He et al., 2015). Examples of VOCs caused by the melting extrusion procedure in recycling are alkanes, alkenes, monoaromatics, oxygenated VOCs (OVOCs), chlorinated VOCs (ClVOCs) and acrylonitrile. Different polymers release different amounts and types of VOCs; Figure 6.3 provides an overview of the VOCs emitted per polymer type.

Figure 6.3. Concentrations (a) and contributions (b) of six groups of VOCs emitted in seven plastic solid waste recycling workshops during extrusion processes



Source: He et al., 2015

6.3.5. Health risks for workers

As can be seen in Figure 6.4, PE and PP release relatively few VOCs[7] (He et al., 2015). The pyrolytic temperature of PE and PP is 350°C, whereas the melt temperature in mechanical recycling is typically between 150 and 250°C. This explains the relatively low amounts of VOCs. Alkanes are the most emitted VOC for these polymers. Table 6.4 shows the most common VOCs emitted for the polymers.

In general, monoaromatic VOCs pose the biggest health risk. According to He et al. (2015) VOCs that are the major contributors to chronic health effects are: benzene, toluene, ethylbenzene, styrene, methylene chloride and trichloroethylene. Inhalation of the monoaromatic VOC toluene, for example, can lead to severe neurological damage. Substances emitted with a major cancer risk (such as causing tumours in the lungs, liver, kidneys and brain via inhalation) are acrylonitrile, styrene, ethylbenzene and 1,2-dichloromethane (He et al., 2015).

Based on the research of He et al. (2015), it can be concluded that the mechanical recycling of PE is safer compared to PP. For mechanical recycling of PET, less information is available concerning health issues. However, it is known that VOCs are emitted when melting rPET (Liu et al., 2018), which is therefore expected to have negative environmental effects. How this compares to other polymers is unknown. A VOC emitted by PET is acetaldehyde, a degradation by-product formed when PET is melted. Acetaldehyde is an extremely flammable liquid and vapour, causes serious eye irritation, is suspected of causing genetic defects and may cause respiratory irritation (ECHA, 2020b).

Additionally, the research of He et al. (He et al., 2015) expects that residents living close to plastic recycling plants with limited safety measures, have a potential cancer risk due to the processing of PS, PA, ABS and PVC. For PE and PP VOCs of particular concern are acrylonitrile, 1,2-dicloroethane, styrene and benzene.

Table 6.4. The three most emitted VOCs for PE, PP, PA, PVC and PET

	PE	PP	PA	PVC	PET
1	i-pentane (20.4%)	cyclopentanone (20.6%)	cyclopentanone (25.1%)	cyclopentanone (33.1%)	acetaldehyde
2	n-undecane (13.5%)	3-hexanone (10.2%)	2-ethyl-cyclopentanone (10.8%)	n-butanol (22.1%)	ethylene glycol
3	toluene (10.3%)	styrene (11.2%)	methyl methacrylate (7.2%)	methyl methacrylate (4.8%)	2-methyl-1,3-dioxolane

Source: He et al., 2015 and Thoden van Velzen et al., 2020

6.3.6. Risk reduction

There are significant differences between recycling facilities in safety measures taken regarding VOC emissions. In many facilities in developing countries these VOCs are discharged directly into the air without any ventilation or treatment (He et al., 2015). Workers in these areas are thus at high risk of health issues. In modern facilities ventilation and air treatment are present that reduces the risks for workers and residents in the area. See the article by Khan & Kr Ghoshal (2000) for the various options for removal of VOCs from the air.

According to Yamashita et al., (2007) fewer VOCs are emitted at lower temperatures, based on the melting of LDPE. When the melting temperature was reduced from 250°C to 200°C, VOC emissions drastically decreased (by over 80%). Lowering temperatures to 150°C resulted in a further reduction of VOCs. Additionally, it was found that lower oxygen levels also reduce the VOCs emitted during the plastic melting process.

Box 18. Polymer considerations

When polymers are melted in an extruder during mechanical recycling, VOCs emerge. Exposure to fumes of any synthetic plastic with no safety precautions can lead to cancer, birth defects and illnesses. Lowering the temperature and oxygen levels during the melting process reduces VOC emission.

a) Select a plastic that produces relatively low emissions of VOCs during recycling.

b) Source plastic for bottle production from a certified recycler that has taken all necessary safety precautions.

6.4. Mechanical recycling – Recyclability of pigments

Pigments are used to give a specific colour to HDPE detergent bottles. Using pigments to colour PET bottles is discouraged. Pigments influence sorting of the bottle and recyclability of the polymer.

6.4.1. Affecting bottle sorting

As elaborated on in Section 6.2, usage of carbon black pigment inhibits recognition of the packaging material in the sorting process. This means that packaging containing carbon black is not sorted in a mono-material stream. Therefore, usage of the carbon black pigment is discouraged for detergent bottles. Alternative pigments are available to create dark colours whilst maintaining recognition by NIR scanners[8]. However, from a recycling perspective dark colours are not desirable in general, because these influence the colour of the whole rHDPE-stream (unless a colour sorter is present).

6.4.2. Dark pigments decrease value of recycling stream

In general, a masterbatch contains 5-10% pigments. In a rHDPE bottle a masterbatch of about 3% is required. Thus the bottle consists of approximately 0.15-0.3% pigment. This percentage is quite small and is regarded as a contamination in the recycling stream. The more pigments that are added and the darker they are, the darker the recycled HDPE stream. Dark-coloured plastics are difficult to recolour with pigments and are thus of less value and in low demand on the market. As this effect is undesirable, it is recommended to use light-coloured pigments, prevent excessive use of pigments, and prevent the use of dark pigments in detergent bottles. This promotes many reuse cycles of the polymer. This recommendation is not solely applicable for detergent bottles, but for all rigid HDPE packaging that ends up in the packaging waste stream.

- **Colour sorting**: High-tech recycling facilities have colour sorters that sort plastic flakes into different colours. Dark colours are separated from light colours and white flakes (containing titanium dioxide) are also sorted. This enables a wider colour range for bottles made from recycled plastic, as lighter flakes are easier to recolour. This reduces the need for pigments in the masterbatch. However, colour sorters are not (yet) common practice in recycling facilities and should thus not be relied upon. Additionally, colour sorting does not improve the recyclability of dark coloured polymers, but merely makes them less disturbing by facilitating their removal from the process (KIDV, 2019). In light of achieving the sustainable design goal of closing material loops it is thus recommended to only use light pigments.

Box 19. Chemical considerations

When mechanical recycling is considered, the following points should to be adhered to:

- Avoid carbon black as a pigment for dark bottles. Carbon black prevents sorting of detergent bottles for recycling (HDPE bottles).
- Prefer light pigments over dark pigments to avoid a dark-coloured recycling stream. Use as few pigments as possible, for example by only using pigments in the outer layer in extrusion blow moulding (HDPE bottles).

6.5. Incineration and landfilling

6.5.1. Incineration of plastics

A huge amount of plastic is still incinerated today, usually for energy recovery. In Europe alone, 42.6% of all post-consumer plastics is incinerated (PlasticsEurope, 2019). However, incineration of plastics is not without risks. Besides the emission of greenhouse gases, there is growing concern about the potential atmospheric release of hazardous substances during incineration. Substances can be released as gasses, soot and residue solid ash (Okunola A et al., 2019; Valavanidis et al., 2008). Substances include halogenated additives, furans, dioxins, polychlorinated biphenyls (PCBs), volatile and semi-volatile organics, polycyclic aromatic hydrocarbon (PAHs) and toxic metals.

- **Gases** are produced with the pyrolysis or combustion of even a simple synthetic polymer (Nkwachukwu et al., 2013), such as hydrogen chloride and hydrogen cyanide. Most of these gases are self-toxic, i.e. interfering with the normal biochemical processes of the body. The type and concentration of gasses differs per polymer.
- **Halogenated additives** can be found in some pigments[9]. During combustion, small amounts of volatile organohalogen compounds will be formed. These combustion products are likely to be persistent, bioaccumulative, and toxic (Cradle to Cradle Products Innovation Institute, 2019). Furthermore, burning of PVC produces halogens which may pollute the air. (Verma et al., 2016)
- **Dioxins, furans and polychlorinated biphenyls (PCBs)** are produced during the manufacture of materials containing chlorine, such as PVC (Nkwachukwu et al., 2013). Burning these plastics can release dioxins. Open burning of such plastics must be avoided. Controlled incineration drastically reduces dioxin release, by controlling the incineration process, cooling of post-combustion gases and reducing the presence of specific metals such as copper (Lali, 2018). Dioxins, furans and PCBs have a high carcinogenic potential for humans.
- **Polycyclic aromatic hydrocarbon (PAHs)** are chemical compounds containing only carbon and hydrogen, composed of multiple aromatic rings. Some PAHs are carcinogenic and mutagenic. PAHs have been detected in soot at relatively high concentrations (Valavanidis et al., 2008), including PAHs known for their carcinogenic potential (e.g. Benz[a]anthracene, Benzo[a]pyrene, Indeno[1,2,3-cd]pyrene and Benzo[k]fluoranthene with fused rings).
- **Toxic metals** such as Pb, Cd, Cr, Cu, Ni are found in soot and residue ashes (Valavanidis et al., 2008), although their concentrations are very low. The highest levels of toxic metals were found when burning PVC.

Health effects

Without suitable safety measures, release of these substances during incineration poses a great threat to human health, in both workers and residents living nearby, and to the environment. Substances are released that are highly toxic and can cause cancer. Soot can end up in the surrounding environments and thus end up in the soil or water. Additionally, the ashes created in combustion are toxic. When these are not disposed of safely these can contaminate the environment.

According to Nkwachukwu et al. (2013) “a few of these pollutants, such as mercury, PCBs and dioxins, persist for long periods of time in the environment and have a tendency to bio-accumulate. In wildlife, the range of effects associated with these pollutants includes cancer, deformed offspring, reproductive failure, immune diseases and subtle neurobehavioral effects. Humans can be exposed indirectly just like wildlife, especially through consumption of contaminated fish, meat and dairy products.”

Safety measures

According to Nkwachukwu et al. (2013), plants compliant with the EU Waste Incineration Directive are not thought to have any significant environmental impact. To prevent pollution of atmosphere, soil and groundwater all incinerators must have a suitable filter system for toxic substances. Additionally, the disposal of fly ashes and slag have an environmental impact. For example, flue gas cleaning residues must often be disposed of as hazardous waste due to the toxicity of the compounds they absorb.

Due to the risks involved in plastic incineration and loss of valuable materials, incineration is a highly undesirable scenario for detergent bottles.

6.5.2. Landfilling of plastics

This section describes the chemical considerations related to the disposal of plastics in landfill. It must be noted that landfilling is not a preferred disposal route and must be avoided at all times. However, globally 80% of plastics was accumulated in landfills between 1950 and 2015 (Geyer, Jambeck and Law, 2017). The capacity of landfills is finite: landfilling of plastics is not an activity that can be sustained over time (Scott & Hannan, 2006). Plastics degradation is extremely slow and thus the material will not quickly decrease in volume. As other types of waste degrade, plastic remains. This means that the volume of plastic in landfills accumulates over time.

Additionally, landfills are an unsafe method for disposing of plastics. Leakage of additive chemicals to the soil and marine environment occurs, transferring these chemicals to animals and humans. In addition, wildlife ingests or gets entangled in plastic waste and microplastics are created (Scott & Hannan, 2006). Because research on the effects of plastics in landfills, and the environment in general, is still relatively new, there remains much uncertainty. The long-term effects in particular are difficult to gauge. However, there is a consensus that plastic in the environment has negative effects and must be avoided.

Microplastics

Over time, plastic in landfills degrades and decomposes over hundreds or thousands of years, gradually fragmenting into microplastics and nanoplastics. Microplastics can migrate beyond the landfill, e.g. through the air or the aquatic environment, and enter the food chain and pose risks for human health for example through:

- Microplastics ingested by fish and shellfish (Thompson, 2015).
- Microplastics can be absorbed by roots of crops (Li et al., 2020).
- Microplastics found in tap water and bottled water (Kosuth et al., 2017).

Much is still unknown about the effects of microplastics and nanoplastics. Large quantities of plastics have only been present in the environment for a relatively short period of time. It is therefore difficult to gauge its consequences.

A type of plastics that causes particular risk for creation of microplastics are degradable, as opposed to biodegradable, polymers (known as oxo-(bio)degradable). According to Thompson (2015) “Oxo-degradable polymers are designed to break down under UV exposure and/or dry heat and mechanical stress, leaving small particles of plastic They do not degrade effectively in landfills and little is known about the timescale, extent or consequences of their degradation in natural environments.” Use of oxo-biodegradable plastics is prohibited by the EU starting 2021, as part of the SUP directive[10]. Therefore, use of oxo-degradable plastic must also be prevented in detergent bottles.

Leakage of additive chemicals into the environment

Additive chemicals in plastic in landfills can leak to the environment. This results in a polluted environment around the landfills and can end up in aquatic environments. Additives of particular concern are phthalate plasticisers, Bisphenol A (BPA), brominated flame retardants and anti-microbial agents (Thompson, 2015). However, as was elaborated pm in Section 4.3, these substances are not present in PP, HDPE and PET for the application of detergent bottles, but are generally present in PVC. Therefore, leakage of these substances to the environment is not relevant for this case study.

Box 20. Design considerations

Promote Design for Recycling to increase chances that packaging will end up in recycling stream. Disposal of plastics in landfill highly undesirable.

Box 21. Polymer considerations

Prevent use of oxo-degradable plastics: degradability of these plastics is not achieved in the landfill environment. These types of plastics also have a negative impact when ending up in the recycling stream. The EU plastics directive will ban use of oxo-degradables in 2021.

Box 22. Chemical considerations

Prevent additives that can leak into the environment: e.g. phthalate plasticisers, BPA, brominated flame retardants, anti-microbial agents.

6.6. Chemical recycling

Chemical recycling of the detergent bottles is included in this case study to refer to the possible future options and restrictions. The current availability of chemically recycled plastics comes from pilot plants and carefully selected and sorted waste. The environmental benefits of the technologies are not yet proven. Chemical recycling promises to be a solution for hard-to-recycle or contaminated plastic waste. However, it is currently not available on a scale that it should be taken into consideration in packaging design or has been developed far enough to be regarded as the sustainable solution for the future. Additionally, mechanical recycling of detergent bottles is always preferred, as it enables larger recovery of material while using less energy.

Chemical recycling is an umbrella term for a range of different processes that break down polymers to monomers or other chemicals that can be used to make new plastics or other useful products. Summarizing from WRAP (2019) Thoden van Velzen et al. (2020), Eunomia, (2020) and Solis & Silveira (2020):

- **Solvolysis**: A process still in development, with a few companies operating pilot plants. PET, PLA, or PA are converted to monomers and oligomers for plastic production. For an efficient process, it requires carefully sorted waste from the targeted polymer as input.
- **Selective dissolution**: A process in which a specific polymer is dissolved from mixed waste, laminates, or from sorted but contaminated plastic waste. The specific polymer can be recovered for plastic production after an elaborate filtration and precipitating process, the rest is still waste. This is also still in the pilot phase.
- **Pyrolysis and gasification**: Mixed plastic waste is broken down into char and gas or oils of smaller hydrocarbons, which can be used as fuel, as a product such as lubricating grease, or can be further refined into monomer building blocks for polymer production. For efficient processes sorted plastic containing predominantly polyolefins is required.

It should be noted that the processes with fuel as output or chemical downcycling should not be regarded as solutions to close material loops. Only processes that result in a secondary raw material that can be used in the production of plastic products should be regarded as truly circular recycling methods. All processes are in theory able to process a mix of plastics. However, for efficiency and an environmental benefit, the waste should be pre-sorted, all other contaminants in the throughput reduce the efficiency of the process.

Box 23. Design considerations

Chemical recycling is currently not a plausible EoU scenario and should not be taken into consideration in the packaging design. When chemical recycling becomes a serious sustainable option, the packaging should contain as much of the specific targeted polymers as possible. In the current technology, those polymers are PET, HDPE or PP.

Notes

[1] NIR is a standard in most recycling plants and thus used as a benchmark.
[2] A full body sleeve can enable the usage of a clear bottle as it also functions as a UV-barrier.

[3] In general, closures are made from a different polymer than the bottle because the materials must have a different hardness to provide a solid closure without needing an inlay. For HDPE bottle PP closures are commonly used. For PET bottles, both HDPE and PP are suitable. In the past, PP was used more frequently, but a trend towards HDPE closures can now be seen.

[4] Use of MICA (pearl effect) or metal flakes (metal effect) in caps and closures is common in detergent packaging to give a more high-end look and feel to the product.

[5] In practice, of course, recycling of detergent bottles is not a closed loop system. Detergent bottles are collected, sorted and recycled along with other plastic packaging waste. This means bottle-to-bottle recycling of detergent bottles also depends on the quality of the other plastic packaging collected.

[6] Food application of rHDPE is possible when it can be proven that the origin of the recycled polymer is food grade. However, this requires a closed loop recycling system, which is not common practice.

[7] ABS and PS release the highest number of VOCs, these contain styrene, benzene and ethylbenzene - these compounds are called cyclic compounds which create a lot of fumes and may cause cancer.

Benzene is a human carcinogen, and styrene and ethyl benzene are probable carcinogens (probable carcinogen means that the compounds have not yet proven to cause cancer).

However, the most dangerous are PVC and PA, as these release the most harmful VOCs when melted.

[8] Pigments 'Black 95491' and 'Black 95491' do not inhibit NIR detectability of the packaging (Dvorak et al., 2011).

[9] Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond.

[10] More information on the SUP Directive can be found here: https://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:52018DC0035&from=EN

Chapter 7. Key considerations and trade-offs

7.1. Key considerations

Key considerations are the most important sustainability aspects on which a material selection should be based. For a detergent bottle, the following hotspots are identified per life cycle stage:

7.1.1. Material sourcing

- Since bottle-to-bottle recycling is feasible for detergent bottles, polymer selection should facilitate this. Therefore, HDPE and PET are regarded as suitable polymers; PP is regarded as unsuitable because recycled PP cannot be used for the production of detergent bottles.
- Prefer recycled (secondary non-renewable) feedstock for the production of detergent bottles. This contributes to a closed material loop and reduces the environmental impact of the packaging. Aim for the highest possible percentage of recycled material.
- Carefully consider using food grade recycled plastic (e.g. rPET) for the non-food application of detergent bottles, as it limits the availability of food-grade plastics for food-grade applications.
- When supplementing recycled plastics with virgin plastics, consider using a bio-based feedstock from residual organic waste streams. This reduces the need for fossil fuels. Validate the environmental benefits of the feedstock with an LCA.
- Recycled polymers have a reduced ESCR compared to virgin polymers. Therefore, packaging concentrated detergents in bottles made from 100% PCR is challenging or unfeasible. A percentage of virgin fossil or bio-based content is required.
- Recycled feedstock can contain impurities or non-intentionally added substances. Evaluate whether expected NIAS are below accepted migration limits and whether potential hazards may occur during the life cycle.
- Only source recycled polymers from certified recycling facilities that take the prescribed safety measures. In this way exposure of hazardous substances to workers and neighbouring residents is avoided.
- Carefully consider addition of chemical substances beyond antioxidants, compatibilisers and pigments in the polymerisation or recycling process as it is likely that these additional substances are not essential. Using fewer additives is beneficial throughout the lifecycle.
- When selecting additive substances, beware that some additives can migrate into the detergent, are volatile, and potentially pose a threat to human health and/or the environment.

7.1.2. Production

- The sustainability of the production method must be considered on a system level during polymer selection. For example, the distance between the bottle-blowing production facility and the filling location can be considered, and transporting empty bottles over long distances can eliminate other sustainability benefits gained in a polymer selection.
- Consider the necessity of using lubricants to release bottles from the mould. These are often not essential, but are used to speed up processing times. Consider the gained benefits versus caused contamination.
- Carefully consider which and how much pigments are used in the bottle. Some pigments pose risks for human health and the environment. Additionally, the value of dark-coloured bottles at end-of-use is lower because these negatively influence the quality of the recycling stream. For PET bottles, any use of pigments is discouraged.

7.1.3. Use phase

- Consider what barrier properties are required to preserve the detergent during its shelf life and which polymer has sufficient chemical resistance to prevent product spoilage. Aim to select a polymer that can offer these properties without requiring additional substances in the material and bottle production processes.
- Avoid transparent PET packaging for UV-sensitive detergents to avoid use of UV absorbers or blockers. Use opaque HDPE bottles for these detergents.
- Aim for an optimised, space efficient bottle design for efficient transportation to reduce transport movements and involved environmental impacts.

7.1.4. End-of-use

- The available waste infrastructure in the intended sales market determines the end-of-use scenario that can be designed.
- Optimise packaging design (including label, adhesives and closures) for effective sorting, washing and mechanical recycling. To facilitate bottle-to-bottle recycling of detergent bottles, compromises on a recyclable design should be avoided. Additionally, also consider applying a digital watermark or fluorescent tracer to the label or bottle to allow sorting of the packaging as part of the HolyGrail project. Follow developments on this project and design accordingly.
- Incineration and landfilling cannot be deemed as sustainable scenarios, and chemical recycling technology is not mature and widespread enough to act as a basis for design decisions.

7.2. Trade-offs

The decisions or constraints in one step of the life cycle influence the possibilities in the other stages. The table below indicates how constraints set in the top row of the table influence the stages in the leftmost column.

Table 7.1. Dependencies between decisions and constraints in one life cycle stage to the other stages.

How → influences ↓	Sourcing	Production	Use	End-of-use
Sourcing		A selected production method requires specific feedstock (and additive substances)	Requirements on barrier properties and chemical resistance limit sourcing options.	Aiming for bottle-to-bottle recycling limits the polymer and sourcing options.
Production	Available polymers might require specific production methods and additives.			Sorting and mechanical recycling of a bottle depends on the bottle design.
Use		Usability of bottles.		
End-of-use	Selected polymers and their required additives might limit the EoU options.		Available EoU scenario in specific sales markets.	

Trade-offs that need to be made concern reduction of material use through primary feedstock versus closing material loops through secondary feedstock. Outcomes of trade-offs depend on local situations.

Reduce material use Light weighting of the bottle to reduce material might require polymers of virgin quality	***vs*** **or**	***Close material loops*** To effectively close material loops recycled content in bottles must be maximised, possibly leading to heavier designs
Reduce material use PET bottles require less material in production compared to HDPE bottles	***vs*** **or**	***Close material loops*** Recycled PET is sourced from a (scarce) food grade stream
Preserve natural capital Highly concentrated detergent leads to fewer transport movements but requires bottle with very good ESCR which can currently not be produced using 100% recycled HDPE.	***vs*** **or**	***Close material loops*** Using 100% recycled feedstock for bottling less concentrated detergent requiring more transport movements.
Prevent product spoilage Using additives and coatings to enhance product shelf life and strength of packaging.	**vs** **or**	**Close material loops** Recyclability of plastic bottle.

7.2.1. Trade-offs on a system level

In the development of bottles, sustainability is not the only topic on which trade-offs are made. The sustainability of a bottle (design) is often in conflict with the desired aesthetics for marketing purposes, or is driven by costs. A few of these trade-offs are highlighted below.

Product marketing	**vs**	**Close material loops**
Transparent bottles have an attractive appearance, but require use of a UV barrier additives when containing UV sensitive detergents.	**or**	UV barriers compromise closing the material loop.
Product marketing	**vs**	**Preserve natural capital & close loops**
Bottles made from virgin feedstock allow for transparent or bright coloured bottles.	**or**	Bottles made from secondary feedstock allow for less bright colours (rHDPE) and might have a grey/yellow discolouration for transparent rPET bottles, but reduce the environmental footprint.
Cost reduction	***vs***	***Close material loops***
Low prices of virgin PET with premium aesthetics.	**or**	High prices for recycled feedstock with slightly reduced aesthetics.

Chapter 8. Material assessment

In this chapter, material assessment is given an example, with criteria and information gathered within the limits of this case study. It is not to be regarded as an all-encompassing advice on the most sustainable plastic detergent bottle design.

The polymer options HDPE, PP and PET are considered, based on the sustainability criteria that emerged from the life cycle analysis. First, the polymers are assessed in Section 8.1, leading to a polymer shortlist. Subsequently, the chemical considerations are addressed in Section 8.2. Finally, Section 8.3 and 8.4 explore the considerations to be made in terms of design and policy.

8.1. Polymer shortlist

8.1.1. First selection

Based on Chapter 4, from a sustainability perspective, polymer feedstocks are prioritised as follows:

- Recycled plastics – Secondary feedstock
- Bio-based plastics – Renewable feedstock
- Virgin plastics – Primary fossil-based feedstock

The required barrier properties and chemical resistance of a detergent bottle can be fulfilled using recycled plastics (secondary feedstock). Therefore, the use of primary fossil feedstock is discouraged to enable closing the material loop and carry out bottle-to-bottle recycling for detergent bottles. In the transition to a circular economy, same-value recycling is essential. Virgin plastics can be used in the masterbatch or to upgrade the quality of the recycled polymer, but for this purpose the use of renewable feedstock should be considered first. However, an LCA should be performed to guide final decision making between bio-based and virgin plastic, as the specific feedstock of a bio-based plastic influences its sustainability.

The shortlisted polymers are first be assessed on the availability of renewable or secondary feedstock, renewability of the material itself and potential for bottle-to-bottle recycling. Based on Table 8.1, it can be concluded that PP is not a sustainable polymer for application in detergent bottle packaging. Recycled PP is not suitable for the production of bottles and renewable feedstock is not available. Therefore, PP is not further considered as a polymer suitable for application in detergent bottles in the context of this assessment.

Table 8.1. Availability of renewable or secondary feedstock of short-listed polymers.

	HDPE	PP	PET
Recycled feedstock available			
Recycled feedstock can be used for bottle production			
Plastic is recyclable			
Bottle-to-bottle recycling			
Renewable feedstock available			
Conclusion	Further investigated	Not further investigated	Further investigated

8.1.2. Polymer assessment

The second sequential selection is conducted by evaluating other sustainability criteria for the more detailed polymers. For both HDPE and PET polymer types, virgin and recycled feedstocks are considered. It is assumed that polymers from a bio-based feedstock have the same characteristics as virgin feedstock.

Table 8.2 shows the different characteristics of HDPE and PET and their recycled variants, indicating which are supporting the considerations between HDPE and PET for application in detergent bottles. The polymers differ primarily in aesthetics (transparency) and chemical resistance. From a sustainability point of view, recycled HDPE is the preferred feedstock for detergent bottles: this feedstock does not require the use of fossil feedstock, bottles from rHDPE can be recycled and its material reused for the production of new bottles (bottle-to-bottle recycling). The predominant concern with regard to rPET is that it is primarily sourced from a food-grade feedstock. While it is technically feasible to recycle PET detergent bottles and produce new bottles of the material, this is currently not common practice.

Table 8.2. Different characteristics of HDPE and PET and their recycled variants.

	HDPE	rHDPE	PET	rPET
Characteristic				
Moisture barrier				
Gas barrier				
Transparency				
UV barrier	*			
Resistance to surfactants				
Resistance to solvents**		***		
Resistance to caustics**		***		
Resistance to acids**		***		
Handle in design				
Can be used in the production of new bottles				
Conclusion		Preferred material		

Note: * Translucent HDPE has no UV barrier, however, adding pigments will provide a barrier
** Not relevant for laundry detergents
*** Expected to be similar to virgin HDPE, but requires validation

8.1.3. Additional considerations on polymer selection

When selecting a polymer, there are other aspects to consider beyond feedstock and technical performance. These additional considerations are listed below:

- Recycled polymers can contain impurities or non-intentionally added substances (NIAS) (e.g. contaminants or breakdown products). Ensure safety of rPET and rHDPE polymers by evaluating if expected NIAS are below the accepted migration limits. A material supplier should facilitate this.
- Consider shedding of microplastics in the polymer selection. HDPE is expected to shed more microplastics during use compared to PET, but for both polymers the released quantities are small. The shedding can also differ based on the polymer composition.
- When polymers are melted in an extruder during mechanical recycling, VOCs emerge. Exposure to fumes of any synthetic plastic with no safety precautions can lead to cancer, birth defects and illnesses. Lowering the temperature and oxygen levels during the melting process reduces VOC emission. Select a plastic that emits limited VOCs during recycling. Importantly, source recycled feedstock from a certified recycler that has taken all necessary safety precautions.

8.2. Chemical considerations

Once a polymer is selected, relevant chemical considerations need to be revisited to make decisions in the production process and guarantee safe and sustainable chemical selection. During the analysis of the life cycle, the following considerations have been encountered.

8.2.1. Barrier properties

- When using additives or coatings, carefully consider how these act in the bottle. If not embedded in the polymer matrix, they can potentially migrate into the detergent.
- A UV barrier can improve the shelf life of a detergent. A UV barrier can be provided by adding pigments to detergent bottles. Use of pigments is preferred over chemical additives or coatings that provide a UV barrier.
- Use of UV absorbers and blockers in transparent PET is discouraged. When extruded in recycling, these cause a yellowing of the material.
- It is recommended to avoid use of colour additives in PET as this compromises the recyclability of the material.
- When using additive substances or coatings on the bottle it is important to carefully consider if these migrate into the detergent. If additives are not embedded in the polymer matrix, migration can take place. If this scenario is likely, safety of the used substances or coating is essential.

8.2.2. Sourcing of materials

- Chemical additives are added to the virgin plastic to serve specific purposes, but can have consequences for the sustainability of the plastic packaging. They might hamper recyclability or pose a toxicity risk to human health or biodiversity at any point in the life cycle. It should be considered whether the addition of the chemicals to the plastic is indispensable or whether more sustainable alternatives can be chosen.
- For detergent bottles, antioxidants (processing stabilisers) are the most relevant. Using antioxidants supports the recyclability of the polymer, as it prevents polymer degradation. Avoid use of the antioxidants BHT and Cyanox 2246, as these can migrate to the detergent and contaminate the wastewater.
- rHDPE: For improving the rHDPE quality substances are added such as antioxidants, compatibilisers for PP contamination and pigments.
- rPET: Carefully consider whether to use blue colourant as an anti-yellowing agent, as this colourant results in a grey haze in the rPET stream.
- rPET: Always conduct SSP on rPET pellets, as this reduces migration of substances during the life cycle.

8.2.3. Production of plastic and bottles

- Avoid using halogen-containing pigments because the combustion products in case of incineration are toxic. Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.
- Pigments containing toxic elements such as lead, cadmium, mercury, vanadium, chromium(VI), cobalt, nickel, arsenic, antimony or selenium should be avoided.

- Azo pigment containing one or more carcinogenic aromatic amines as defined in European regulation 76/769/EEC should be avoided.
- Carefully consider the necessity of using lubricants to release bottles from the mould.

8.2.4. End-of-use

- Pigments: Avoid using carbon black as a pigment, because it prevents correct sorting of detergent bottles and thus inhibits recycling.
- Pigments: Prefer light pigments over dark pigments to avoid a dark-coloured recycling stream. Use as few pigments as possible, for example by only using pigments in the outer layer in extrusion blow moulding (HDPE bottles).
- HDPE and PP: Ensure the density of HDPE and PP used in bottles is not above 1g/cm3. Otherwise, the plastic will not be sorted for recycling. Therefore, use a mono-material and avoid fillers.
- Additives: Prevent additives that can leak to the environment: e.g. phthalate plasticisers, BPA, brominated flame retardants, anti-microbial agents.

8.2.5. Guidelines for the safe selection of chemical additives

- For safe chemical selection, see the methodology set out in Section 2.2.

8.3. Design considerations

8.3.1. Space-efficient design

Optimise bottle design for efficient transportation to reduce transport movements and thus preserve natural capital. This means excessive curves, headspace and ‘shoulders’ should be avoided. Additionally, it is recommended to only use a handle for bottles larger than 2 litres.

8.3.2. Design for recycling

Design for recycling is essential to enable reuse of the materials. When a bottle is mechanically recycled, investigate the local sorting and recycling process. In general, when mechanical recycling is considered the following design rules need to be adhered to, to allow sorting of the plastics in pure mono-streams:

- Labels: Avoid the use of full-body sleeves and PVC labels.
- Labels: Select the material and size of the label to enable sorting and recycling of the detergent bottle.
- Closures: Avoid fillers in PP and HDPE closures that increase the density above 1g/cm3 to enable the closure material to be separated from the plastic bottle. Use of fillers in PP and PE can increase the density of the polymer, causing it to sink instead of float. The recycling process is based on the floating properties of PP and PE.
- Adhesives: Select adhesives for the label that are soluble or can be released in the washing process.

Chapter 9. Policy considerations

This case study leads to insights about current practices that inhibit genuinely sustainable use of plastic detergent bottles. Five considerations for policy and research by regulatory bodies are proposed.

Note that these considerations mainly concern the safe and circular application of plastic packaging. However, it should be kept in mind that a circular economy is a means to an end of a sustainable future, not a goal in itself. The ambition should focus on minimising resource use and overall environmental impact.

Encourage the use of recycled plastics

Detergent bottles are very suitable for the application of recycled plastics. Currently, 'costs' are a dominant driver in polymer selection. A lower material price for virgin feedstock versus recycled feedstock inhibits large-scale demand for recycled plastics. To stimulate the uptake of recycled plastics, for this (and other non-food) application(s), different approaches can be considered, such as a mandatory minimum percentage of recycled content or a positive monetary incentive, e.g. by reducing taxes on recycled feedstock or by increasing taxes on / incorporating negative impacts in the price of virgin feedstock. Procurement can also play a role here by demanding a minimum recycled content.

Encourage recyclable design of detergent bottles

Bottles must be recyclable by design, based on the local EoU scenario, to enable bottle-to-bottle recycling. Increasing the recyclability of the bottle both enhances its circularity and increases the volume, and thus the availability of recyclable plastics. Recyclable design can be stimulated through a positive monetary incentive, such as taxes or extended producer responsibility. For example, in the Netherlands, a waste management contribution is paid for all packaging that enters the Dutch market. The contribution is reduced by approximately 50% for recyclable plastic packaging. Procurement can also play a role here by demanding a recyclable design.

Discourage the use of potential hazardous substances

Some substances with known or suspected hazards are used to perform functions in detergent bottles despite the existence of alternative substances. One drawback of these alternatives is that they are not commercially attractive due to higher costs, lower process efficiency, or incompatibility with currently installed machinery. Policies should be developed to discourage, or in some cases ban, the use of potential hazardous substances, either through financial instruments such as taxes, extended producer responsibility, or by prohibiting the use of the substance (either completely or in certain applications, depending on the nature of the hazard and the exposure risk) unless it is demonstrated that the substance causes no harm.

Mandatory safety standards for plastic recyclers and waste incinerators

Poor recycling and waste management practices can lead to the emission of hazardous substances. This poses risks both through occupational exposure of workers as well as through emissions to the environment and to nearby residential areas. The risks can be reduced with solutions such as vacuum extrusion, strict control of extrusion temperatures, proper ventilation and air treatment. Regulatory bodies should create mandatory standards for recyclers and waste incinerators based on best available practices. EuCertPlast is an example of European certification of plastic recycling processes.

Encourage transparency within the supply chain

Encourage full disclosure of information on material composition and additive substances used in the packaging within the supply chain. As such, purchasers would gain more insight into the current use of material for their bottle (or other packaging) and could steer towards more sustainable and recyclable material compositions. One method to promote transparency could be the certification of recycled plastics. Prices of recycled materials are sometimes higher than their virgin alternatives, which is especially the case for PET. In the market, virgin PET is sometimes sold as recycled PET. To prevent such practices, it is recommended to promote development of certificates for recycled plastics with chain-of-custody traceability.

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This case study on detergent bottles was developed to provide input to and inform the development of general considerations for design of sustainable plastics from a chemical perspective. Four case studies were developed as concrete examples and included two in the plastic packaging sector (biscuit wrappers and detergent bottles) and two in the construction sector (flooring and insulation). For this purpose, the case studies start from the premise that plastic material will be used and therefore alternative material selection is not considered. They identify the key considerations regarding environmental/health sustainability that should be examined along the product life cycle when chemicals are selected at the design stage, as well as the potential trade-offs between these considerations.

The examples of material selection within the case studies are developed in the context of the information gathered for the case studies to exemplify the sustainable design process and to highlight key considerations. To make actual decisions about material selection other factors would also need to be considered and the analysis could be further informed by elements such as life cycle assessment comparing alternatives and a full review of regulatory restrictions.

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