



# Level 3 Industrial Case Study

## Water Containers and Plastic Waste

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## Summary

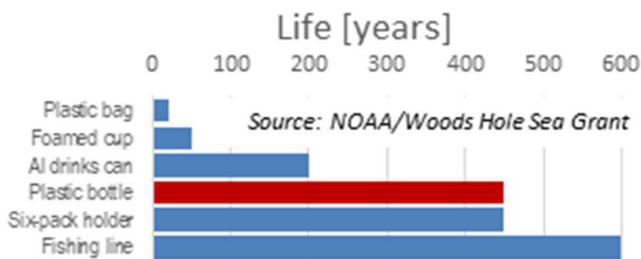
In order to engage students of today, it is important to find topics that are perceived as relevant to them. The Granta EduPack platform has data and tools that enable investigations into many material decisions, both in design of new products and re-design of existing ones. It can also be used to assess and understand different approaches and options within product development and design, not least when it comes to environmental properties. This advanced industrial case study highlights the problem of plastic waste and we have used the Eco Audit tool to investigate material options for water containers. It contains ideas and information useful for performing a practical exercise in the classroom in the shape of a computer-aided, interactive group activity.

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## 1. Scope

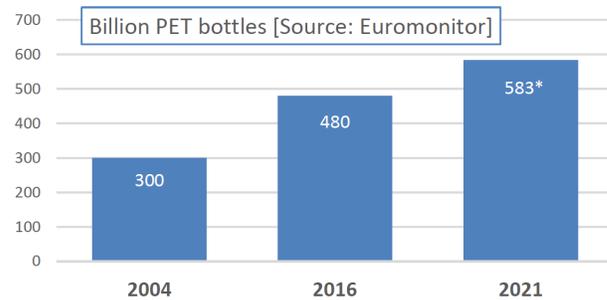
The BBC documentary, *The Blue Planet II*, has raised awareness and sparked a debate about the use of plastics in our society and the consequences to the marine environment. Up to 12 million tonnes of plastics end up in the sea every year. The concerns range from whole objects to microplastic particles as well as chemicals associated with these products. Around 1 million tonnes per year enter as primary microplastics, but most of it is larger plastic litter from land-based sources. In particular, packaging, such as drinks bottles, and various disposable plastics have been highlighted as problematic [1].



Plastic bottles are likely to be floating, but only 1% of marine plastics are found near the surface of the ocean, with an average global concentration near 1 kg/km<sup>2</sup>. The highest concentration is recorded in the North Pacific Gyre at 18 kg/km<sup>2</sup>. This patch is clear evidence of the accumulative effect of plastics as waste. One main problem is that plastics are very long-lasting [2] and not part of any natural cycle.

Rather than to blame the material alone, we must look at the product design and how we use plastics in packaging. Well over one million plastic bottles are bought around the world every minute and the number may increase by up to 20% by 2021 [3]. Most plastic bottles used for soft drinks and water are made from polyethylene terephthalate (PET), which is highly recyclable. However, it is estimated that globally only around 9% of plastic waste is recycled. A further 12% is incinerated, and 79% is deposited in landfills or in the natural environment [2]. It is a question of life-cycles.

### We produce almost 20 000 bottles per second



It is important that material life-cycles are discussed in engineering and design courses, to enable future generations of product developers to consider long-term effects, such as this waste problem. Different materials need to be considered and alternative concepts, which minimize negative environmental (and social) impact. In this case study, we show that Granta EduPack can be used to aid discussion and help informed decision-making in product development. We provide a life-cycle comparison of PET bottles and some alternative water containers using the Eco Audit and propose a classroom exercise/practical that can be done with students in small groups.

## 2. What can EduPack do?

**The material**

The name polyester derives from a combination of 'Polymerization' and 'esterification'. Saturated polyesters are thermoplastic - examples are **PET** and PBT; they have good mechanical properties to temperatures as high as 175 C. **PET** is crystal clear, impervious to water and CO<sub>2</sub>, but a little oxygen does get through. It is tough, strong, easy to shape, join and sterilize - allowing reuse. When its first life comes to an end, it can be recycled to give fibers and fleece materials for clothing and carpets. Unsaturated polyesters are thermosets; they are used as the matrix material in glass fiber/polyester composites. Polyester elastomers are resilient and stretch up to 45% in length, they have good fatigue resistance and retain flexibility at low temperatures.

**Environmental notes**

**PET** bottles take less energy to make than glass bottles of the same volume, and they are much lighter - saving fuel in delivery. Thick-walled bottles can be reused; thin-walled bottles can be recycled - and are, particularly in the US.

**Supporting information**

**Design guidelines**

There are four grades of thermoplastic polyesters: unmodified, flame retardant, glass-fiber reinforced and mineral-filled. Unmodified grades have high elongation; flame retardant grades are self-extinguishing; glass-fiber reinforced grades (like Rynite) are some of the toughest polymers but there are problems with dimensional stability; and mineral-filled grades are used to counter warping and shrinkage although some strength is lost. The **PET** used in carbonated drink containers is able to withstand pressure from within, it is recyclable and lighter than glass. The limits of the material's permeability to oxygen is overcome by sandwiching a layer of polyethylenediacetate between two layers of **PET** giving a multi-layer material that can still be blow molded. Polyester can be optically transparent, clear, translucent, white or opaque; the resin is easily colored.

Granta EduPack has materials data covering a relevant range of materials for water containers; glass, aluminum, cardboard, and polymers, such as PET. The database includes eco-data (embodied energy, carbon footprint, water consumption), as well as recycling and biodegradation information. A search for **PET** in the database results in a datasheet with a useful overview of this plastic with basic facts, such as composition, as well as support for design decisions, both at Level 2 and Level 3.

Another polymer that would be familiar to most people is a material used for plastic bottle caps, *polypropylene* (PP). There is an abundance of applications for this plastic, as can be seen in the datasheet at Level 2. This rich information is useful when searching for specific applications within design and product development, looking for inspiration and materials for similar concepts. It means that PP will be one of the materials suggested upon searching for *containers or packaging*, for example.

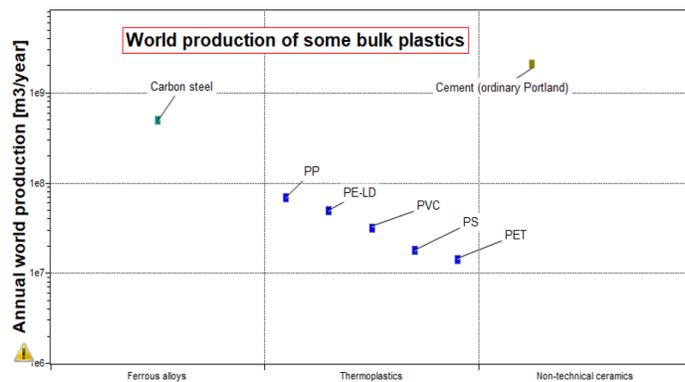
**Typical uses** ⓘ

Automotive interior parts, appliance components, electrical/electronic applications, packaging, cosmetic, cosmetics, coating applications, automotive under the hood, parts, thin-walled, compounding, containers, shipping, consumer applications, household goods, bags, packaging, food, sheet, clear, color concentrates, fabrics, industrial applications, laminates, containers, thin-walled, cups, packaging, media, toys, parts, engineering, mining applications, coatings, fabric, coatings, foil, coatings, non-wovens, coatings, paper, coatings, wovens, packaging, rigid, appliances, lids, furniture, sporting goods, tool/tote box, kitchenware, general purpose, lawn and garden equipment, automotive exterior parts, outdoor furnishings, containers, food, outdoor applications, bathroom accessories, automotive bumper, automotive instrument panel, packaging, thin-walled, washer, parts, industrial, trays, support, luggage, audio tapes, film, cast, film, multilayer, vials, film, bi-axially oriented, film, oriented, hypodermic syringe parts, labware, parts, transparent or translucent, hinges, living, bonding, containers, industrial, hospital goods, batteries, buckets, bowls, general mechanical parts, bottle crates, medical components, washing machine drums, pipes, battery cases, bottles, bottle caps, films for packaging, fibers for carpeting and artificial sports surfaces.

**Composition overview** ⓘ **Design support for PP at Level 2**

**Compositional summary** ⓘ

Random copolymer of propylene (CH<sub>2</sub>CH(CH<sub>3</sub>))<sub>n</sub> small amounts of ethylene (CH<sub>2</sub>CH<sub>2</sub>)<sub>m</sub> or other comonomer, forming a single phase material. Ethylene content up to 7% but typically 2-4%.



The data can also be used to discuss resources. For example, to illustrate the magnitude of the annual world production of plastics, and how the most common polymers compare with other bulk materials. To the left, production *volumes* from the database is shown. Although polypropylene is one of the most produced polymers in the world, a quick look at the *Recycling and end of life* information in the datasheet, seen below, reveals that there is less than 3% of recycled PP in the industrial supply and that PP is not biodegradable.

Eco-properties are, of course, interesting in themselves, but for fair comparisons, the whole life-cycle of, *e.g.*, a water container, has to be considered. In circular economy, several life-cycles needs to be included. An Eco Audit takes into account feedstock and end-of-life options for the materials, as well as the manufacture and use phases of a product. The feedstock can be virgin material, reused material (no energy required), or, any specified mixture of recycled and virgin fractions of the materials.

**Material recycling: energy, CO<sub>2</sub> and recycle fraction**

Recycle	ⓘ	✓
Embodied energy, recycling	ⓘ	* 22.3 - 24.7 MJ/kg
CO <sub>2</sub> footprint, recycling	ⓘ	* 0.94 - 1.04 kg/kg
Recycle fraction in current supply	ⓘ	2.57 - 2.84 %
Downcycle	ⓘ	✓
Combust for energy recovery	ⓘ	✓
Heat of combustion (net)	ⓘ	* 44 - 46.2 MJ/kg
Combustion CO <sub>2</sub>	ⓘ	* 3.06 - 3.22 kg/kg
Landfill	ⓘ	✓
Biodegrade	ⓘ	✗
Toxicity rating	ⓘ	Non-toxic
A renewable resource?	ⓘ	✗



At Level 2, all thermoplastics indicate recycling marks. The full range of end-of-life options in the Eco Audit are: *Landfill*, *Combust*, *Downcycle*, *Recycle*, *Re-manufacture* and *Reuse*. These utilize the eco-property data for virgin and recycled materials in the datasheets, as shown above.

### 3. Level 2 vs Level 3

Our advanced industrial case studies normally make use of the Level 3 databases and showcase advanced features of the Granta EduPack. When it comes to eco design, the Level 2 database is also powerful, and has access to the Eco Audit tool similar to advanced databases. Some features, such as the *images* of materials and manufacturing processes in typical applications can only be found at Level 2.



**General information**

**Overview** ⓘ

**PET** was originally only used to produce fibers for clothing (polyester). In the last three decades, its use for blow-molded drinks/food containers has become highly significant due to its generally good properties and superiority to glass for such applications (particularly in terms of brittleness and strength to weight ratio).

**Strengths** ⓘ

Good water vapor and oxygen barrier. High strength and stiffness (for commodity/engineering thermoplastic). Excellent transparency/clarity, practical and established recycling, low friction. Good low frequency electrical properties, good melt flow, good resistance to gamma radiation (allows for sterilization), very good surface finish. Easily colored, can be optically transparent, clear, translucent or opaque.

**Limitations** ⓘ

Unfilled **PET** is problematic to injection mold compared with PBT. Very susceptible to heat degradation in amorphous form (less so when semi-crystallized), burns easily (unless fire retardant grade used), can release harmful fumes during processing, poor heat distortion temperature. High mold shrinkage, limited resistance to hydrolysis, limited usefulness below 0 °C (32 °F) (becomes brittle). Cannot be steam sterilized due to low hydrolysis resistance.

**Designation** ⓘ

Often the specific polymer referred to as polyester, even though polyesters are a broad class.

**Typical uses** ⓘ

Amorphous: Blow-molded bottles, packaging film, film, photographic and X-ray film, audio/visual tapes, industrial strapping, capacitor film, drawing office transparencies, fibers. Semi-crystalline: Electrical fittings and connectors, audio/visual tapes, industrial strapping, capacitor film, fibers.

**Composition overview**

**Compositional summary** ⓘ

(CO-(C6H4)-CO-O-(CH2)2-O)n

Material family	ⓘ	Plastic (thermoplastic, semi-crystalline)
Base material	ⓘ	<b>PET</b> (Polyethylene terephthalate)
CAS number	ⓘ	25038-59-9

**Effect of composition** ⓘ

Amorphous grades have better clarity and barrier properties than semi-crystalline grades. Voluminous comonomers such as isophthalic acid or 1,4-cyclohexane dimethylol are used to lower crystallinity for production of transparent parts. Gas barrier properties can be further improved for specialized application by multi-layering with polyvinyl alcohol. Unmodified grades have high elongation. Glass-fiber reinforced grades are tough and strong though dimensional stability can be problem. Mineral-filled grades are used to counter warping and shrinkage, but some strength is lost.

Whereas there is some general information on, for example PET and PP, as well as design guidance at Level 2, there is more detailed folder-level information at Level 3, shown to the left. The information is naturally more grade-specific in the datasheets of Level 3 and when it comes to material properties covered, there is an extended number of mechanical properties, such as Rockwell hardness, as well as more optical and thermal properties, for example thermal shock resistance and heat deflection temperatures. There are also additional absorption and permeability attributes compared to Level 2. The number of materials in Level 3, around 4100 of them, means that we cover many more alloys, heat treatments and grades, which is essential for realistic project work and advanced teaching. In the case of PET bottles, for instance, it enables a distinction between unfilled *amorphous* PET, which is transparent, and unfilled *semi-crystalline* PET, which is opaque.

External polymer databases like *Global Polymer Plastics* are available only in the *Polymer* database at Level 3 and refer to industrial suppliers of specific grades. These contain contact details for further investigation, like product datasheets. In the *Polymer database*, there is also around two hundred additional chemical resistance properties from the Rapra *ChemRes* database.

The advanced *Sustainability* database in Granta EduPack has additional data-tables that, for example, summarizes Legislation and Regulation relevant to packaging, covering regions (EU) and nations (USA, China, UK etc) both at Level 2 and 3 shown to the right.



**Bio-data**

Biocompatible	ⓘ	✓
Medical grades	ⓘ	✓
Food contact	ⓘ	✓

Another advanced database, *Bioengineering*, has bio-data on, for example compliance with food contact protocols and directives (FDA, EU etc) for certain materials, such as polymers for packaging.

## 4. Eco Audits of water container options

The containers that are included in our comparison at Level 2 are (the brands are irrelevant to the results):

1. PET (500 ml)



2. PLA (500 ml)



3. Al can (330 ml)



4. TetraPak (500 ml)



Transport ?

Name	Transport type	Distance (km)
Transport	14 tonne (2 axle) truck	405

Use ?

Product life: 1 Years

Country of use: United Kingdom

Static mode

Product uses the following energy:

Energy input and output: Electric to mechanical (electric moto)

Power rating: 0.12 kW

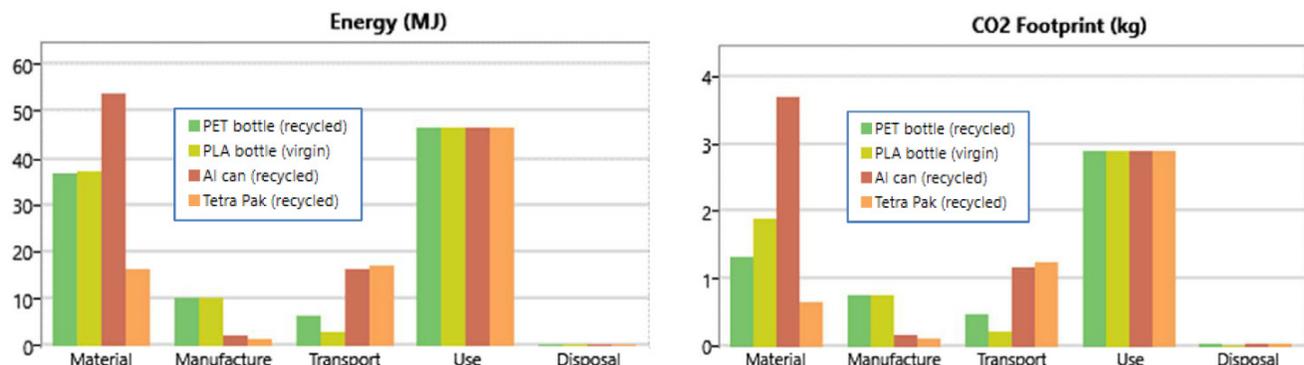
Usage: 2 days per year

Usage: 24 hours per day

This selection represents a main PET bottle, as reference, and some options that can be compared and discussed in a life-cycle perspective, e.g., Polylactide (PLA) a biopolymer. We have excluded glass bottles that can be cleaned and reused instead of recycled. The masses were measured using baking scales with an accuracy limited to approximately +/- 0.5 g. The use phase is represented by refrigeration for 2 whole days (static mode) using a UK electricity mix. An average power use of 120 W is assumed in this example. Actual distances for transport are entered, with information from the Internet concerning where the water has been sourced. For example Armathwaite (see first picture inset) to Cambridge in the UK: 404.5 km by road via A1 and A1 (M). Don't forget to add water.

Container	1. PET (0.5 l)	2. PLA (0.5 l)	3. Al-can (0.33 l)	4. TetraPak (0.5 l)
Units for 10 liter [#]	20	20	30	20
Material (bottle+cap)	PET+PP	PLA+PP	Wrought Al non-aged	Cardboard+PP
Mass [g] (bottle+cap)	23+3	30+3	12.5	20+3
Mass [kg] (dummy)	0.5	0.5	0.33	0.5
Recycled [%]	21	0.3	42.5	71.9
Transport [km]	405	188	936(road)+ 41(ship)	1082(road)+ 41(ship)
Source	Armathwaite, UK	South Downs, UK	Perrier, France	Fläming, Germany
Energy [MJ]	100	97	118	81
CO <sub>2</sub> [kg/kg]	5.4	5.7	7.9	4.9

The results are displayed as *Summary* charts for Energy and CO<sub>2</sub> footprint, below:



The numerical values can be found within *Detailed report*, but it is clear from this summary that the use phase (refrigeration) is considerable and that the Al can, using a recycled fraction taken from the typical industrial supply (43 %), has a CO<sub>2</sub> footprint for the material part twice that of any of the other options. It is easy to explore what happens if you were able to reach 100% recycled Al by adjusting the recycled fraction in the BOM. This hypothetically brings down the material CO<sub>2</sub> footprint to below the current PET footprint (and 2% less total CO<sub>2</sub> footprint for the whole lifecycle). This highlights the importance of a reliable system for recycling.

Overall, the Al can has the largest total energy use (18% higher than PET) and CO<sub>2</sub> footprint (45% higher than PET). The Tetra Pak option has the lowest, 19% less energy and 10% lower CO<sub>2</sub> footprint than PET. It can also be seen that the transport phase may be significant, although both imported water containers (Al and Tetra Pak) have moderate relative energy consumption and emissions. The manufacturing phase is relatively small for all containers. Now, these results, or similar results that you generate yourselves, are open for interpretation and discussion in the classroom.

## 5. Reality check

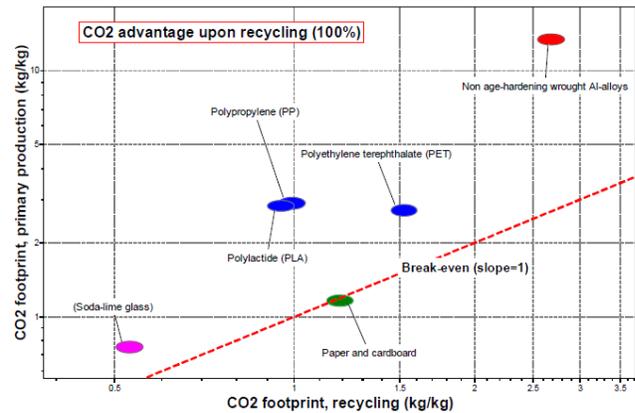
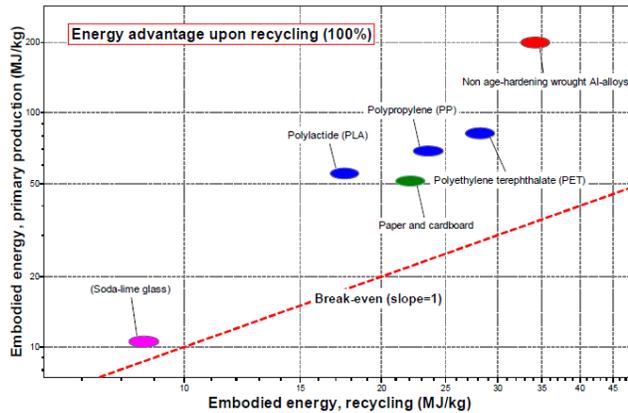
The Tetra Pak option comes out as the clear winner regarding lowest energy use and CO<sub>2</sub> footprint as well as being made of a highly recycled, renewable material. TetraPak has a publicly available CO<sub>2</sub> calculator online for a more in-depth investigation of its performance [4]. This container does present a challenge to the recycling industry, though, since it contains a thin plasticized Al barrier, which cannot be easily recycled as is. Tetra Pak cartons are made from of typically 6 layers of material. Paper accounts for up to 78% (by weight) of the package and recycled paper has recently been introduced. Aluminum foil in some packages weighs between 5 and 7%, the rest is made up of Polyethylene (PE) [5]. If 3 g of paper/cardboard is replaced by 1 g of Al and 2 g of PE in the Bill-of-Materials of the Eco Audit, the energy and CO<sub>2</sub> footprint increase by around 5 percentage units but the general picture does not change.

Due to the hybrid nature of the packaging, TetraPaks can't be recycled with normal paper or even plastic waste streams and need to be collected and sorted separately. In the UK, for instance, there are only few recycling plants that currently handles all the cardboard packaging. The challenge of separating the layers means that the PE and Al and usually left together as another form of hybrid material and then used in construction materials. The pure Al can, however, does offer great recycling benefits, since it has an integrated cap and recycled Al require 85-95% less energy than virgin Al. The *European Aluminium* packaging industry reports an encouraging 73% recycling rate of Al beverage cans [6].

Biodegradable plastics like PLA would be another solution. The amount of recycled PLA in supply is very low. This might be attributed to that they are composted and not recycled, but the actual story may be a bit more complex. Composting PLA *can* still leave behind particles that do not decompose but act as contaminant. While PLA can be recycled like other plastics, the presence of the bio-polymer actual contaminates the recycling stream of other polymers [7]. The presence of a biodegradable polymers damages the stability of polymers like PET and PP. For these reasons, PLA is more likely to go to landfill than composting or recycling. Moreover, although PLA can be considered 'compostable', it will only biodegrade under specific industrial conditions. It takes up to 90 days to break down in an industrial composting facility, 12 months to degrade in a home composter and between 100 and 1000 years if left in the environment [8].

A partial solution to the problem of plastic waste is to improve the current recycling systems, for example by introducing a deposit (refundable fee) on PET bottles at purchase and a way to refund this money upon returning the bottle. This already exists in some countries, for example Sweden, which have resulted in recycling levels for both PET bottles and Al cans of around 85% [9]. Recycling is an important tool both to reduce waste and CO<sub>2</sub> emissions. This can be seen from the charts below, showing benefits of recycled material compared to virgin.





The container materials (except glass, included for comparison) show at least 50% less energy required for recycled material than virgin. An interesting observation from the second chart is that new Paper/cardboard has the same CO<sub>2</sub> footprint as recycled. This is because renewable material based on wood captures CO<sub>2</sub> from the air by photosynthesis during growth and therefore generate no fossil emissions that adds to the footprint of the material.

What can be done about the plastic waste already polluting the marine environment? One idea could be to collect it and use it as solid fuels for heat generation or to power the collection itself. The Heat of combustion for PET is more than 23 MJ/kg, ranking between Wood (around 15 MJ/kg) and Ethanol (around 30 MJ/kg) in comparison. PP has even higher energy content, around 45 MJ/kg for a random copolymer, matching Diesel fuel! It is clear from the expected degradation times (hundreds of years) that active measures must be taken.

## 6. What does Granta EduPack bring to the understanding?

Granta EduPack is a versatile tool for studying issues related to sustainability. Materials decisions can be scrutinized and discussed in assignments or in the classroom and many current topics can be covered. The starting point for this case study was to use materials data and the Eco Audit to understand alternatives to PET bottles as water containers. This was triggered by recent reports about plastic waste in the environment. Granta EduPack suggests the following conclusions around this issue:

- Granta EduPack has proved helpful in investigating the environmental challenge of plastic waste by comparing PET bottles with alternative options; PLA bottles, Al cans and TetraPak.
- Both level 2 and level 3 have useful data that can be employed to assess the containers, for example regarding recycled fraction in current supply of materials as well as embodied energy and CO<sub>2</sub> footprint of virgin or recycled materials. This data provides a good platform for discussion in the classroom.
- Using the Eco Audit, you can easily explore the impact of recycling, as demonstrated by changing the recycled fraction in the Al can feedstock, for instance. This highlights the consequences of materials decisions.
- The Energy/CO<sub>2</sub> footprint of the *Use phase* of the Eco Audits are considerable and of the same order as the other phases combined. Although this is just an example, it implies that major reductions can come from decreasing the refrigeration but with minimal influence of the container choice.
- The combination of the software with a practical activity offers an engaging learning opportunity in the classroom.

We do emphasize that the results are estimates from an Eco Audit, which is a streamlined life-cycle inventory. It contains approximations and is based on eco data that has considerable uncertainties. The results are intended to be used as a basis for discussion and has limited quantitative accuracy [10].

## Practical classroom exercise

The simple Eco Audit comparison is a suitable exercise to perform in small classes, as a practical lab for groups of 2-3 students. This has been tested with students of a European Winter School, during a session in Cambridge. All you need is digital scales of the type used for baking with a precision of about 0.5 g, or better. Containers can be contributed by the students or the educator and the results can be posted on the blackboard/ whiteboard in real-time during the session, in a table similar to the one we used. Glass bottles, soft waterbags or camping flasks for tap water can be used in the comparison. It can be interesting to compare the influence of different transport options, so try to find a diverse set of sources, domestic and exotic (Fiji, Canada, Switzerland, Italy, France etc, depending on your location) and research the distances and logistics involved.

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