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INGENIERO INDUSTRIAL

FEASIBILITY STUDY ON ALTERNATIVES FOR THE BOTTLED WATER INDUSTRY

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Madrid
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FEASIBILITY STUDY ON ALTERNATIVES FOR THE BOTTLED WATER INDUSTRY

BY

EMILIO DE LAS HERAS PÁEZ DE LA CADENA

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Resumen ejecutivo

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Entidades colaboradoras: Illinois Institute of Technology, Universidad Pontificia de Comillas – ICAI

El objetivo principal de este proyecto es la realización de un estudio de viabilidad sobre los materiales y procedimientos alternativos disponibles para comenzar a sustituir el plástico de tereftalato de polietileno (PET) en el embotellado de agua. En su comienzo, este proyecto se centraró en la esferificación, una técnica que consiste en encapsular el líquido en una película en forma de esfera hecha de algas. Esta alternativa biodegradable demostró, incluso de manera cualitativa, ser demasiado temprana en sus etapas de desarrollo, pero despertó la idea de que deberíamos buscar materiales biodegradables. A partir de este escenario inicial, llegamos a unos cinco materiales alternativos (tanto biodegradables como no biodegradables), con los que analizar sus posibilidades en este tipo de mercado.

Para asentar bases para la realización del proyecto, se realizó una investigación de mercado para compilar un estado del arte actual. Se sabe que el PET es, por mucha diferencia, el líder indiscutible del mercado, pero ¿Cómo llegó a tal posición? Al observar la relación histórica de los humanos con el agua y particularmente con el agua embotellada, este proyecto detalla cómo hemos llegado a nuestra situación actual para poder analizar cuáles son las consecuencias de las tendencias actuales en el consumo de agua embotellada.

Habiendo detallado las consecuencias que están ocurriendo actualmente con el mercado actual de agua embotellada, y las que pueden ocurrir como resultado de este tipo de consumo, se proponen algunos materiales alternativos. Estos materiales son: PET reciclado (rPET), PET de base biológica (BioPET), esferificación, ácido poliláctico (PLA) y polihidroxialcanoatos (PHA). Cada uno de los materiales propuestos es único en algún aspecto, lo que hace una comparación compleja. Para establecer una comparación inicial, se realiza un análisis cualitativo basado en un análisis SWOT (Fortalezas, debilidades, oportunidades y amenazas). Debido a la naturaleza de un análisis

cualitativo, llegar a una conclusión en términos de viabilidad sería excesivamente subjetivo y sesgado. Como consecuencia, para abordar este problema, se decidió que era necesario realizar un análisis más cuantitativo y racional. En esta etapa, se llegó a un periodo de reflexión para averiguar cómo se podría cuantificar estos aspectos para ayudarnos a tomar una decisión más objetiva e imparcial.

De cara a la cuantificación de datos para nuestro objetivo, la idea de usar indicadores clave de rendimiento (KPI) se postuló como una técnica a tener en cuenta. Durante años, las empresas han estado usando más los KPI (cada vez con más frecuencia) para poder medir su proximidad a un objetivo comercial específico. Esto nos llevó a pensar, ¿Y si pudiéramos crear algo similar a un modelo de KPI para nuestro objetivo específico? Nuestro objetivo final es que comparemos diferentes materiales con el PET y contemplar alternativas. Sin embargo, antes de crear el modelo, necesitábamos establecer un denominador común para determinar qué inputs serían necesarios para el modelo. Para hacerlo, se determinó tras ver todos los ciclos de vida del producto para los materiales, se podría determinar una serie de inputs comunes.

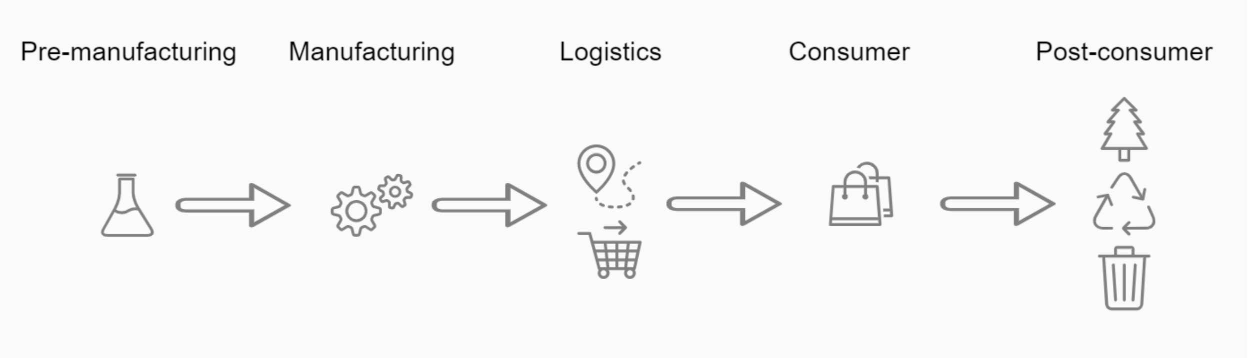
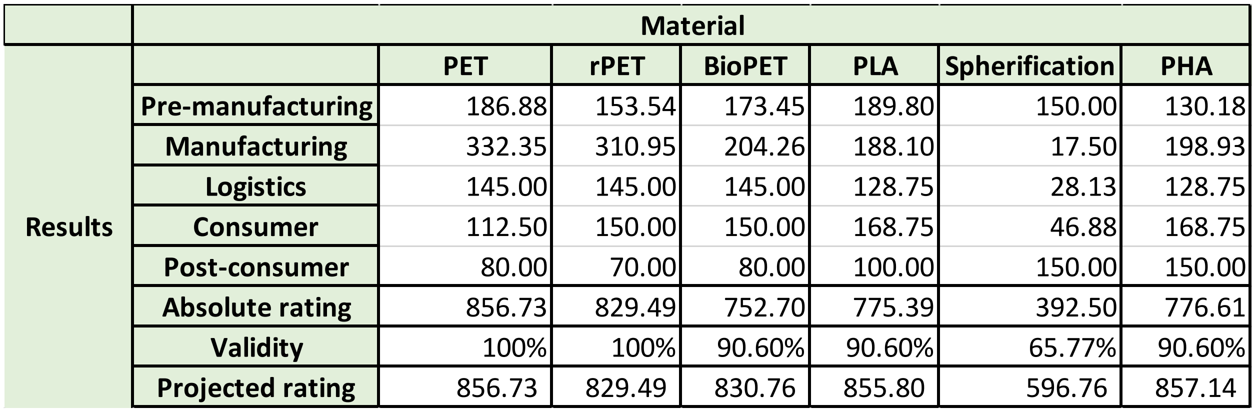


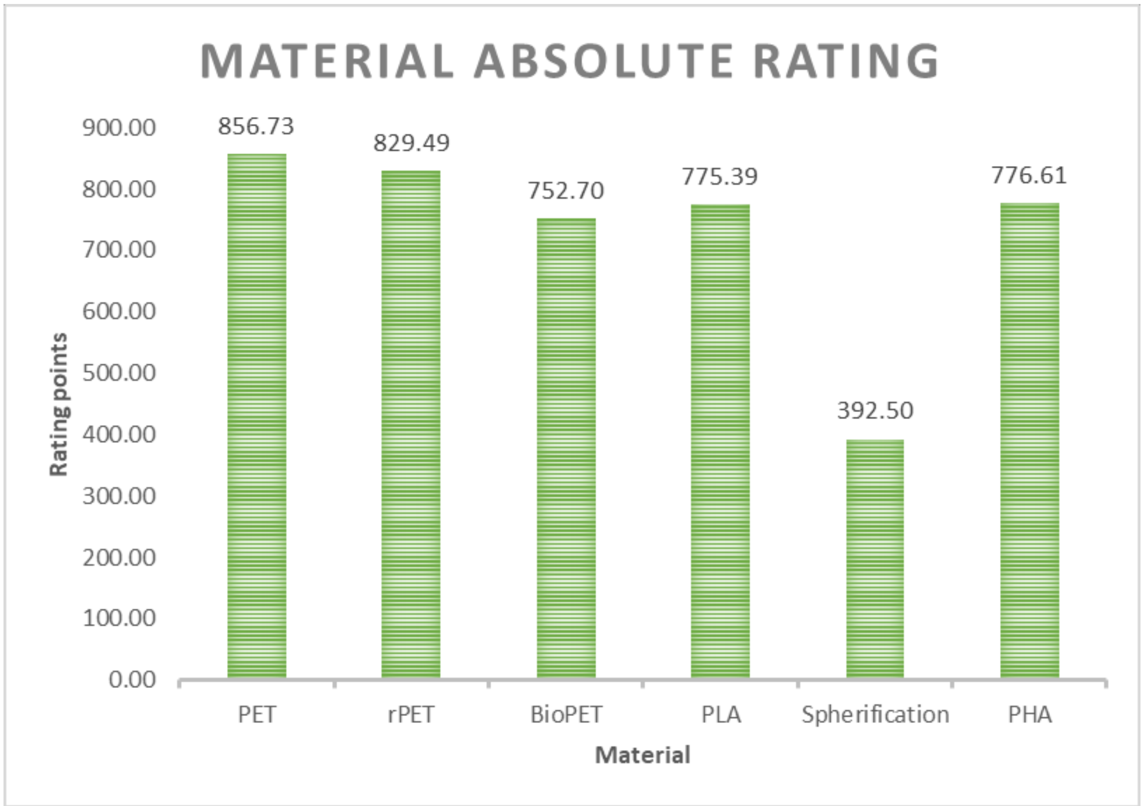
Imagen 1: Las cinco etapas de ciclo de vida de las cuales se determinan los inputs al modelo.

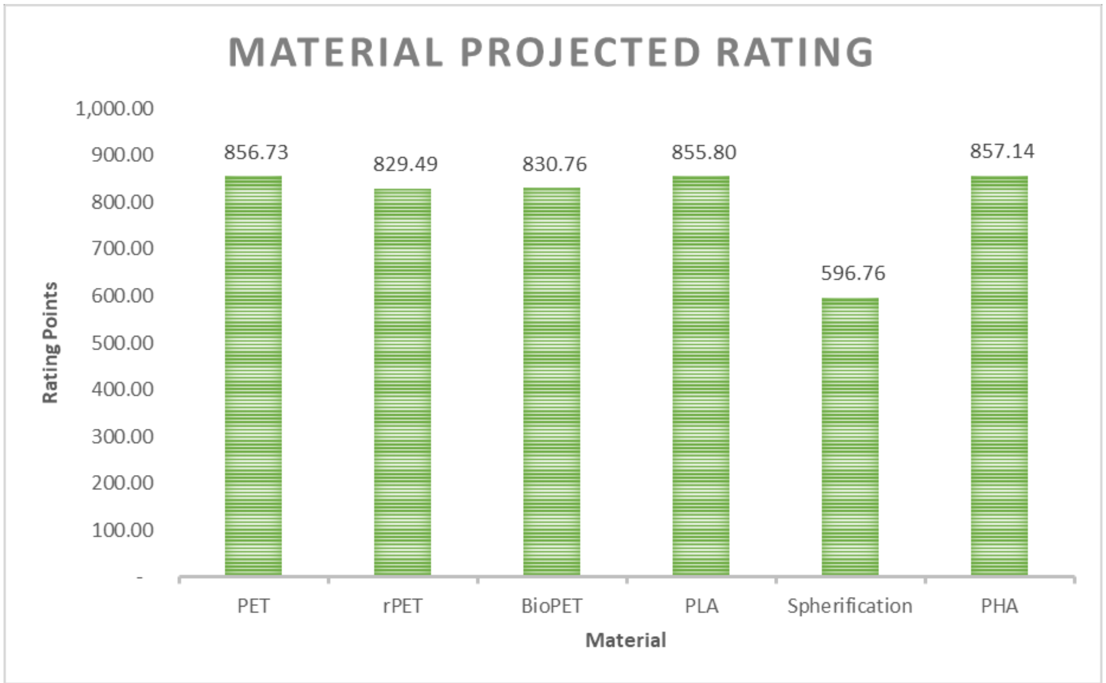
De las etapas del ciclo de vida de la imagen anterior, se seleccionaron un total de 18 entradas o inputs. A partir de esos inputs, el modelo diseñado asignaría una cierta cantidad de puntos a los sobre las variables de entrada disponibles. La suma total de los puntos asignados a cada una de las variables de entrada se denominará "puntuación absoluta" del material. Dado que todos los materiales se encuentran en diferentes etapas de madurez, cada uno de los inputs tendrá un porcentaje de validez además de los puntos de calificación asignados a ellos. Si para un determinado material, uno o varios de los insumos no están disponibles, ese material no tendría puntos de clasificación otorgados ni validez otorgada para esos insumos específicos. La validez permite al usuario saber que falta algún tipo de información para un determinado material siempre que su validez sea inferior al 100%. En el caso de que a un material le falten entradas, el material optaría por una puntuación o clasificación absoluta inferior a la de un material que tenga toda la información disponible para ser introducida. Para compensar esto, el modelo estimaría una calificación potencial o proyectada. Esta estimación se calcularía juzgando la clasificación del material en función de los insumos disponibles y utilizando ese promedio para calcular los insumos que faltan. A continuación, se muestran los resultados de pasar todos los materiales por el modelo.

Imagen 2: Resultados obtenidos tras la utilización del modelo.



		Material					
		PET	**rPET**	**BioPET**	**PLA**	**Spherification**	**PHA**
Results	**Pre-manufacturing**	186.88	153.54	173.45	189.80	150.00	130.18
	Manufacturing	332.35	310.95	204.26	188.10	17.50	198.93
	Logistics	145.00	145.00	145.00	128.75	28.13	128.75
	Consumer	112.50	150.00	150.00	168.75	46.88	168.75
	Post-consumer	80.00	70.00	80.00	100.00	150.00	150.00
	Absolute rating	856.73	829.49	752.70	775.39	392.50	776.61
	Validity	100%	100%	90.60%	90.60%	65.77%	90.60%
	Projected rating	856.73	829.49	830.76	855.80	596.76	857.14





Cabe señalar que este modelo debe utilizarse para comparar dos materiales y debe analizarse caso por caso. Esto significa que las clasificaciones obtenidas del modelo deben examinarse

cuidadosamente para cada uno de los materiales que se comparan. Este proyecto utilizó el modelo para comparar 5 materiales alternativos al PET ya establecido y para juzgar cada uno de sus potenciales para dar forma al futuro del mercado de agua embotellada. Al comparar las "calificaciones absolutas" queda claro que, de momento, ninguno de los materiales presentados podría erradicar al PET por completo del mercado. Sin embargo, cuando se observan las clasificaciones proyectadas para los materiales, dos opciones biodegradables parecen ser igual de competitivas (PLA y PHA). Este modelo no prueba objetivamente que estos materiales puedan superar al PET en el mercado del embotellado. Sin embargo, refleja que hay esperanzas de que las alternativas biodegradables desempeñen un papel en este mercado, especialmente en el futuro, una vez que los costes de las materias primas sean más bajos. La conclusión final de este proyecto es que, aunque no hay un candidato claro para una botella de agua más sostenible, la solución puede consistir en utilizar varios materiales que se complementen entre sí en una botella de agua menos "monopolística". En comunicación con los fabricantes de PET, así como con los vendedores de bioplásticos, debido a la información de propiedad de la empresa, sólo pudieron aludir a sus intenciones, lo que es coherente con los resultados de este proyecto. Las alternativas necesitan comenzar a impactar una pequeña fracción de la enorme posición de mercado del PET en las botellas de agua.

Executive summary

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Director: Nicholson, Myron

Collaborating entities: Illinois Institute of Technology, Universidad Pontificia de Comillas – ICAI

This project's main objective was to perform a feasibility study on the alternative materials and procedures that are available to begin to substitute polyethylene terephthalate (PET) plastic in water bottling. To start with, this project was going to focus on spherification, a technique that involves encapsulating the liquid in a sphere-shaped film made from algae. This biodegradable alternative proved, even in a qualitative way, to be far too early in its development stages but sparked the idea that we should look into biodegradable materials. From this initial scenario, we came to about five alternative materials, (both biodegradable and non-biodegradable), with which to analyze their feasibilities in this type of market.

To set the project up, a market research was conducted in order to create a current state of the art. It is known that PET is by far the market leader, but how did it get to such a position? By looking at human's historical relationship with water and particularly bottled water, this project details how we have reached our current situation in order to then be able to analyze what are the consequences of current trends in bottled water consumption.

Having detailed the consequences that are currently occurring with today's bottled water market, and those that may occur as a result of this type of consumption, some alternative materials are proposed. Those materials are: recycled PET (rPET), bio-based PET (BioPET), spherification, polylactic acid (PLA) and polyhydroxyalkanoates (PHA). Each of the proposed materials is unique in some regard, which makes for a difficult comparison. To begin the comparison, a qualitative analysis based on a SWOT (Strengths, weaknesses, opportunities and threats) analysis is conducted. Due to the nature of a qualitative analysis, jumping to a conclusion in terms of feasibility would be excessively subjective and biased. So, in order to address this issue, it was decided that a more quantitative and rational analysis needed to be conducted. At this stage, we

were left considering thinking how could we quantify these aspects to help us come to a more objective and unbiased decision.

When looking at quantifying data towards a certain objective, the idea of using key performance indicators (KPIs) became quite realistic. Businesses have been increasingly using KPIs in order to be able to measure how close they are to a specific business goal, and so we thought, what if we could create something similar to a KPI model towards our specific goal? Our final goal is for us to compare different materials to PET and see how they match up. However, before creating the model we needed to draw some common ground to determine which inputs would be needed for the model. To do so, we theorized that if we were to look at all of the materials from their respective product life cycles, a series of common inputs could be made.

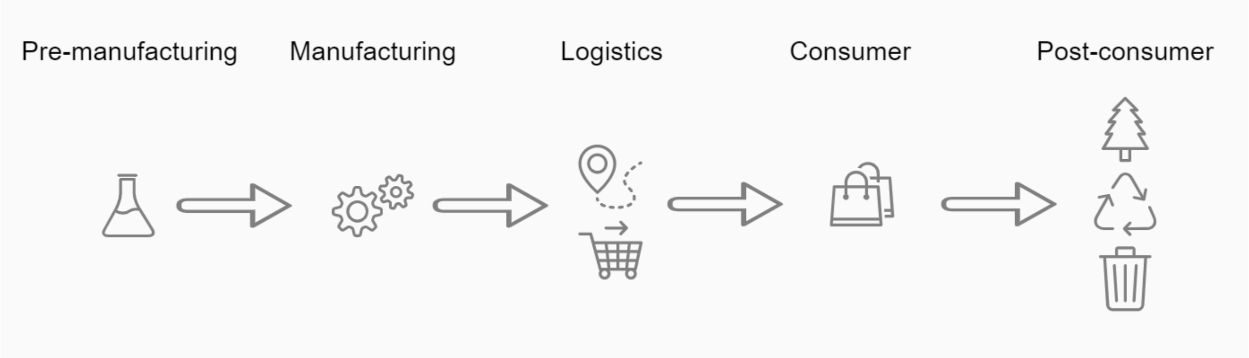

Image I:5 lifecycle stages from which inputs were drawn.

From the lifecycle stages in the image above, a total of 18 inputs were selected. From those inputs, the designed model would allocate a certain amount of points to the available inputs. The total sum of the points allocated to each of the inputs would be referred to as the material's "absolute rating". Since all of the materials find themselves to be at different maturity stages, each of the inputs will have a percentage validity in addition to the rating points assigned to them. If for a certain material, one or several of the inputs are not available, that material would have no rating points awarded and no validity awarded for those specific inputs. The validity lets the user know that some information is lacking for a certain material whenever its validity is lower than 100%. In the event that a material could be missing inputs, the material would opt for a lower absolute score or rating than a material that does have all the information available to be entered. To make up for this, the model would estimate a potential or projected rating. This estimation would be calculated by judging the material's rating on the inputs that were available and using that average to calculate the missing inputs. The results of running all of the materials through the model are shown.

Image II: Results obtained through model

		Material					
		PET	**rPET**	**BioPET**	**PLA**	**Spherification**	**PHA**
Results	**Pre-manufacturing**	186.88	153.54	173.45	189.80	150.00	130.18
	Manufacturing	332.35	310.95	204.26	188.10	17.50	198.93
	Logistics	145.00	145.00	145.00	128.75	28.13	128.75
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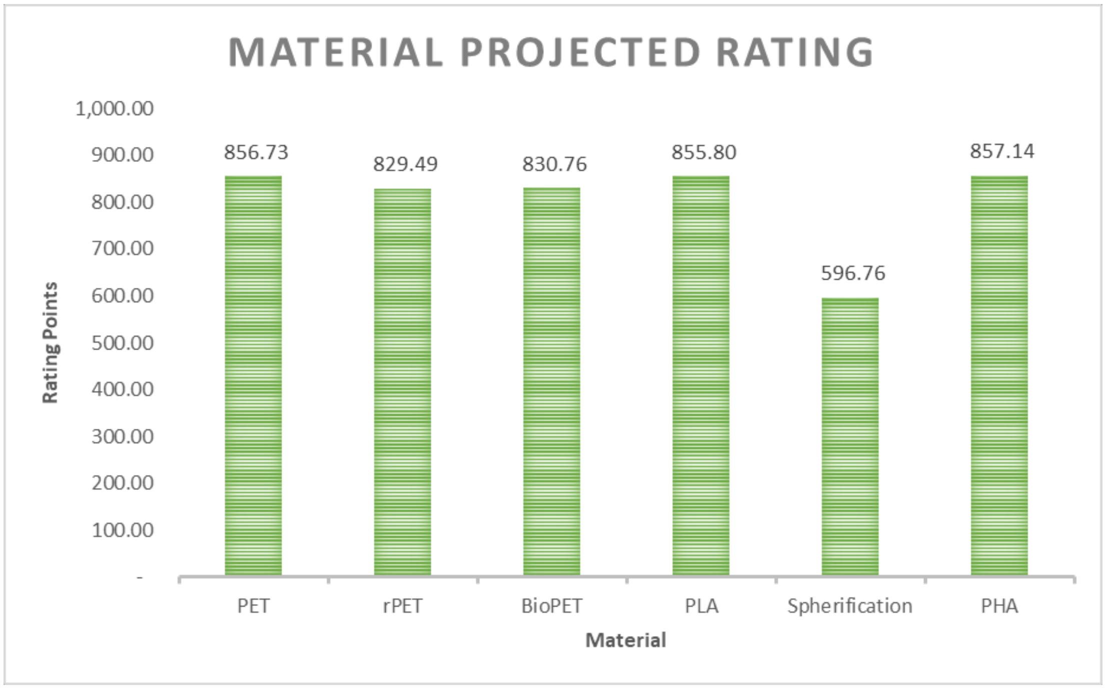

It should be noted that this model should be used to compare two different materials and should be analyzed on a case by case basis. This means that the ratings obtained from the model should be carefully looked at for each of the materials being compared. This project used the model to compare 5 alternative materials to the already established PET and to judge each of their potentials to shape the future of the bottled water market. When comparing "absolute ratings" it becomes clear that not one of the presented materials could overcome PET totally just yet. However, when looking at the projected ratings for the materials, two biodegradable options seem to prove to be just as competitive (PLA and PHA). This model does not objectively prove that these materials will likely overcome PET in the bottling market. However, it does reflect that there is hope for biodegradable alternatives to play a role in this market, especially in the future once raw material costs are lower. The final conclusion to this project is that although there is not one clear candidate towards a more sustainable water bottle, the solution may lie in using several materials that complement each other in a less "monopolistic" water bottle. In communication with PET manufacturer as well as vendors of bio plastics, due to business proprietary information, they could only allude to their intentions which is consistent with the results of this project. Alternatives need to begin to impact some small fraction of the huge PET market position in water bottles.

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1. Historical introduction to the water bottle industry

1.1 Introduction

In order for life to remain existing as we know it, there are several conditions that must be met. Among those conditions lie a healthy rate of consumption of the resources available, keeping in mind their replenishing rates, as well as the consequences of consuming those resources. When analyzing which resources are critical for life, more specifically for human life, a few of those resources stand out. Energy and how we produce it is certainly one of them, as well as, shelter, food, air and water. The latter two are notably important because without clean breathable air humans would survive for minutes and without clean, available, drinkable water humans would only survive for a few days. Not all life forms are as dependent on air as humans are, however how we currently handle water absolutely affects all life forms on planet Earth. This project focuses on one aspect of water consumption, which is how we have gotten to our current state of portable water consumption, and how feasible it is to implement other, more sustainable alternatives, in order to effectively satisfy consumer demands and trends, as well as the environment and the resources being used to do so.

1.2 Historical relationship between humans and water distribution systems

To arrive at the current state of human water consumption we must first see how water and human history have coexisted. The human race, as have the other living creatures, quickly realized the importance of water to their survival, which is why water storing and distribution dates back centuries, even over a thousand years in some civilizations. It is known that the human race has been nomadic before the arrival of agriculture and great civilizations. While being nomadic (in the days where people lived as hunters/gatherers), the natural source of drinking water was river water, it was once people started to settle in specific locations that the actual storing and distribution of water really began. At first, logically, humans settled near rivers or lakes in order to have easier access to water. Whenever this was not a possibility, humans opted to dig and build wells to extract water from the ground. Several examples are shown ahead.

Approximately 7000 years ago, in Jericho (Israel), water was being stored in wells for later use. In this city, there was also a development of a system that would help transport and distribute the water (Figure 1). The means of water transportation were simple channels that were dug in the rocks or the sand, hollow tubes were occasionally used. Other regions that hollowed out materials to transport water in this time frame were, Egypt, where they hollowed out palm trees and China and Japan where bamboo was used for this same function. Throughout practice the selected materials ended up mainly clay, wood and sometimes, metal.

Figure 1: Simple water distribution systems found in Jericho, Israel (Lenntech, n.d.).

Other practices done approximately around 3000 BCE is in the Persian empire, where people searched for underground rivers and lakes. The water would go through holes and cracks in the rocks into the wells. Also, during this time, in what today is Pakistan a very vast water supply was being used, including to supply public bathing facilities.

The first complex water distribution systems came from the Greeks and Romans. Both of these cultures used spring, well and rain water from very early on. On Greece's part, due to a rapid increase in their population, the Greeks needed to store water in wells and transport it to those who needed it through their distribution systems. These were made up by sewers that transported the already stored water along with the rainwater. The Greek empire was amongst the first to become interested in water quality. The Greeks incorporated the use of aeration basins to address this issue. On the other hand, the Romans were the most revolutionary constructors of water distribution networks. While they used river, spring or groundwater for provisioning, they built dams and aqueducts (Figure 2) to improve the previous set systems.

Figure 2: Roman aqueduct in Segovia, Spain (Lenntech, n.d.).

With the fall of the Roman empire came the end of aqueducts, and people went back to using a water system based on mainly on wells. In the Middle Ages water from wells would start to mix with sewage water. To avoid contamination people started drinking water from outside their cities, where the sources were not polluted. Water-bearers were the people responsible for bringing this unpolluted water back into the city. It was not until the nineteenth century that similar systems to those that we have today came about. It was when, in 1804, John Gibb built the first drinking water supply for the city of Paisley in Scotland.

1.3 Historical evolution for bottled water

The focus of this project is to analyze where the future of the bottled water industry could be. Having already stated briefly how water and humans have coexisted historically, this section aims to analyze how the first bottles have come about and how it has evolved to get to today's situation.

In the 1620s came about the first water bottle for sale in the United Kingdom. The rest of Europe and the US quickly followed in the 1700s, with the bottling of mineral spring water (it was believed that the natural springs had healing and therapeutic properties). Due to this bottled water was sold as a medicinal solution in pharmacies until the 1900s.

Carbonated water gained popularity in the US after Joseph Hawkins receives a patent to produce a type of water called "imitation mineral water". This coincided with decreases in glass costs and advances in the efficiency of bottling speed, and hence, production increased. In addition to this, there was a growing fear in contracting cholera and typhoid, which led to millions of bottles sold in an annual basis in the US by the mid-1800s. In the early 1900s the demand for purified bottled water diminished after an English doctor ended the typhoid epidemic through chlorination (using chlorine to eliminate the bacteria).

A turning point in history (and the leading factor that led us to where we are today) happened in 1973, when Polyethylene terephthalate (PET) bottles were patented. They were the first plastic bottles that were able to contain and maintaining the desired pressure for carbonation. This meant that there now was a much cheaper alternative to the traditional glass bottles.

Figure 3: PET water bottle (ScoopWhoop, n.d.).

Around the end of the 20th century bottled water became the fastest-growing beverage category in the world. In the United States, such a prosperous market involved several companies, which will be discussed later.

As previously mentioned, the bottled water industry by the end of the 20th century was a booming and highly competitive market that involved a variety of companies. In the United States alone, 700 different brands of bottled water were being produced by 430 bottling facilities. Although this seems to be a high number of brands, and even though the bottled water market is a global market, 75% of the entire market was controlled by three different types of local companies.

The first of these types of companies were those that were created to run and market only one specific brand. Although brands like Perrier or Evian have been family owned for nearly a century, most of the brands that have been present in the market are now under the control of a major multinational food company (Nestlé or Danone for instance). These two companies have a rich experience in selling natural mineral water. Just before the turn of the century, in 1999, Nestlé was the number 1 company on the world market for bottled water with a turnover that reached US$ 3.5 billion. This turnover represented 15.3% of the entire world's market share. Nestlé managed this feat by owning well-known brands in 17 countries, such as, Perrier in France, Poland Spring in the US, or San Pellegrino in Italy. Danone, on the other hand, held 9% of the global market share with a turnover around the US$ 1.5 billion mark. Both of these major corporations started to consider marketing purified water at this point to gain a competitive edge.

Figure 4: Nestlé waters is undoubtedly one of the biggest companies involved in the market through several brands in different countries (Nestlé Waters, n.d.).

The second type of companies that tapped the bottled water market were the soft drink companies that in the 90s turned to this profitable market. Massive corporations, such as Coca Cola and PepsiCo, managed to take advantage of their already established world-wide distribution networks and bottlers to enter this prosperous market. Through both of these factors they gained an incredibly quick access to this market. They proceeded to successfully enter this market by using some of their ingredients for soft drinks (purified and aerated water only needed to have a concentrated solution of minerals added to be sold as enriched purified water). Proof of their quick success was that, just two years after the launch of Aquafina (1995), PepsiCo reached the top ten companies in the market with sales rising an incredible 126% increase from one year to the next, making sales reach more than US$ 52 million in 1997. On Coca Cola's side of the picture, just some years after launch (in 1999) Dasani was 9th in the American market.

Figure 5: Dasani and Aquafina quickly managed to make room for themselves in this highly competitive market (DK USA Inc, n.d.).

Lastly, companies that provide tap water have become the last major player in the bottled water industry. Since they already have extensive knowledge and experience in water purification and pipe distribution, they started to look towards a more profitable way to distribute their water. Most of these companies started to sell their water in carboys but quickly were faced with a dilemma. How can they sell carboys and at the same time distribute their water through public municipal distribution networks without giving the impression that tap water is not of a good quality? They also had to find out what sort of pricing strategy they wanted to use for their carboy packaged water. Regardless of these sorts of boundaries, tap water-providing companies have managed to enter the bottled water market, although not to the same scale as the two other types of companies.

With a growing demand for bottled water, companies started to look for increasing efficiencies. Newer technology and better efficiencies suppressed pricing and made bottles more accessible by consumers worldwide. This led to a battle between tap and bottled water, with beverage companies playing to consumers' fears of falling ill from contamination from tap sources. When we add this to the fact that people enjoy the convenience of having fully portable water, we can understand why plastic bottles are so popular today. We are still facing this battle today and it comes with a series of consequences that we are facing and will worsen if we continue to act in the same manner.

2. Current State of the Art

2.1 Introduction to bottled water today

In the past 50 years bottled water consumption has grown at a relatively steady rate (an average of 7% each year in terms of volume of water consumed). It is because of this, that this market is regarded as the most dynamic out of the food and beverage industry. The fact that bottled water increases at such a rate becomes even more exceptional when we compare its price to the price of tap water. In order to fully understand this phenomenon, we must make some distinctions on the main different types of bottled water (natural mineral water, spring water and purified water).

1. *Natural mineral water*

According to the European Union (EU) this product is to meet certain expectations, making it a very specific product. It is referred to as a "microbiologically wholesome water" that originates from an underground source and emerges from a spring tapped in natural or bore exits.[1] Natural water, whether it is still or aerated, presents two major differences when being compared to other types of bottled water. The first of the two different aspects that natural mineral water has is its nature. It is characteristic of this type of water to have a constant level of minerals and trace elements. As a result, natural mineral water can provide health benefits. The second difference this water presents is its original state. Due to the fact that it is found in underground sources, this water is preserved in a pristine state, and thus, for the EU for water to be considered natural mineral is must remain under these conditions. To verify this, EU member states assess the water characteristics from several points of view, including, physical, geological, hydrological, chemical and microbiological. It should be noted that since this type of water is not sterile, there is a possibility that it contains natural microflora.

On the other hand, in the United States, this type of water carries fewer restrictions. The International Bottled Water Association (IBWA) claims that this type of water should be limited to containing less than 250 parts per million (ppm) total dissolved solids. The IBWA also defines that this sort of water should come from come from a source that is either tapped at one or more bore-holes or springs that originate from a physically and geographically protected underground water source. Natural mineral water is differentiated from other types of water by its constant level and relative proportions of mineral and trace elements at the point of emergence from its original source.

2. *Spring water*

Spring water is found in underground sources and is protected against pollution hazards, microbiologically safe, and suitable for human consumption without any additional treatment (some exceptions include aeration). In Europe this water is different from natural mineral water as it must stand up to the same standards applicable to drinking water.

In the United States, this water is defined as “water derived from an underground formation from which water flows naturally to the surface of the earth”. It is to be collected only at the spring or through a bore hole tapping the underground formation so that it finds the spring.

3. *Purified water*

Purified water (also named drinking water) is the water that is retrieved from bodies of water, such as rivers, lakes or underground springs that has undergone some form of treatment prior to consumption. Processes that produce purified water include, distillation, reverse osmosis or deionization. It is still considered purified water when it undergoes chemical treatment to diminish undesired components. It also allows for water with different components to be mixed. Keeping in mind how it is produced there is little difference between purified water and municipal tap water, with the exception of their distribution methods and retail price.

4. *Well water*

Well water is bottled water that comes from a hole bored, drilled or constructed in the ground which taps the water from an aquifer (which is a water-bearing underground layer of rock or sand).

5. *Artesian water / artesian well water*

This type of bottled water, as its name suggests, has is retrieved through a well that taps a confined aquifer, in which the water level stands at some height above the top of the aquifer.

6. *Drinking water*

This type of bottled water is the type that is sold for human consumption in sanitary containers and contains no additives or flavor modifying components (such as sweeteners). It must be sugar and calorie-free but it can contain very low amounts of sodium, although this is not necessarily the case.

7. *Sparkling water*

Sparkling water is water that after treatment and possible replacement with carbon dioxide contains the exact amount of carbon dioxide that it had at the emergence of the source.

If these waters contain a minimum required amount of mineral content they can be referred to as ¨mineral waters¨ according to United States' standards.

Figure 6: Different brands for different types of water in the US (Business Insider, 2016).

2.2 Overview of the current situation: PET.

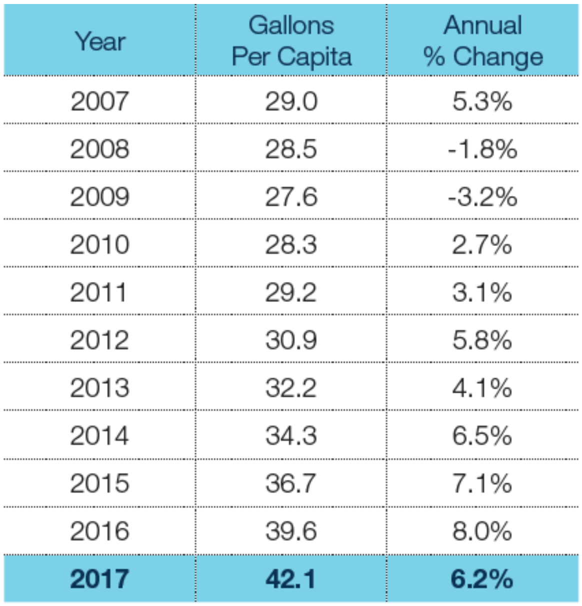
Bottled water consumption has been growing steadily in the US for decades. Back in 1976 Americans drank an average of 5.7 liters of bottled water each year, 17 liters in 1986 and 35 liters in 1999 and it has kept on rising since. But how has bottled water raised its popularity so steadily? As we all know, bottled water is often regarded as the leading alternative to tap water. Consumers reject the taste of certain components that are sometimes found in tap water, specially chlorine (which is used in the purification process). Customers also want for their water to taste exactly the same, regardless of the location where they are drinking and as it is known, tap water taste varies depending on location due to having different treatments and chlorine concentrations and due to it traveling different distribution networks. Consumers are also looking for safety, in both emerging and industrialized countries. People who travel to very different countries know that it is not usually recommended to drink tap water as your stomach may not be used to the local tap water composition, so consumers tend to mistrust tap water tend to fall on bottled water as a safer (or at least more familiar) alternative.

Bottled water's population can also be linked to the increase in urbanization in the past years. It is shown that the more populated areas and cities have a population that consumes more liters per year than the more rural areas of the country. With more urbanized regions, came bigger shopping centers and more frequent supermarkets with more convenient locations for the consumers. This does not only imply that there is a more distributed network for bottled water but also a wider range of brands available to the consumer.

This tremendous increase in bottled water consumption would be impossible without the rise of a material with the right properties and capabilities to cover all of the demand. PET (polyethylene terephthalate) became that material rather quickly. It is a transparent, lightweight, strong, shatterproof, safe and recyclable plastic that has been first safely implemented in the 1970s. PET is used to package beverages, food, household items and personal care items since its introduction in the 70s. Technically, Polyethylene terephthalate is derived from terephthalic acid (otherwise known as dimethyl terephthalate) and mono ethylene glycol. In order for the mix of both to be considered PET, the sum of terephthalic acid and mono ethylene glycol reacted must make up at least 90 percent of the mass of the monomer reacted to form the polymer. In addition to that, it must have a melting peak temperature between 225ºC and 255ºC. There are two main ways that PET packages can be made: blow molded to create bottles or thermoformed from sheet. PET also has recycling capabilities, which initially made it an ideal material for food and beverage packaging.

Products that have been packaged for more than 35 years include beverages, water, peanut butter, salad dressing, sauces, beer, wine, spirits, produce, deli items, candy, baked goods and non-food items (for instance health and beauty products and household cleaners). From its introduction, the United States Food and Drug Administration (USFDA) and other equivalent regulating agencies throughout the world have approved of PET as a safe material to package food or beverage. Packaging designers and manufacturers have chosen this material, not only because of its low production cost, but also because of its properties. PET is a strong plastic, it is transparent (allowing to see the contents inside) and versatile. It also allows for the product to retain its freshness and taste. From the consumer standpoint, people have chosen to consume products in PET packages due to it being a lightweight material, with resealable capabilities and shatter-resistant.

As mentioned before, bottled water consumption has grown for several decades, in fact, with the exception of 2008 and 2009, where small reductions in consumption were seen, since 1977, bottled water volume consumed has grown every year.



Year	Gallons Per Capita	Annual % Change
2007	29.0	5.3%
2008	28.5	-1.8%
2009	27.6	-3.2%
2010	28.3	2.7%
2011	29.2	3.1%
2012	30.9	5.8%
2013	32.2	4.1%
2014	34.3	6.5%
2015	36.7	7.1%
2016	39.6	8.0%
2017	**42.1**	**6.2%**

Figure 7: United States bottled water market per capita consumption (Bottled Water, US & International Developments and Statistics, 2017).

As a result, per capita consumption of bottled water has exceeded 160 liters (42 gallons). Overall bottled water volume consumed grew from 48 billion liters in 2016 to nearly 52 billion liters (13.7

billion gallons), a 7 percent increase from the previous year. This rise in bottled water coincides with a decrease in soft drink consumption.

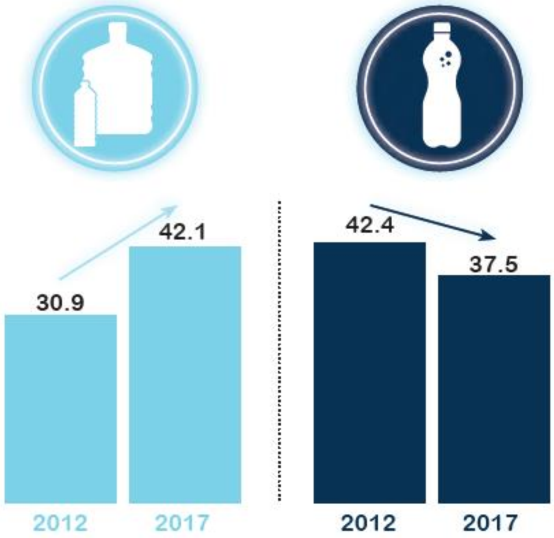


Figure 8: Consumption per capita in gallons for bottled water and soft drinks (Bottled Water, US & International Developments and Statistics, 2017).

As a result, the American bottled water market has become highly profitable in the past few years, as can be seen in the following figure.

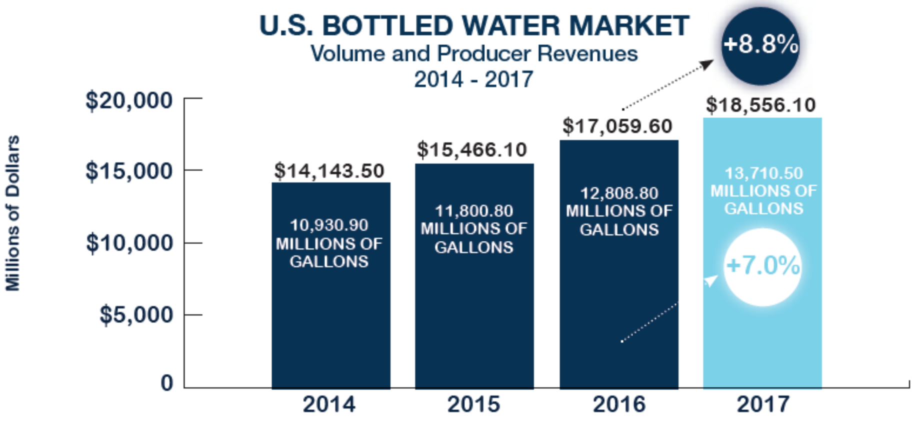


Figure 9: US bottled water market (Bottled Water, US & International Developments and Statistics, 2017).

As can be seen previously, the resulting increases in bottled water consumption in the United States has managed to increase revenues accordingly to more than $18.5 billion. This is especially interesting because the increase in revenue for producers since 2016 (8.8%) surpasses the percentage increase in the volume consumed since that same year (7.0%).

When analyzing the United States packaged water market, the individual segment that remains the most prevalent is the domestic non-sparkling water. This segment represents 92.5% of the total volume of bottled water consumed in the US (12.7 billion gallons). PET is largely attributed to this feat since most water packages fall under the PET spectrum. By 2009 PET volume had grown to 5.2 billion gallons, more than 4.1 billion gallons higher than 10 years earlier, in 1999. In 2009, the share of total bottled water rose all the way to 61%, compared to the 24% it held in 1999. It was, however, in 2010, when PET experienced its biggest growth of any bottled water segment. It grew by 6.8% reaching 5.5 billion gallons consumed. This tendency continued up until 2017, when PET came close to 9.2 billion gallons consumed and its share of the market, compared to other segments rose to roughly 70%. It should be noted that in this case, it is for single-serve PET meaning that other (less used) materials would fall into some of the categories. For instance, glass containers for water can be present in the sparkling, imports and retail bulk (restaurants tend to buy bottled glass water).

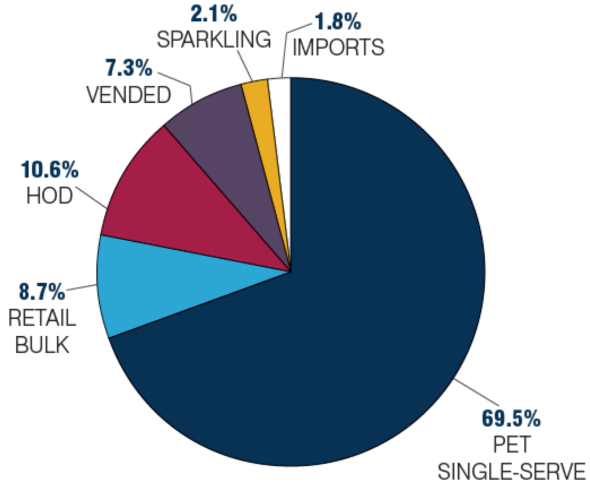


Figure 10: Volume market share by water segment in 2017 (Bottled Water, US & International Developments and Statistics, 2017).

This has been the case as part of a global phenomenon where the United States is located just second in terms of millions of gallons consumed, despite the fact that there are many countries that are far more populated, only China has been capable of consuming more gallons of bottled water and also capable of outgrowing the United States since 2012, as it can be seen in Figure 11.

2017		Millions of Gallons		CAGR*
Rank	Countries	2012	2017	2012/17
1	China	14,579.9	25,468.9	11.8%
2	United States	9,711.4	13,710.5	7.1%
3	Mexico	7,516.3	8,682.9	2.9%
4	Indonesia	4,966.4	8,158.2	10.4%
5	Brazil	4,611.9	5,794.5	4.7%
6	India	3,623.6	5,759.0	9.7%
7	Thailand	3,135.4	3,966.3	4.8%
8	Germany	3,024.1	3,131.5	0.7%
9	Italy	2,904.8	2,917.5	0.1%
10	France	2,287.9	2,445.7	1.3%
	Top 10 Subtotal	**56,361.7**	**80,034.9**	**7.3%**
	All Others	16,532.8	19,520.7	3.4%
	WORLD TOTAL	**72,894.5**	**99,555.6**	**6.4%**

*Compound annual growth rate
Source: Beverage Marketing Corporation

Figure 11: Global bottled water consumption and compound annual growth rates (Bottled Water, US & International Developments and Statistics, 2017).

Interestingly enough, even though the United States places second in overall bottled water consumption (in terms of volume) it places fourth in per capita consumption from 2012 until 2017. With Mexico, Thailand and Italy ahead of the US (see Figure 12). This consumption trend is likely to continue its growth. In fact, it is estimated that global bottled water consumption is to surpass the 100-billion-gallon mark (378.5 billion liters) by 2018.

2017		Gallons Per Capita	
Rank	Countries	2012	2017
1	Mexico	62.2	67.2
2	Thailand	46.9	57.5
3	Italy	47.7	48.2
4	United States	30.9	42.1
5	Germany	36.6	37.9
6	France	35.8	36.4
7	Belgium-Luxembourg	34.6	35.1
8	United Arab Emirates	25.3	33.9
9	Spain	30.9	32.6
10	Indonesia	20.1	30.9
11	Saudi Arabia	27.8	30.5
12	China, Hong Kong SAR	25.3	29.5
13	Hungary	28.4	29.2
14	Korea, Republic of	20.1	28.5
15	Brazil	23.2	27.7
16	Poland	21.3	25.6
17	Argentina	28.2	24.9
18	Austria	25.3	24.6
19	Pacific Islands	21.3	24.4
20	Switzerland	25.0	24.3
	Global Average	10.3	13.2

Source: Beverage Marketing Corporation
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Figure 12: Per capita bottled water consumption 2012-2017 (Bottled Water, US & International Developments and Statistics, 2017).

It is undeniable that not only has the overall bottled water consumption increased due to an increasing human population but also that it has mainly increased due to consumers consuming more bottled water on average each year (per capita consumption has increased by nearly 12 gallons in just five years, and the global average has increased by nearly 3 gallons). Having this sort of growth of such a basic and fundamental asset in everyone's life poses a series of challenges and threats, especially regarding the materials that we use to package water. The following section of this project aims to see why this sort of growth is not sustainable just through increasing the amount of PET we produce each year.

2.3 The PET lifecycle

Through the arguments previously displayed, it is quite clear why PET had risen to the top of the list in terms of materials being used for packaging food and beverages. Particularly for bottled water, where consumption steadily rises each year. Polyethylene Terephthalate has amazing properties for packaging and can even by recycled multiple times, however there are a couple of aspects of the PET bottle lifecycle that we should analyze.

PET is the most common thermoplastic polymer resin worldwide. Polymers are substances that are made out of particles with long successions of one or more types of molecules (gathering of atoms connected to each other typically by covalent bonds). Polymers are considered to be macromolecules with a high atomic weight. PET is the most commonly used polymer and derives from ethylene glycol and terephthalic acid. Its origins are predominantly petrochemical (coming from crude oil processes, such as distillation), there are however PET products that are also plant based. Traditionally, after collecting the ethylene glycol from crude oil distillation, it undergoes a series of processes to reach the final product.

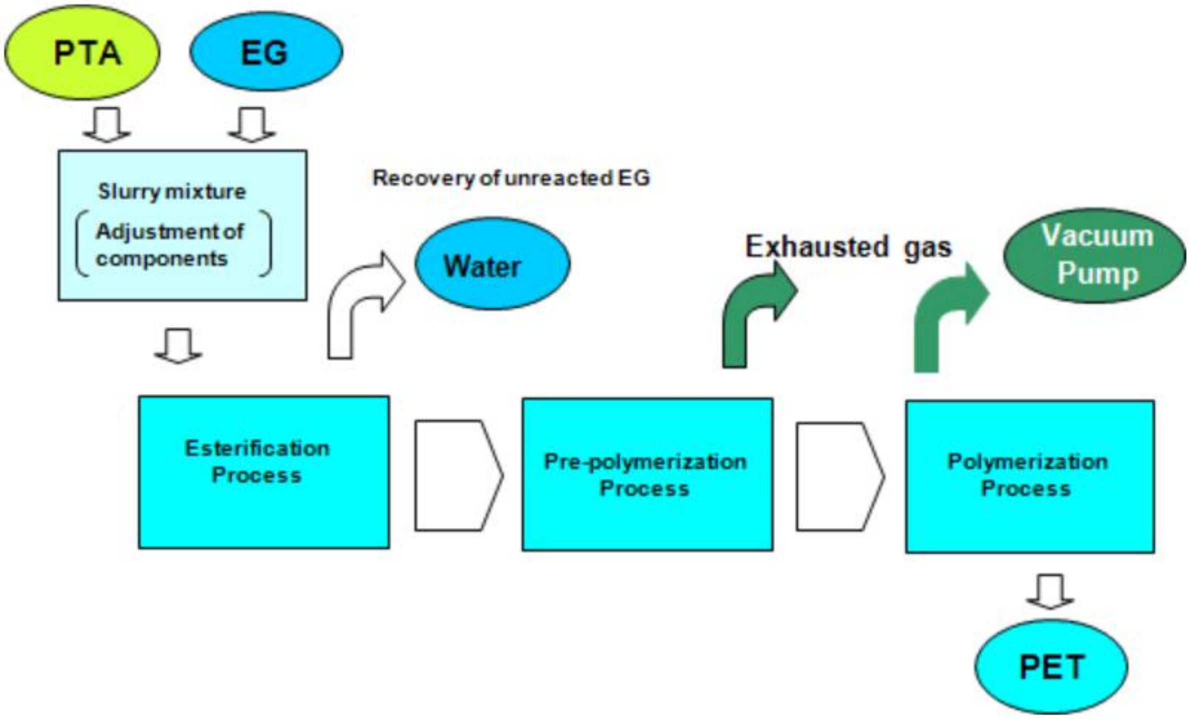


Figure 13: PET production process (Hitachi Global, n.d.).

Esterification is conducted directly and at high temperatures (ranging from 220 to 260 ºC) and moderate pressures of 2.7 to 5.5 bar. Then, a pre-polymerization process begins to prepare for the polymerization, where these components of PET are combined under high temperatures and low pressures to form long polymer chains. Once the desired length of polymer chain is obtained the reaction is stopped. As a result, PET flake or resin is formed. Before heading off to the bottling facility, the PET resin or flake has to undergo certain procedures of washing and grading in order to comply with the corresponding standards for food and drink in the country of bottling.

When it comes to PET´s use in water bottles, depending on the source and the water type to be bottled the process varies. This can be seen in the following process map.

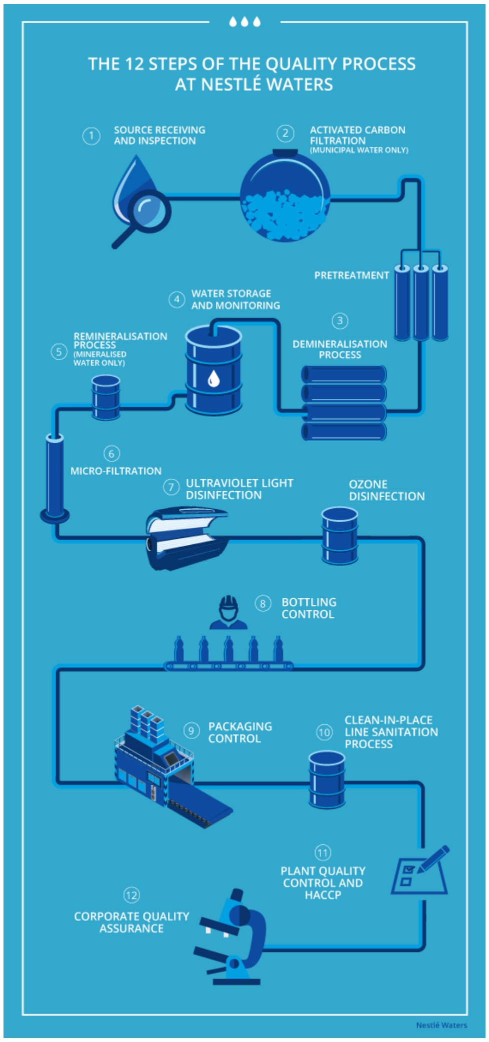


Figure 14: Water bottling process Nestlé (Nestlé Waters, n.d.).

The main objective for this process is to comply to the quality standard required by the legislation in the country where the bottled water will be consumed, with that in mind the process steps are described ahead.

1. Water is received and collected through stainless steel pipes that arrive from a variety of sources (municipal water supply or a local well).
2. This step focuses on the removal of chlorines and trihalomethanes (THMs) through an activated carbon filtration process. Water softener is used in order to reduce the hardness of the water.
3. Demineralization is used to remove unwanted minerals (by means of reverse osmosis or distillation).
4. Water storage and monitoring for further quality control.
5. Selected minerals are introduced to the water to cater to the demand.
6. Micro-filtration is responsible for removing small particles and potential microbiological contaminants.
7. UV filtration provides an additional removal of contaminants. Ozone disinfestation uses highly reactive form of oxygen.
8. Bottles are then filled in the filling room.
9. Finally, bottles are packaged and sent out.

For this process there are a number of resources and energy being used as well as waste and pollution being created. In order to get a better understanding of the water bottling process as a whole, we must evaluate inputs and outputs that are involved in the process.

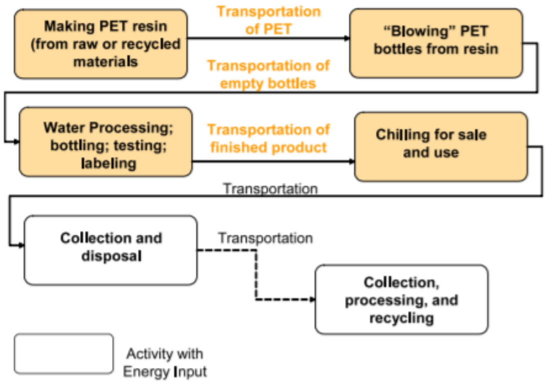
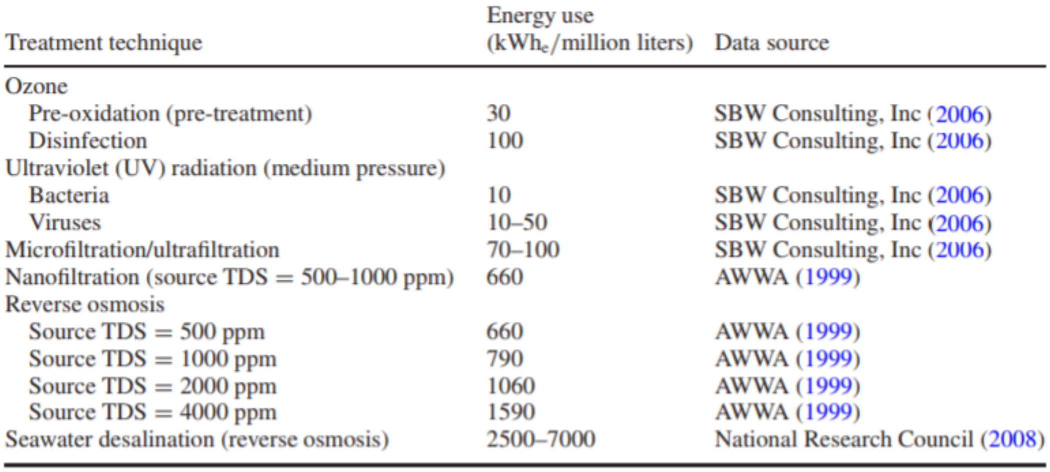


Figure 15: Water bottling inputs (P H Gleick and H S Cooley, 2009).

The first inputs occur in the manufacturing of the PET bottle, where it is estimated that in order to produce the PET resin would take approximately between 70-83 MJ (thermal)/kg, and turning the resin into bottles requires an extra 20MJ/kg (this is obviously dependent on the thickness and weight of the bottle). Considering the average weight of a plastic bottle (approximately 40g for 1 liter), the average energy consumption per bottle is 4 MJ. The following estimations for energy consumption in the water treatment needed prior to bottling can be seen in *Figure 16*.



Treatment technique	Energy use (kWh_e/million liters)	Data source
Ozone		
Pre-oxidation (pre-treatment)	30	SBW Consulting, Inc (2006)
Disinfection	100	SBW Consulting, Inc (2006)
Ultraviolet (UV) radiation (medium pressure)		
Bacteria	10	SBW Consulting, Inc (2006)
Viruses	10–50	SBW Consulting, Inc (2006)
Microfiltration/ultrafiltration	70–100	SBW Consulting, Inc (2006)
Nanofiltration (source TDS = 500–1000 ppm)	660	AWWA (1999)
Reverse osmosis		
Source TDS = 500 ppm	660	AWWA (1999)
Source TDS = 1000 ppm	790	AWWA (1999)
Source TDS = 2000 ppm	1060	AWWA (1999)
Source TDS = 4000 ppm	1590	AWWA (1999)
Seawater desalination (reverse osmosis)	2500–7000	National Research Council (2008)

Figure 16: Energy requirements for water treatment methods (P H Gleick and H S Cooley, 2009).

Considering the variability between the needs of different water to obtain different treatments, it is estimated that the energy required for treatment per bottle is between 0.0001 and 0.02 MJ (far less than that of producing the PET bottle). Lastly, the total energy that would be required to clean, fill, seal, label and package the water is approximately 0.014MJ. This obviously excludes the energy used for transportation, which is highly dependent on the origin and destination, as well as, the transportation method. It should also be noted that in producing a PET bottle, on average, it is estimated that it requires 3 times as much water to actually make the bottle as it does to fill it. As this data suggests, the majority of the energy used in the bottling process is used to actually make the PET bottle.

PET's properties do show that although it does require many resources to make them, there is potential for reutilizing and recycling this material. In the past years, recycling has become increasingly popular. However, for the first time since 2009, the volume of PET bottles that were available for recycling in the United States declined in 2017. Most likely, this decline is a direct result of the bankruptcy of M&G Polymers, a major PET resin producer in the late stages of the year. As a result of their closure of some of their plants 800 million pounds of annual capacity were wiped off the map. The total weight for that amount of PET bottles was 5,913 million pounds, which interestingly represents a 4% decrease from the previous year. The total number accounts for the total amount of PET resin used by American bottle manufacturers from all sources (US, foreign and recycled). Although in 2017 there has been a decrease in the weight of total PET resin produced in the US, due to the consumer trends shown in ***2.2 Overview of the current situation: PET*** we are led to believe that this would spark larger and larger volumes of PET resin produced each and every year in the future. With that in mind, in the following page, *Figure 17* shows a PET material flow in the United States for 2017.

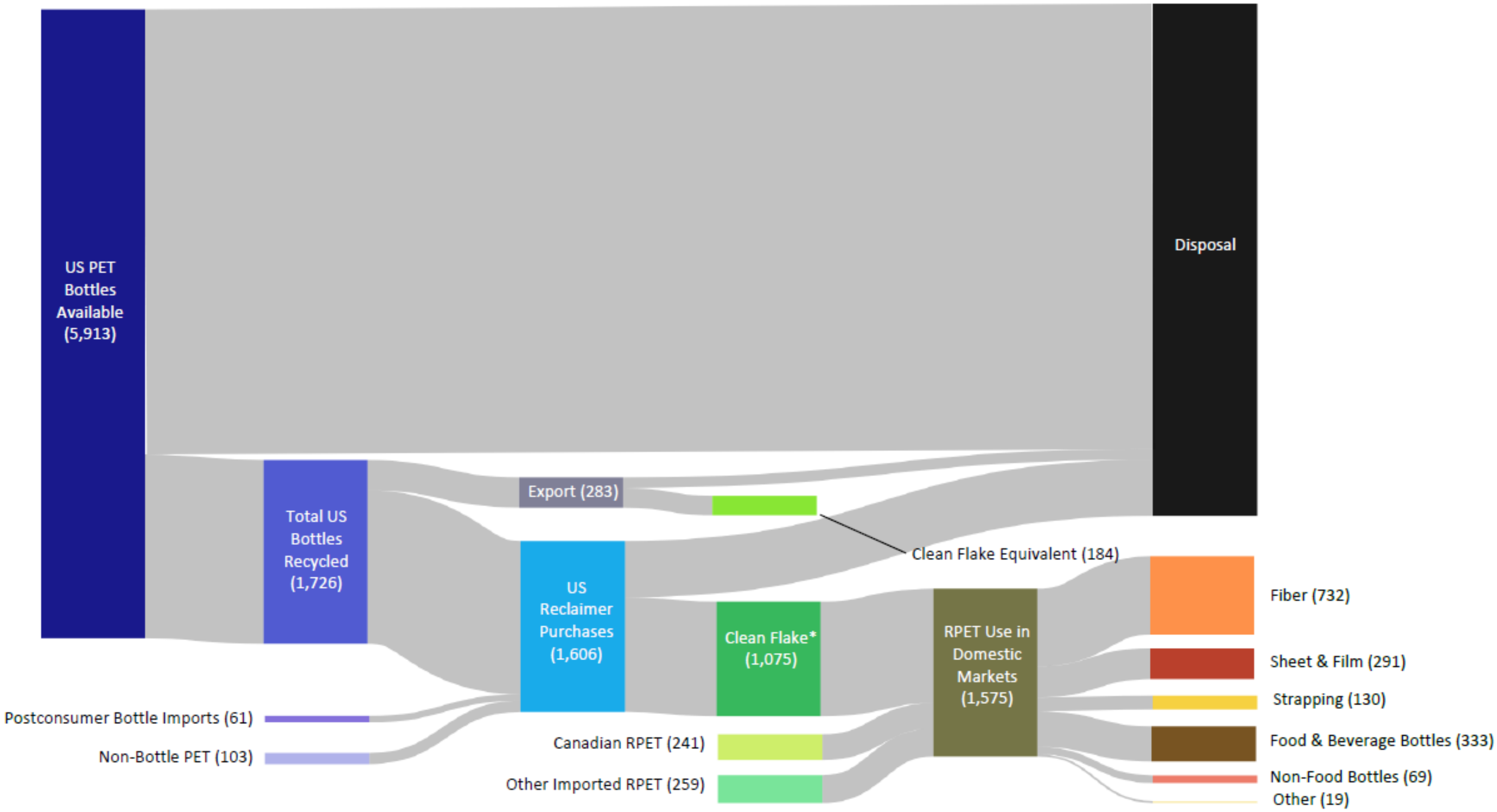


Figure 17: 2017 PET Material flows in the United States (MMlbs) (NAPCOR, 2017).

As can be seen in *Figure 17*, a massive part of the American PET bottles that were available in 2017 ended up disposed. This sort of life cycle can be defined as a cradle-to-grave lifecycle, where a product is designed and manufactured (in a sense "born") only to be used once and ultimately end up in the trash (or "dead"). Of the 5,913 million pounds of PET resin available in 2017 in the US, only 1,726 million pounds managed to undergo a recycling process. That accounts less than 30 percent of the total weight and of that total amount of US bottles that are recycled, roughly 90% of it makes it to the domestic market in the form of recycled PET (also known as rPET). It is quite alarming, in my opinion, to know that over 70 percent of the PET produced in the United States ends up as a waste, and this can be due, mainly, by two causes. The first, and perhaps easier to fix cause of this problem could be that the United States does not have the recycling capacity to tackle such a large amount of PET bottles, and although I believe there is some degree of truth in that, the underlying issue that is causing the majority of PET to end up as disposal are the consumers.

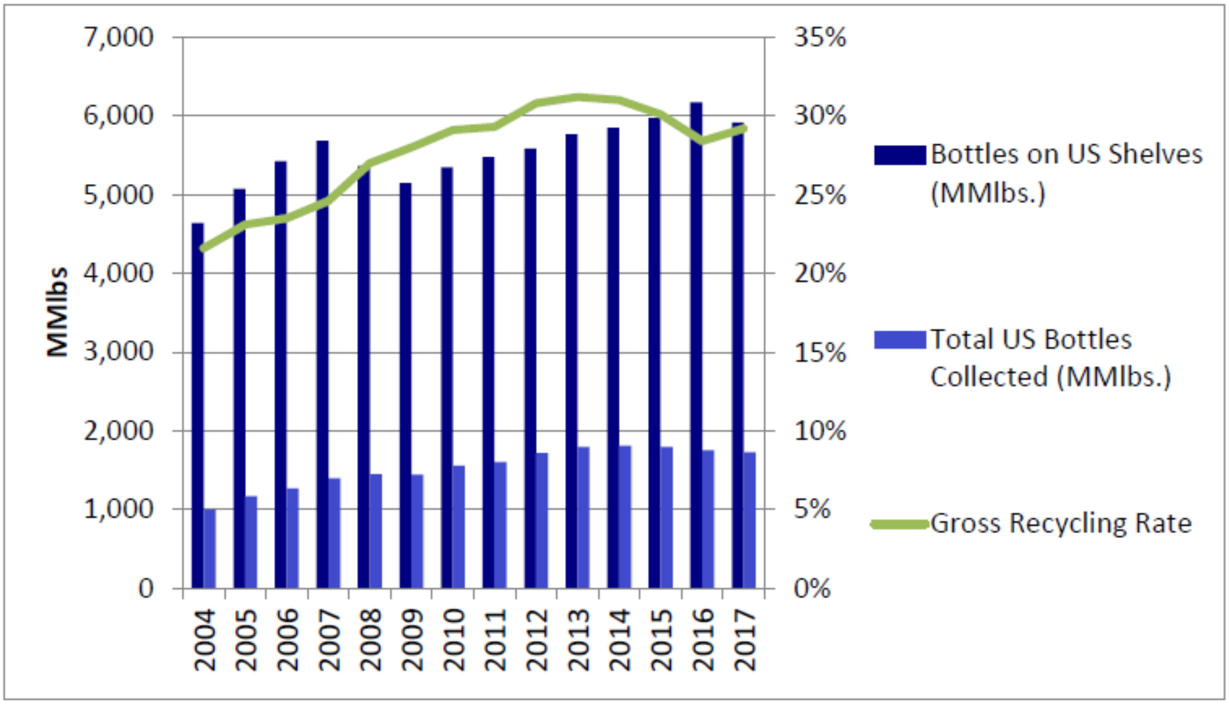


Figure 18: Gross Recycling rates from 2004 until 2017 (NAPCOR, 2017).

As can be seen in the image above, the number of American bottles collected for recycling are nowhere near the number of American bottles on shelves available for consumption. Consumers have grown accustomed to disposing of water bottles in the trash and in other non-recyclable disposal destinations, and as a result, it becomes harder to collect bottles for proper recycling.

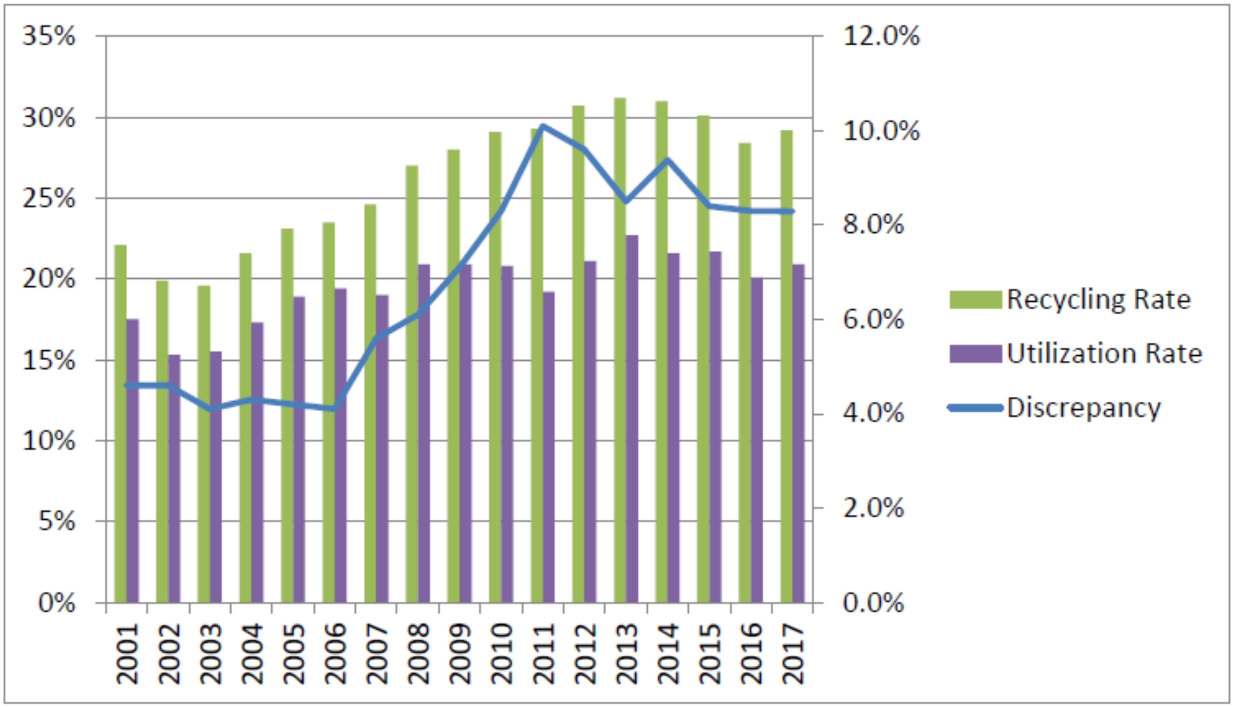


Figure 19:PET recycling & PET Material Utilization rates (NAPCOR, 2017).

To reassure that the recycling process, once collected, is actually reasonably effective we must look at the graph above (*Figure 19*). The utilization rate, which compares the amount of usable end product (clean flake) produced from American bottles to the volume of bottles available for recycling (collected bottles), is reasonably efficient when we compare it to the recycling rate. Once recycled PET has many uses for several different industries, ranging from creating new bottles or packages to creating fibers for clothes (*Figure 20*).

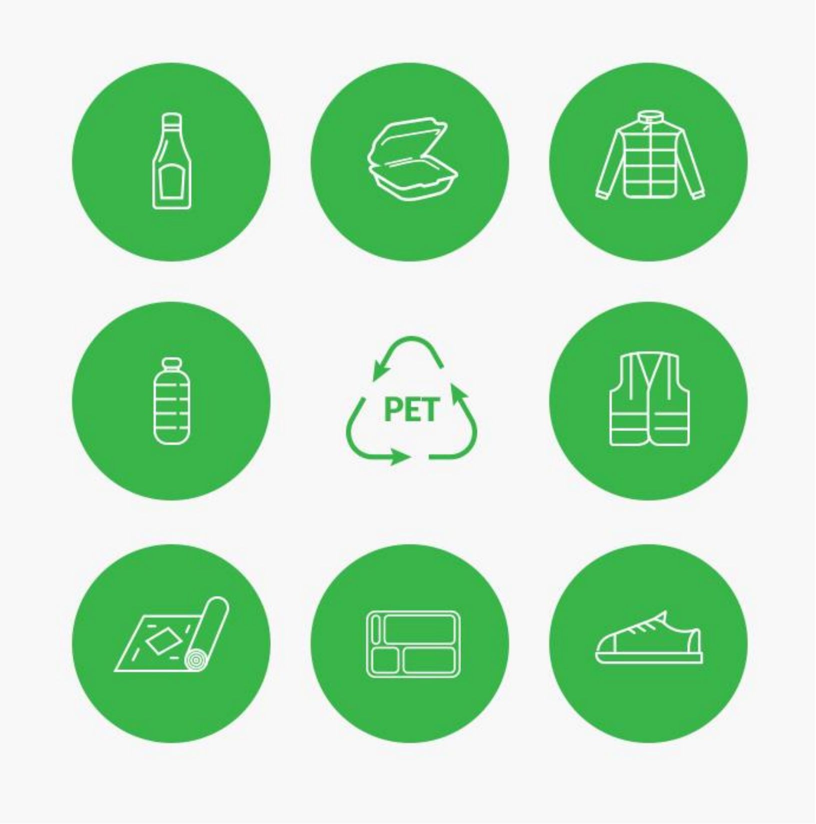
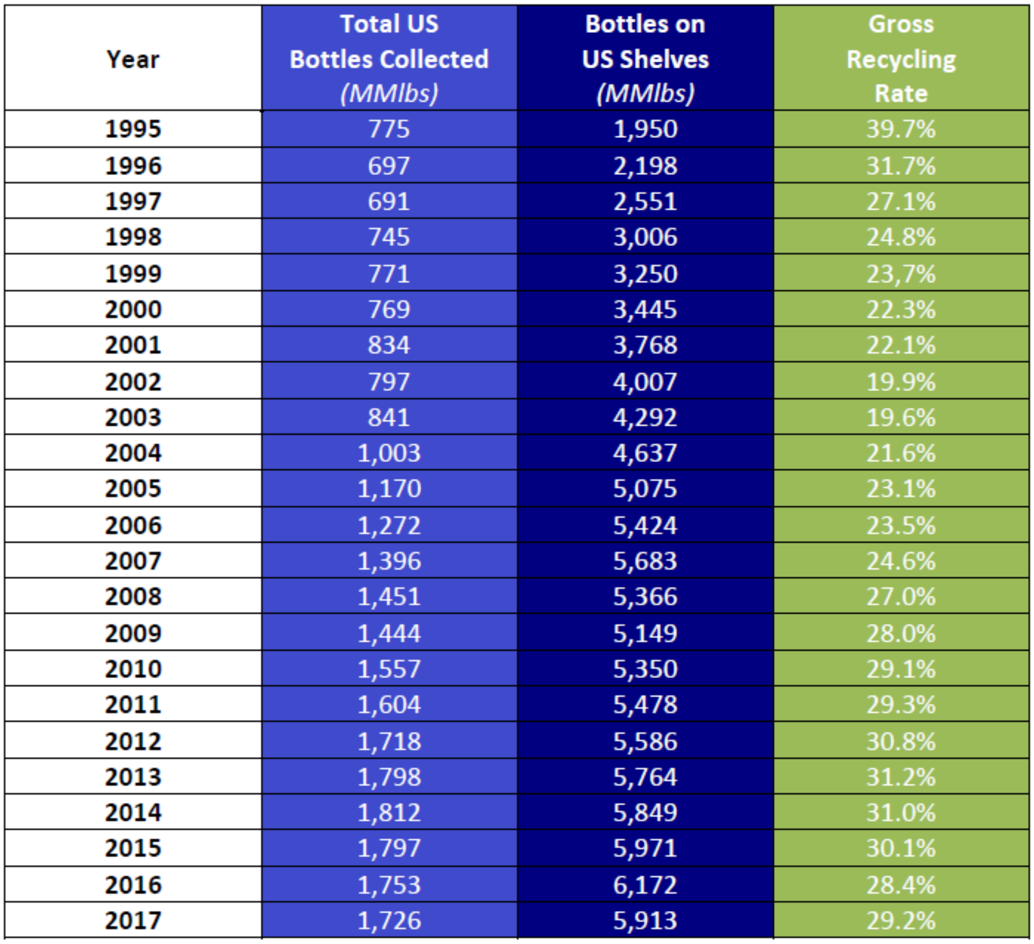


Figure 20: Different applications of rPET (NAPCOR, n.d.).

Keeping in mind that the number of bottles being collected grows each year, the utilization rate remains fairly efficient, the gross recycling rates, however, struggle to keep up with the growth of PET bottles that are being produced (*Figure 21*). This highlights that the main issue is not necessarily a lack of an efficient or effective process for recycling PET bottles, but rather a lack of an effective method of collection, and that is ultimately down to the masses that consume bottled water and other beverages frequently. If recycling facilities were truly overwhelmed with the number of bottles, they had to recycle they would surely increase their recycling capacity seeing as they profit from this activity.



Year	Total US Bottles Collected *(MMlbs)*	Bottles on US Shelves *(MMlbs)*	Gross Recycling Rate
1995	775	1,950	39.7%
1996	697	2,198	31.7%
1997	691	2,551	27.1%
1998	745	3,006	24.8%
1999	771	3,250	23,7%
2000	769	3,445	22.3%
2001	834	3,768	22.1%
2002	797	4,007	19.9%
2003	841	4,292	19.6%
2004	1,003	4,637	21.6%
2005	1,170	5,075	23.1%
2006	1,272	5,424	23.5%
2007	1,396	5,683	24.6%
2008	1,451	5,366	27.0%
2009	1,444	5,149	28.0%
2010	1,557	5,350	29.1%
2011	1,604	5,478	29.3%
2012	1,718	5,586	30.8%
2013	1,798	5,764	31.2%
2014	1,812	5,849	31.0%
2015	1,797	5,971	30.1%
2016	1,753	6,172	28.4%
2017	1,726	5,913	29.2%

Figure 21: Bottles available, collected and gross recycling rates since 1995 (NAPCOR 2017 Report).

2.4 Consequences

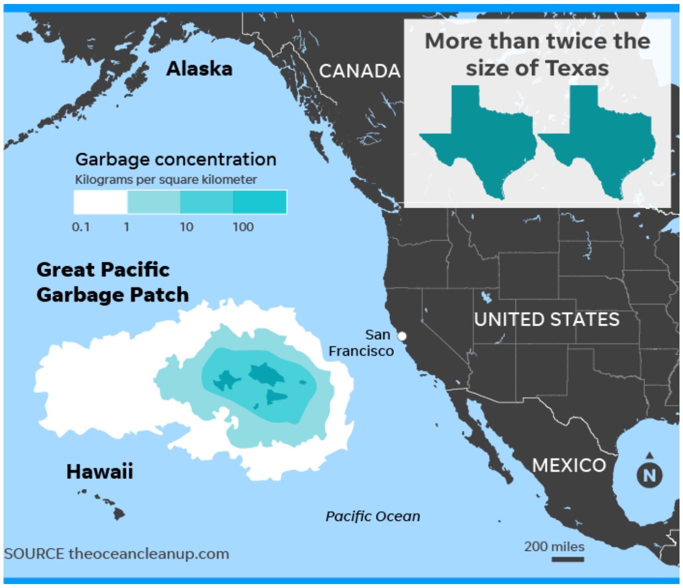
Having analyzed PET's lifecycle, we can begin to analyze the consequences of mass-producing bottles from this material.

Like other industrial activities, bottled water presents a series of impacts on the environment. In its production, PET derives from a petroleum product which requires a large amount of fossil fuel in order to make and transport. It is estimated that, on average, it takes approximately 17 million barrels of oil to meet the yearly American demand for bottled water. This amount of oil is equivalent to filling one million cars a year with fuel.

In my opinion, the most significant impacts come from the consumption of PET water bottles. According to Peter Gleick's *Bottled and Sold* there are 1,000 bottles being opened and thrown away in the United States every single second. As we saw previously, the vast majority of the PET produced in the last few years has ended up disposed, which, as it turns out, is problematic. Disposal is defined as the act or process of throwing something away or getting rid of something. But what exactly is “throwing something away”? When it comes to the disposal of water bottles, there is no such place as “away”. This is the main issue that we as consumers need to fix. “Away” in this context means bottles end up somewhere where they are not seen. Incineration or clustering massive amounts of PET plastic in the sea are common techniques to “dispose” of plastic bottles. Both of these techniques have negative implications.

When incinerated pollutants are left in the atmosphere contributing to the greenhouse gas effect and other potential respiratory health hazard. On the other hand, when throwing large quantities of plastic in the sea, some of PET’s positive attributes become negative ones. PET’s preservative properties translate into the plastic taking a very long time to decompose, it could in fact surpass 1,000 years, leaving pollutants in the soil and in the water. This of course has negative implications for all of the lifeforms that require soil or water to survive.

This is outcome is concerning because of the rate at which plastic is building up in the ocean. If we were to continue “disposing” of water bottles in this way by 2025 there will be one ton of plastic for every three tons of fish in the ocean, according to the Zoological Society of London (ZSL). Just a year ago, Scientific Reports published a study where they detail their findings of a massive floating island made from plastic, located between California and Hawaii. The island is rapidly growing and is currently approximately three times the size of France. It covers an area of approximately 1.6 million square kilometers (617,800 square miles) and contains 79,000 tons of plastic that was supposedly thrown “away”.



SOURCE theoceancleanup.com

Figure 22: Great pacific plastic patch (D. Rice, 2018).

These are the main reasons that lead me to believe that consumers are not being responsible enough or sustainable enough for things to remain operating as they are. Several nations have caught on to the fact that changes need to be made in order to make this a more sustainable practice. Countries, such as Germany and Sweden, have implemented policies to incentivize recycling of PET, like the introduction of refundable deposits in supermarkets. These deposits allow for consumers to return their empty bottles and in return they receive a small economic compensation (anywhere from 5 to 25 cents). As a result, Germany has recorded the highest recycling rate for bottles in the world as can be seen in *Figure 23*.

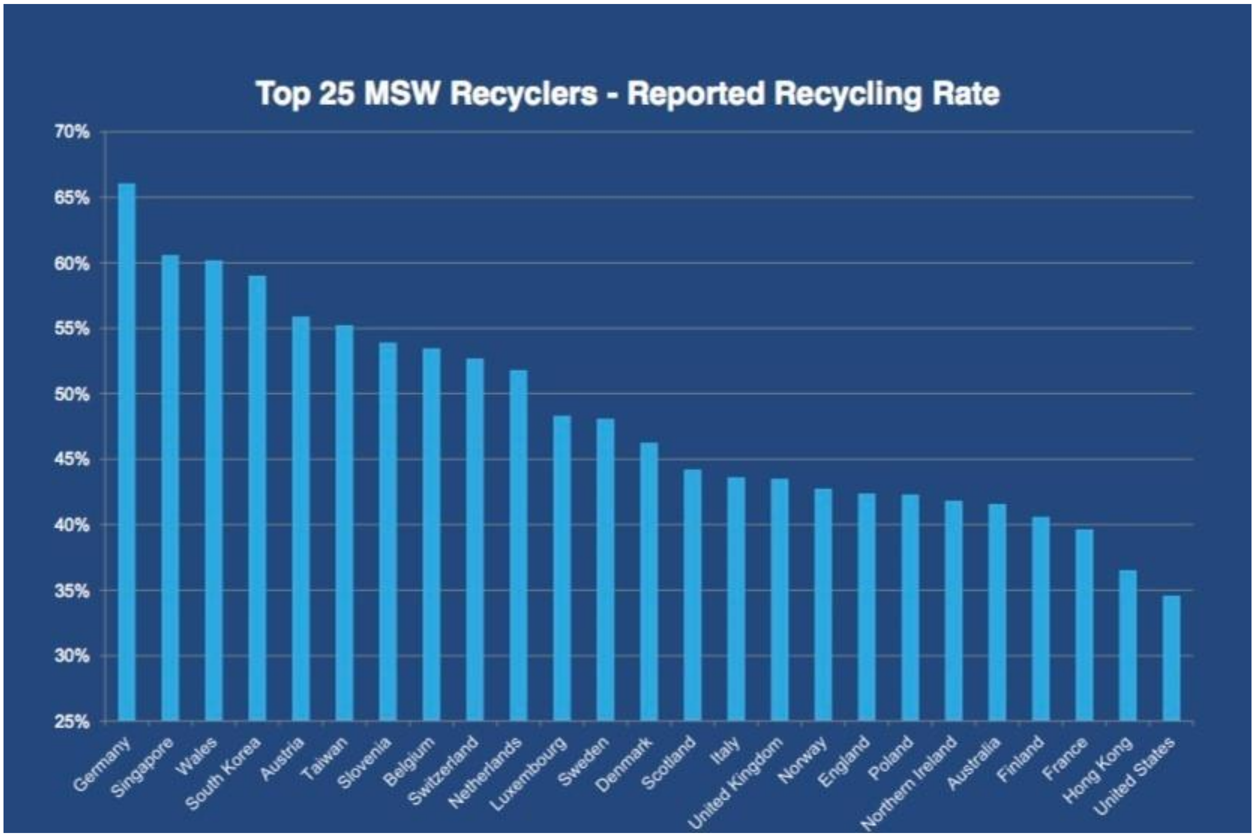


Figure 23: Top 25 MSW recyclers (A. Gray, 2017).

The United States seems to have more barriers to implement these sorts of policies due to beverage and retail industries and their trade association being powerful forces in state legislatures and the US Congress. Through campaign contributions, high-powered lobbyists and expensive public relations firms, these companies are able to keep these sorts of policies out of both state and national committees. Although these sorts of policies are likely to be a large part of the solution, this project aims to study the different alternatives to PET bottling and seeing how feasible (economically, physically and in terms of energy) it would be to introduce one of these alternatives into the market. With all that being said, for the alternatives that will be explored not all of them share the same properties or qualities. Some are still in development, and as a result, lack of verified and established data, in order to tackle this, prior to the quantitative analysis, a qualitative assessment of each of the alternatives will be conducted.

3. Alternatives to PET bottling: Qualitative Assessment

3.1 Introduction

Having seeing the rise of PET and what consequences it has caused through becoming such a widely used material, this section of the project attempts to display some of the available alternative materials that could, potentially, begin to substitute some of the PET being produced each year. Plastic (PET more specifically) historically has shown many advantages when compared to metals or glass containers, so this section will focus mainly on other plastic alternatives, of which, some, display different properties.

Plastics can be defined as materials that consist of a wide range or either synthetic or semi-synthetic organic compounds. Plastics are usually organic polymers of high molecular mass that often contain synthetic substances. As is the case with PET, substances derived from petrochemicals are the ones being mixed with the organic polymers in order to produce it. There are, however, some plastics (known as bio-based polymers) that are derived from renewable biomass sources. These sources include: vegetable fats and oils, corn starch, sugar cane and food waste. However, this does not imply that all bioplastics are biodegradable, meaning that they are capable of being broken down into innocuous products by the action of living organisms.

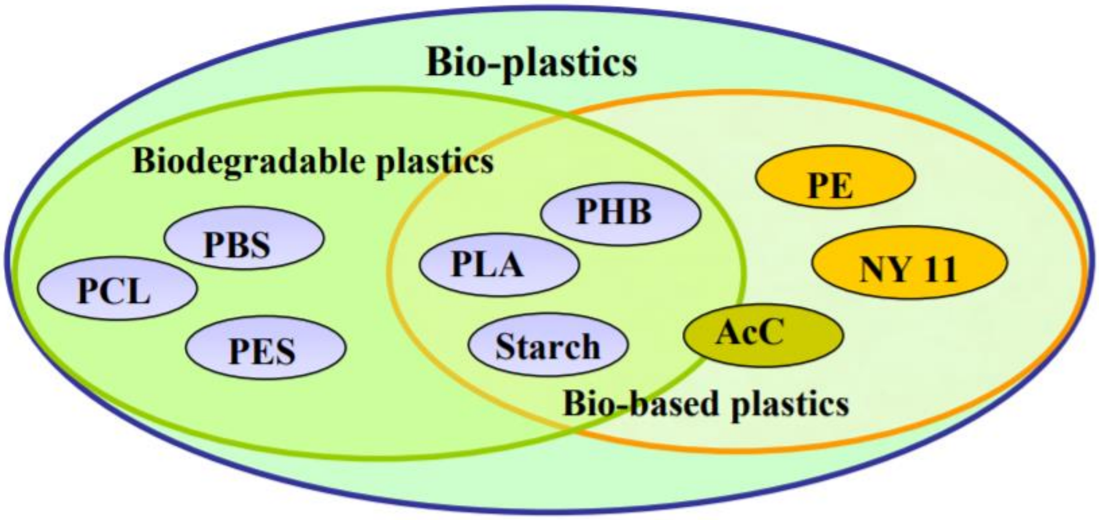


Figure 24: Plastics regarding their biodegradability and origins (International Journal of Molecular Sciences, 2009).

Keeping in mind that there are many alternative materials and the magnitude of this idea, this project will narrow down its scope onto the bottle production process while acknowledging the resin production process and the disposing or recycling processes that could be in place for said material. This project will also have as its main objective, to develop a tool or methodology that allows us to reach a rating (with its corresponding degree of validity) in order to quantify how feasible of an entry a material has when it comes to the water bottle industry. To do so, a number of key performance indicators (KPIs) are to be established with their respective importance or weight in the material's rating. Having said that, the following sections show a qualitative assessment of each of the alternative materials to be considered for future implementation. This qualitative assessment will be conducted by means of a SWOT (Strengths, Weaknesses, Opportunities and Threats) analysis for each of the alternative materials.

Figure 25: Traditionally used in business-related contexts, the SWOT analysis allows for a simple way to analyze internal and external factors for a specific company or item (LUCCA AM, n.d.).

3.2 Recycled Polyethylene Terephthalate (rPET)

Recycled Polyethylene Terephthalate (rPET) is the first and most obvious candidate that should be considered. There are already companies that package and bottle with percentages that can technically reach 100%, meaning that you can potentially make an entire usable drinking bottle from just rPET. In addition to this, there are currently some legislative strategies to enforce a minimum of 50% rPET in new PET bottles. For instance, in Spain, there are initiatives to enforce bottling companies to ensure that each PET bottle they manufacture holds at least 25% of rPET by the year 2022 and 50% by 2025. It presents a series of advantages compared to the rest of the alternatives that will be discussed. Firstly, the process implemented and the machinery used to produce rPET bottles would be identical to traditional PET bottle manufacturing. With rPET resin being nearly identical to PET resin, the process would suffer very few and subtle changes. Since the starting product is of very similar properties, the final product would also be very familiar to anyone who comes in contact with it. This means that transporting it from the facility to a supermarket and that having consumers interact with rPET bottles would turn out to be identical.

Figure 26: rPET flake (Sorema, n.d.).

This means that this is the alternative that presents the least amount of changes, or so it seems, as there are also a series of disadvantages or weaknesses that this material brings. Having a growing presence of rPET in our water bottles is undoubtedly a good sign. In fact, I would personally go as far as to say that without rPET as a major player of the future market it is extremely unlikely that the water bottle market would survive at all. We absolutely need to push for rPET but in order to do that we would need to change and educate a society where bad recycling tendencies have sprouted and led to our current situation. In conclusion, while rPET will be a critical part to making this a more sustainable market, to make the most use of it we would need societal changes and therefore will not stand as a solution on its own. Having said that, I believe that rPET is the basis for a future sustainable market with the sort of demand that will be expected. From our qualitative analysis we can reach the following SWOT analysis:

- **Strengths:** Presents the same properties that consumers are used to, once the flake is obtained all of the same machinery is used (from manufacturing standpoint costs would be the same in this respect)
- **Weaknesses:** This material is still from petrochemical sources and cannot be infinitely recycled so it would still add up to the major amounts of waste located in the oceans and wastelands. It also requires for people to correctly recycle them or for a restructure of waste management in the country of implementation.
- **Opportunities:** Could incentivize better recycling rates (more plastic being recycled as opposed to being thrown elsewhere) from both technical and political standpoints.
- **Threats:** Recycling capabilities of a country might be limited and could require massive investments (opening new facilities). It might also be challenging to establish a community of people that effectively recycles. Other threats include policies against petrochemical-based materials, global warming or environmental-related treaties or agreements.

3.3 Bio-based Polyethylene Terephthalate (BioPET)

Bio-based Polyethylene Terephthalate (BioPET) is a polyethylene terephthalate resin manufactured from the same terephthalic acid, and ethylene glycol from a bio-source. Ethylene glycol is obtained from plants such as, sugar cane or sugar beet. When it comes to bottle manufacturing, bottles come as a blend composed of approximately 70% conventional PET (fossil fuels) and up to a maximum of 30% plant based (sugar cane). Famous companies such as, Coca-Cola uses it in its Dasani bottles to claim a greener, more sustainable product. The strengths of this product are similar to rPET, where the final product and even the raw material is the same, so the process does not require as much of a change in terms of adapting machinery and facilities and the consumer receives a product of the same characteristics and properties. It is also a slightly more sustainable alternative to standard PET due to the fact that it is not entirely made from petrochemical sources, however it may bring an ethical debate regarding using crops to manufacture rather than to feed the people. It should however be noted that this material has experienced a growth of use and will gain popularity as consumers look for more sustainable alternatives. The United States, particularly, has been one of the major consumers of BioPET, where its main use is for bottles (as mentioned in Aquafina and Dasani).

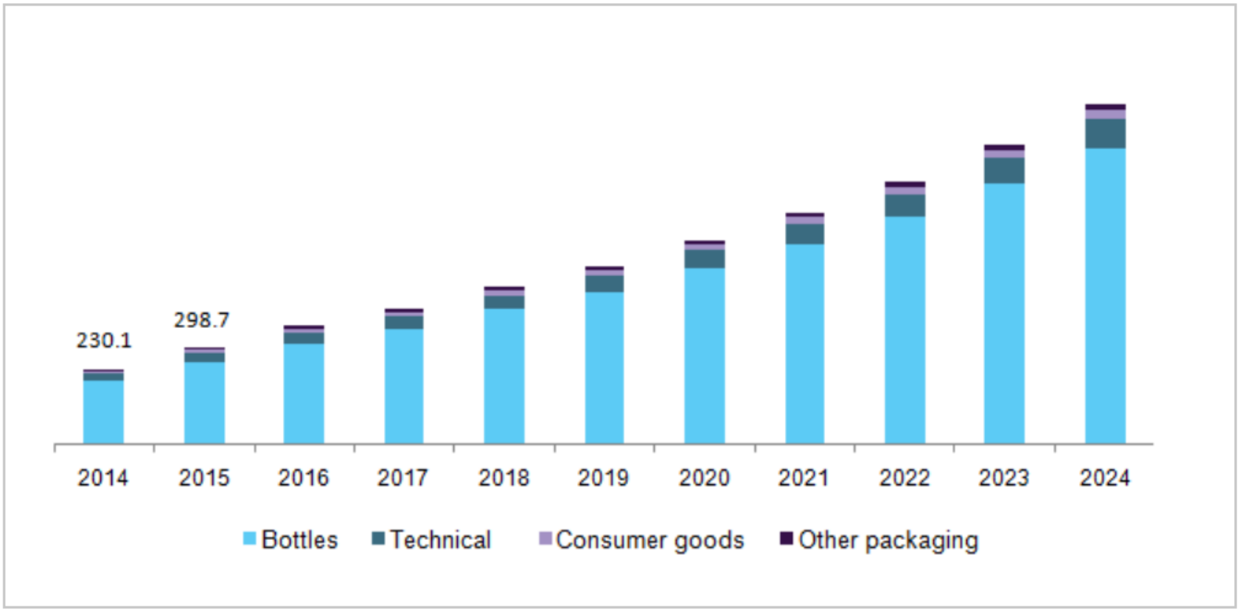


Figure 27: U.S bio-based PET market (by application) 2014-2025 (USD Million) (Grand View Research Inc, 2017)

Most importantly, BioPET remains as a non-biodegradable alternative and it will therefore, contribute to the unsustainable tendencies and customs of the consumers (unless these decide to change). This information leads us to the following SWOT analysis:

- **Strengths:** Presents the same properties that consumers are used to, once the flake is obtained all of the same machinery is used (from manufacturing standpoint costs would be the same in this respect). Lower carbon footprint and from a non-petrochemical source (if the entire bottle is made from BioPET).

- **Weaknesses:** Generally, most of the bottle is still made from petrochemical sources (usually 70%). Although its origin is from a plant it still results in a non-biodegradable product and so it would mean that crops and other forms of plant life would be used to create a non-biodegradable product.
- **Opportunities:** Could spark better recycling rates (so that not as much plant life is used to manufacture plants) from both technical and political standpoints. Could bring new technologies for other methods of manufacturing PET.
- **Threats:** Other threats include policies against petrochemical-based materials, global warming or environmental-related treaties or agreements.

3.4 Polylactic Acid (PLA)

Polylactic Acid (PLA) is a plastic that is both bio-based, that is from renewable sources (corn starch) and is biodegradable. It is a polymer made up by small lactic acid units. Lactic acid is an organic acid that is present in our daily lives. It expresses itself in our daily lives as pain in our muscles when they are overworked and even the taste of sour milk. Anything that is glucose-based can be turned into PLA. Its sources include both natural (corn starch, sugar cane...) and non-natural sugar sources, such as, sugar byproducts of other processes such as sweeteners for soda production. Bioactivity from bacteria turns the sugar source into a starting product for polymerization. For instance, in PLA production from corn starch, upon harvesting the corn, it is sent to a wet mill, where the starch is segregated from the rest of the corn. Once that is done, the starch is converted into dextrose by enzymatic hydrolysis (a process through which enzymes incentivize the cleavage of bonds). Then, a fermentation process for the dextrose takes place to create lactic acid after acidulation and a series of different purification steps. Once lactic acid is obtained, there are two main methods to produce polylactic acid. The first is through direct condensation polymerization of lactic acid and the second is ring-opening polymerization though the lactide intermediate, where the following steps are made. Water is eliminated (without the use of solvent) to provide a prepolymer that has a lower molecular weight. Then, it is catalytically depolymerized into a lactide which is purified by distillation to obtain a polymer. This completed process forms pellets of polylactide, which can be produced at different levels of purity in order to be capable of producing different molecular weights depending on the applications of PLA.

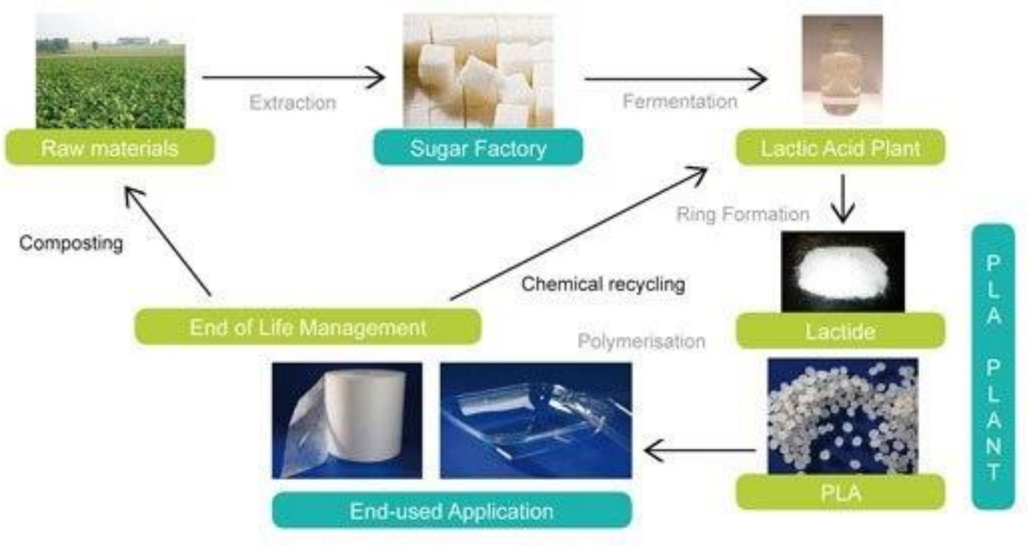


Figure 28: PLA production process (BioPlastics News, n.d.).

PLA presents itself as a transparent plastic with similar superficial properties to petrochemical-based mass plastics. Its main applications include 3D printing, cutlery and other container applications as is the case for bottles in some countries (already in the market in Italy and Chile). Out of the alternatives being explored, this is the first one with biodegradable capabilities. PLA biodegrades at different rates in different scenarios. For instance, it degrades in a matter of months in composting environments (hot, humid and highly bacteria-populated environments), however it does not biodegrade in marine environments.

If we analyze this alternative comparing it to PET through a SWOT analysis standpoint we can come to the following conclusions:

- **Strengths:** Non petrochemical origins (lower carbon footprint than PET), biodegradable in composting conditions
- **Weaknesses:** Not as prolific in sealing water vapor, O_2 or CO_2 when compared to PET, shorter shelf life than PET and PLA is not biodegradable in marine environments, which means it would still contribute to ocean polluting.
- **Opportunities:** Possibility to introduce new bottle manufacturing methods such as 3D printing could potentially make this material extremely feasible especially in localized bottling.

- **Threats:** using crops for producing plastics may be frowned upon, especially in developing countries where food might be scarce.

3.5 Spherification

By far, the most innovative and revolutionary alternative to PET water bottling would be a process called spherification. Spherification is a technique that comes from the culinary world, where foods are encapsulated in algae-based film to be eaten as a whole. When applied to portable water consumption, this would imply having the water encapsulated in that same algae-based film to then be distributed and eventually consumed by the consumer. These spheres can be made in various sizes and firmness, which would allow these spheres to hold liquids within them. There are two main components used for this technique: calcium chloride and sodium alginate, which is used to gel the chosen liquid. In this process the sodium alginate is dissolved directly into the chosen fluid. After mixing the liquid is left set in order to get rid of air bubbles that were caused in the mix. Once it is ready, the liquid is dropped into a bath that is prepared with calcium chloride and water. As a result of the gel coming in contact with the calcium chloride, a membrane is created, encapsulating the liquid within the membrane. This process is referred to as direct spherification and results in a thin gel shell. This thin gel shell means that the spheres are more subject to breaking and therefore should be consumed as early as possible. As a result, this method is commonly used in the kitchen to prepare elaborate dishes. There is another method known which is called reverse spherification. In this second method of spherification, the gelling stops and does not continue into the liquid orb. This means that as a result, thicker shells form, leaving a more resistant sphere. If we were to consider spherification as a feasible alternative to PET bottling, it would be through reverse spherification.

Figure 29: The result of spherification with water (ThoughtCo, 2019).

From a product life cycle analysis standpoint, this method would mean that every single aspect of water bottling would be changed, from the containers, to how they are distributed and finally how they are being consumed. So, in order to assess its possibilities, I have decided to conduct a brief SWOT analysis, reaching the following conclusions.

- **Strengths:** Bio-based source which is not crops (algae), smaller carbon footprint, biodegrades in 4 to 6 weeks
- **Weaknesses:** It would require a revolution from a manufacturing standpoint. Needs far more efficient methods that can compete with this rate of production. It requires a mindset change from consumers who would now need to overcome how they carry their water and how they overcome the unfamiliar taste of the biodegradable film.
- **Opportunities:** Could spark a complete revolution in the industry with almost no carbon footprint and without consumption of crops that could be otherwise used to grow food.
- **Threats:** Transportation and logistics within a supermarket could be extremely challenging in terms of fragility and preserving what is inside of the algae films (shorter shelf life).

3.6 Polyhydroxyalkanoates (PHA)

Polyhydroxyalkanoates (PHA) are polyesters that are produced in nature. Polyesters are a specific type of polymers that contains ester in its main functional group. This means that at least one hydroxyl group has been replaced by an alkoxy group. PHAs are a type of natural polyesters that derive from bacterial fermentation. These bacterial fermentations of sugar or lipids mean that microorganism synthesize polyesters in nutrient-deficient conditions. The fermentations occur in bio-reactors where the bio-source and the bacteria meet in the correct conditions for the process to happen. As a result of fermentation, the PHAs are formed and can be harvested and collected by means of separation, purification and drying. Once the PHA powder is obtained it is turned into pelletized biopolymer resins through an extrusion process. Once the resin is pelletized it can be treated as other plastics to shape and contour the desired product. Contrary to PLA production, for PHA production, fermentation is used to produce the entire polymer within the organism. Then, it must be harvested from cells and purified to obtain the desired polymer. Whereas in PLA production it is the monomer that is produced in the fermentation process.

PHAs are obviously bio-based and are also biodegradable not only in composting environments but also in other environments, such as, marine ones. Other properties of PHAs include good ultra violet (UV) resistance but poor resistance to acids and bases. This would not be a problem, since we are to be containing water within PHA and water is neither basic nor acidic. In addition to that, it is a nontoxic plastic that sinks in water, facilitating its anaerobic biodegradation in marine water. PHA applications are usually medical applications such as, sutures, slings and also single-use food packaging.

Figure 30: PHA flake prior to molding (Bio-Based Press, n.d.).

PHAs' properties bring an interesting perspective as can be seen in the following SWOT analysis:

- **Strengths:** Bio-based source, smaller carbon footprint, bacteria used to ferment the polymer can be reused, cheaper in terms of injection molding (lower fusion temperature needed). Biodegradable in several environments including in marine ones.
- **Weaknesses:** It would require a revolution from a manufacturing standpoint, harvesting polymers as opposed to other plastics having a monomer and creating the polymer with a reactor and a catalyst. Higher material costs and slower production methods.
- **Opportunities:** Could help those who aim to clean the oceans by not adding extra plastic to the already contaminated sea. Could lead to newer technologies to harvest this material more efficiently and could potentially use the nutrients from the plastic to plant more crops and feed the bacteria to create more PHAs.
- **Threats:** It is an opaque (non-transparent) material, which could draw away some consumers that would like to clearly see the contents of the bottle. Could face backlash due to the fact that crops would be used to manufacture a product as opposed to feed people.

3.7 Conclusion

From all of these assessments reaching certain and solid conclusions is nearly impossible. While qualitative analysis sets the basis for comparison, it becomes quite apparent that it is not enough to establish a comparison between alternative materials that are different in so many ways. Due to this, we came to the realization that this project, in order for the comparison to fully make sense, had to be able to give a number rating to each of the alternative materials so that they become easier to compare. The following section of the paper, aims to explain what this quantification process is, as well as, how and why it takes place.

4. Quantification method

4.1 Introduction

As previously mentioned, having reached the end of the previous assessment, it is hard to draw conclusions from just a qualitative analysis. As humans, we are a rational species that, in order to compare, need some sort of rationality to make it a more objective comparison. To do this we have decided to create a model, that relies on some input data, and returns a certain rating for that given material. The reason why this methodology was chosen is due to the fact that not all of the materials presented in this paper find themselves in the same maturity levels and so, not all have the same amount of data available. Having said that, of course those entries with more input data would result in a more solid and structured rating, meaning that its rating would have more validity behind it. This means that from the input data would result in two output numbers, one being the rating of that material, with its corresponding validity or strength. In order to develop a tool that would have its use in the future, as well as other parts of the world, the rating would not have a finite scale, whereas the validity or strength of the ratings will be ranked out of 10. The validity will be a number that depends on both the amount, and the type of input data being provided. To create this model, we would need to figure out the input data to be received and in order to find these inputs the lifecycle of water bottles must be analyzed.

This section of the paper will firstly define what Key Performance Indicators (KPIs) are, how they are determined and how that would translate to the water bottle business. To see how these KPIs are determined for water bottles, the product life cycle of this product must be closely looked at, as to establish certain inputs that carry importance in determining a materials feasibility (their rating). Later in this section, since the same KPIs might carry different weights or degrees of importance, which is why, as well as identifying the KPIs we must understand which impact they will have on both the rating (some input data is more relevant towards the feasibility) and the validity of that rating (without certain crucial inputs it would be impossible to determine that a rating has a certain degree of strength behind it). Both of these impacts are also highly dependent on the specific place where these materials are to be studied (availability of resources, policies, GDP, among others) which is why for section *4.4 KPI weights and model*, the framework will be based on the current United States market.

4.2 KPI analysis and determination

Key Performance Indicators, otherwise known as KPIs, are measurable values usually used to quantify and demonstrate how a business or a company is performing effectively towards achieving their key objectives or goals. As just mentioned, KPIs are usually used to quantify an organization's (or a specific department's) performance towards a business goal. These include financial metrics, such as, *profits, earnings before interest taxes depreciation and amortization* (*EBITDA*), *cost of goods sold* (*COGS*), *sales* used to measure how close a business is towards their financial goals and objectives. Other examples are customer metrics and process metrics. For instance, *customer acquisition costs* and *percentage of product defects* are two measures that a company could use to quantify how close they are to reaching objectives in terms of customers and processes respectively.

Figure 31: KPI are becoming widely popular, especially in business applications (EALDE Business School, n.d.).

One may think that this project is not necessarily related to how a business operates, however, the concept of measuring certain values to make an assessment as to how close to a certain objective, are certainly ideas that can translate towards this project's focus. Traditionally KPIs are easily measured values that can then be used to assess proximity towards a larger business goal, this is where this project deviates from the standard key performance indicators. Although these KPI models were used as inspiration to continue making progress in this project, since our goal is to quantify feasibility within very different materials and thus, very different amounts of data available (some have barely been discovered or are vastly different from other materials), we have decided to develop a tool that with a certain number of inputs would give a resulting rating. Since our aspiration is for this tool to be able to be used in the future, in different countries and regions where different aspects of bottling might be prioritized, the tool should not return a value that is limited by a scale. This is because having the rating limited could lead to ratings that could exceed that limit. For example, if this tool were to be used in the future, where material costs might drop due to new extraction techniques or incentives might be placed to benefit a specific group of materials, values could exceed the limit. In other words, contrary to traditional KPI models, there is no specific "goal" or "objective" but rather, this tool should allow for its user to compare different materials by introducing certain values that are known and comparing their resulting rating.

As mentioned previously, the materials that we are planning on comparing not only possess very different characteristics but are also at different stages of their maturity. Some have been in place for close to a hundred years while others have barely made it to production, which means that the data pools available for each of the materials are also very different, not only in the size and the amounts of data, but also the quality of the data. This has several implications, first we must carefully analyze and draw KPIs that these materials can have in common to address physical differences between the materials. In order to address the varying amounts of information available for each of the materials, just one output in the form of a rating would become an insufficient comparison. For example, if we are to compare two materials (for the sake of this example material *A* and material *B*) and the user has provided ten different inputs for material *A* and only one input for material *B*, comparing just the rating on its own would not provide a fair comparison. This is because each of those ratings do not have the same amount of information supporting it. To address this concern, the tool should also give some sort of indication to the user of the rating's validity.

Each of the KPI inputs will have different importance in the material's feasibility for the chosen market, therefore, those KPI inputs that weigh more towards the rating, will also share a larger contribution towards the rating's validity. The model would of course be limited as to the amount of inputs the user has available to him/herself and therefore the validity of each rating will be expressed as a percentage. It should be noted that, the percentage displayed for the model is by no means an absolute measure, meaning that a rating with 100% validity would not guarantee 100% certainty in that rating, but rather, 100% validity would let the user know that all of the model's inputs have been used to determine the rating. How true and valid a rating is, depends more on the quality and the certainty of the data that is being introduced to the model, rather than the sheer volume of inputs being introduced (although by increasing the amount of inputs the rating would have a more solid foundation).

Apart from rating each of the materials, there are other goals for this tool. As it was mentioned, this tool would allow the user to rate each material (with its corresponding validity) but if the analysis is taken a step further, the tool can allow the user to perform sensitivity analysis on each of the materials. For example, if a user sees that a certain material has a higher rating compared to another material, the user can use the tool to see which thresholds or benchmarks have to be reached for each of the KPI inputs in order for the lower rated material to surpass the higher rated material. In doing so, the user would discover which sort of conditions have to be met for one material to surpass the other.

Having addressed that this model should give a rating and a validity towards that rating (2 outputs with variable inputs) and that it can be used to analyze materials in several ways; what should be studied is which and how many inputs there should be. To do so, we must analyze our five alternative materials along with PET, and we must do so from a product lifecycle perspective in order to draw some similarities and features that are more comparable.

4.3 KPIs in the water bottle life cycle

As previous sections have stated, in order to achieve a more fair and logical comparison some similarities must be drawn and some common ground must be reached as to establish certain parameters that could be shared by most (if not all) materials that are going to be analyzed. To do that, the decision that was made was to breakdown a bottle´s life cycle into different sections and then seeing which sort of information would be desirable towards knowing if that material could result in a feasible product. Upon analyzing each of the product's lifecycle the figure below displays the five categories in which it has been decided to split the inputs.

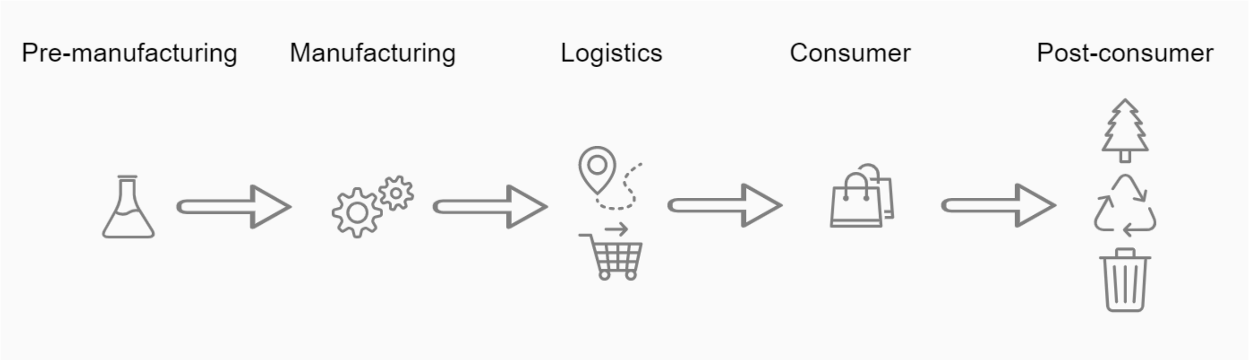


Figure 32: The chosen five stages for bottled water lifecycle.

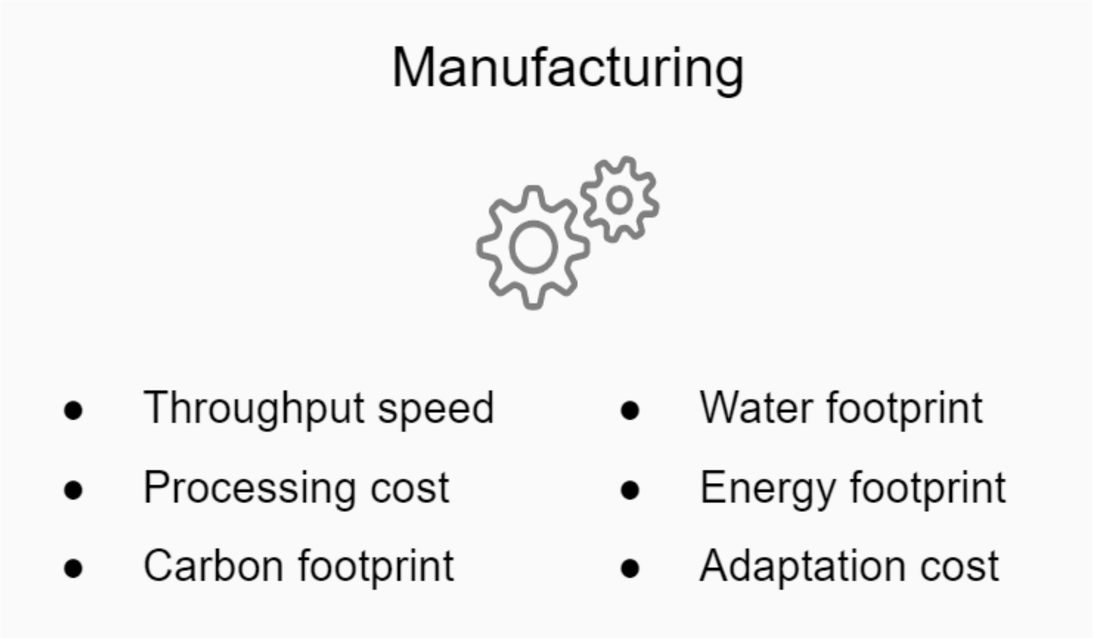
As a result of the analysis these are the resulting categories for the inputs:

- **Pre-manufacturing:** Even though all of the materials we have chosen to study have different sources and procedures to follow before becoming the recipient where water is stored, they all have to undergo a stage where raw materials are turned into the corresponding product that will later hold water. Taking into consideration all of the elements of this stage we reach the following set of inputs for the model.

Figure 33: Pre-manufacturing inputs.

Obviously when considering what is necessary before manufacturing bottle products that differ in the raw materials, the following questions arise. What raw materials are needed in order to create this product? Where does it come from (or what type of source is it)? And finally, how available is it? These are the sorts of questions we are to answer in order to assess an alternative's strength in the "pre-manufacturing" stage of the lifecycle. How each of the inputs are introduced and how each of them contributes towards computing a rating will be shown in the section *4.4 KPI weights and model construction*.

- **Manufacturing:** In this particular stage of the product lifecycle, it is where each of the materials undergo different processes, resulting in different products. To account for these differences and to make the best possible judgement of this particular section, the following inputs will be considered:



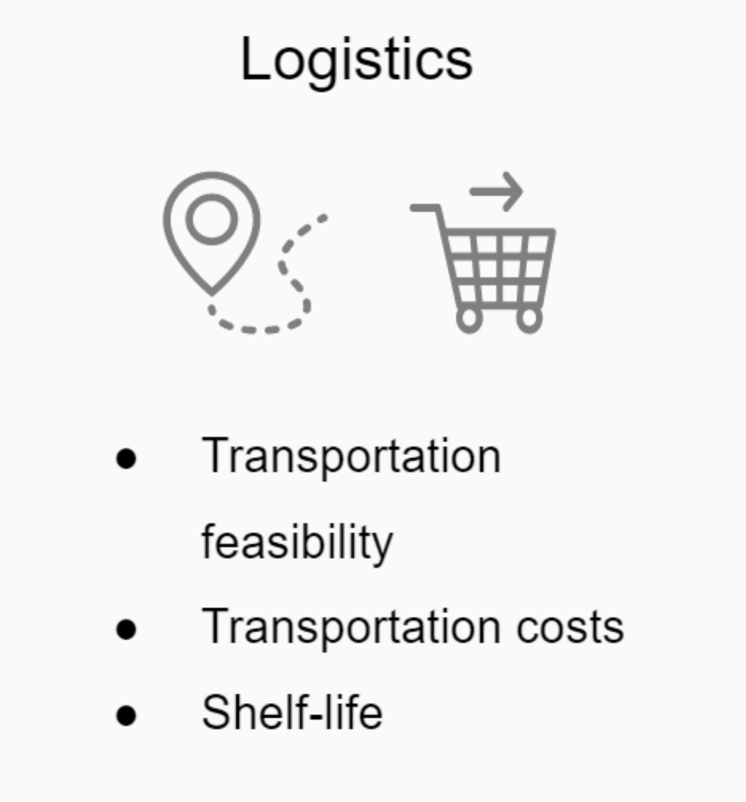
Manufacturing

- Throughput speed
- Processing cost
- Carbon footprint
- Water footprint
- Energy footprint
- Adaptation cost

Figure 34: Manufacturing inputs.

When it comes to manufacturing the main questions we want to solve are, how much is this stage going to cost as well as how many units will be able to be produced. In addition to these matters, it becomes useful to know not only how much money is being spent but also how many resources (carbon emissions, energy emissions and energy expenditure) as well as knowing, if it would be possible to adapt our current manufacturing facilities and networks (PET facilities and networks) to the other materials. As with all other inputs, how each of the inputs are introduced and how each of them contributes towards computing a rating will be shown in the section *4.4 KPI weights and model construction*.

- **Logistics:** This section of the of the product life cycle corresponds to those steps that the product takes between leaving the manufacturing facility and reaching the consumer. In this case, although the products will be different due to the materials being used, this stage would be fairly similar for all of the products. This stage involves transportation, storage and retail (at supermarkets or other stores) and all of the possible issues and concerns that may surface in any of these areas for each of these materials. With that being said, here are the inputs for the lifecycle stage titled "Logistics":



Logistics

- Transportation feasibility
- Transportation costs
- Shelf-life

Figure 35: Logistics inputs.

The first issue to address is to see how feasible it is to transport each material, since different materials require different environments to ensure that they maintain and preserve their contents. For example, some biodegradable materials may experience certain conditions of humidity and heat causing them to decay quicker than wanted. The second question to answer is how much would be the transportation/storage cost when compared to today's standard PET bottle. And finally, the last question to answer is what sort of shelf-life each material has in order to assess their effectiveness in a supermarket scenario where it might take several days or even weeks to be sold to a consumer.

- **Consumer:** Naturally, the stage that follows would be how the consumer interacts with the product and the experience that consuming the water in the bottle would cause them to have. With that being said, this section has only two, but very important inputs as can be seen in the following image:

Figure 36: Consumer inputs.

Willingness is an input meant to describe and measure how likely a consumer is to consider and purchase each of the products. It should account for preference in the composition of its properties, such as recyclability or biodegradability. Without taking into consideration what the consumers want, it would be impossible to determine whether a product would let alone be successful, but be a feasible alternative. Having addressed that we must quantify how willing a customer is to change to a product or to simply consume that product, it should also be accounted for how likely that customer is to adapt to the changes necessary for that product to be used in their daily lives.

- **Post-consumer:** The fifth and final section of our product lifecycle would be the aspects involved after the consumer has made use of the product and has ingested the water within it. Due to the physical differences between all of the products, each of these may follow a different path depending primarily on each material's composition and decomposition. Taking all of that into account, these are the inputs chosen for the "post-consumer" stage of the product lifecycle:

Post-consumer

- Biodegradability
- Recyclability
- Collection costs
- Incentives

Figure 37: Post-consumer inputs.

Keeping in mind the aspects previously mentioned, these four inputs are meant to evaluate and determine what each of the materials future would be, as well as, account for any policies or political measures that would be in place to favor any specific material in the form of adding collection costs or incentives (like would be the case in countries like Germany or Sweden).

Having broken down the different stages of the products' lifecycles and each stages' corresponding inputs, the following section will break down how each of the inputs are introduced and how they interact in order to compute a rating for a specific material entry.

4.4 KPI weights and model construction

4.4.1 Introduction

Having made the decision on the type of inputs to be used for each of the stages of a bottle's lifecycle this section has two main objectives. Firstly, this section aims to determine how important each of those inputs is towards a final absolute rating, and its corresponding validity and also what tool is to be used towards creating the model and how that model is to be constructed. It should be noted that for this model to be effective these weights and inputs have to be carefully studied for the desired region, seeing as a country like the United States of America would have different policies and priorities when compared to countries such as, Germany or Sweden.

4.4.2 KPI input structure & weights for the US

As it can be seen from previous sections where the inputs have been displayed, not all of them will have the same importance in determining the rating of the material. Nor do they require the same type of inputs, seeing as some inputs will require a number and others a qualitative comparison to the standard that we have chosen (PET). Since for this particular feasibility study, it is to be performed in the United States of America. It should be taken into account which of the inputs should be more highly valued towards the development of the rating. Throughout the US market research that was performed by talking to American companies involved in water bottling, plastic recycling, plastic manufacturing as well as other European companies that do business in the United States, the following weights have been awarded to each of the inputs.

Table 1: KPI Inputs with their corresponding weight.

Lifecycle stage	KPI Input	KPI Input weight
Pre-manufacturing	raw material cost (cents / lb)	170
	Origin	50
	Availability	100
Manufacturing	Throughput speed	80
	Processing cost (cents/lb)	150
	Carbon footprint (kg CO2 / kg produced)	50
	Water footprint (liters)	50
	Energy footprint (MJ/liter)	90
	Adaption cost	60
Logistics	Transportation costs	70
	Transportation feasibility	90
	Shelf-life (weeks)	65
Consumer	Willingness	150
	Adaptability	75
Post Consumer	Biodegradability (type)	90
	Recyclability	40
	Collection cost	60
	Incentives	50

It should be noted that for the majority of the inputs, their respective weight is the maximum amount of points that can be awarded for that specific input. These inputs are the ones that require a non-numeric entry but are rather a comparison to the standard in place today, PET bottles. The other inputs (the ones that require a numeric entry) have room for improvement, for instance raw material costs can severely drop leading to a much higher rating. Doing this leaves room for this tool to be used in the future in the event that one of those numeric inputs experience notable changes from today's current situation. From the table above we can tell that in this current market the most important aspects are: raw material costs, followed by consumer willingness, processing costs, availability and then other lesser aspects such as degradability and other resources being consumed for production. The majority of the non-numeric inputs will have several options ranging from "Unknown", "Very Low", "Low", "Standard", "High" and "Very High" depending on how they compare to the industry standard of PET bottles. This is done to account for those inputs that would otherwise be hard to quantify for comparison. These inputs can therefore be defined as "subjective data", where the inputs would be up to the consideration of the user and which require contrast and expertise from said user. The rest of the non-numeric inputs (Origin and Biodegradability) have different types of entries where, for instance, a material that biodegrades in marine environments would be awarded more points than those who only biodegrade in compost environments and a lot more points than those who do not biodegrade at all. The remaining inputs (numeric) have been scaled so that the current market leader PET is close to receiving maximum points, leaving room for improvement for future and alternative scenarios. The latter part of the non-numeric inputs along with the numeric inputs can also be defined as "objective data" meaning that the inputs are factual, as opposed to being estimated or obtain through judgement.

4.4.3 Model construction and modifications

Like it was discussed throughout earlier sections of the paper, the tool to be used to create the model is Microsoft Excel as it allowed for flexibility in a number of aspects, such as, different types of inputs for the system, flexibility in modifying the model, and ability to produce graphical representations.

For each of the inputs' validity, it was decided that as long as the information being introduced was anything other than "Unknown", that particular KPI input would be awarded with its corresponding validity. This means that as long as an input is valid, it would receive the corresponding validity. The inputs with higher weights also carry a bigger percentage of the total validity seeing as those inputs have a larger significance in the result, and therefore as long as the entry is a known input, the full validity should be awarded to that input- To illustrate how the model works see *Table 2* for an example on an imaginary material.

Table 2: Example inputs with awarded points and validity.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	85	170	124.00	170
	Origin	Petrochemical	50	0.00	50
	Availability	Unknown	100	0.00	0
Manufacturing	Throughput speed	Standard	80	40.00	80
	Processing cost (cents/lb)	90	150	86.67	150
	Carbon footprint (kg CO2 / kg produced)	2	50	12.50	50
	Water footprint (liters)	Unknown	50	0.00	0
	Energy footprint (MJ/liter)	Unknown	90	0.00	0
	Adaption cost	Standard	60	30.00	60
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	Standard	65	32.50	65
Consumer	Willingness	Standard	150	75.00	150
	Adaptability	Standard	75	37.50	75
Post Consumer	Biodegradability (type)	No	90	0.00	90
	Recyclability	No	40	0.00	40
	Collection cost	Unknown	60	0.00	0
	Incentives	Unknown	50	0.00	0

To develop an output and to provide more additional information on each of the five stages, a rating is assigned to each of the five lifecycle stages. This rating is a sum of the points awarded for each of the inputs of that category, each of those stage ratings with their own validity percentage (see *Table 3*).

Table 3: Example five stage ratings with % validity.

Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	124.00	68.8%
Manufacturing	169.17	70.8%
Logistics	112.5	100.0%
Consumer	112.5	100.0%
Post Consumer	0	54.2%

By doing this prior to constructing the complete absolute rating, a viewer can analyze and see how their selected material compares in each stage to another material and can also provide a visual representation as to how each of the stages contribute towards the material's rating. To illustrate this, *Figure 38* shows how each of the five stages contribute towards an absolute rating for an imaginary material.

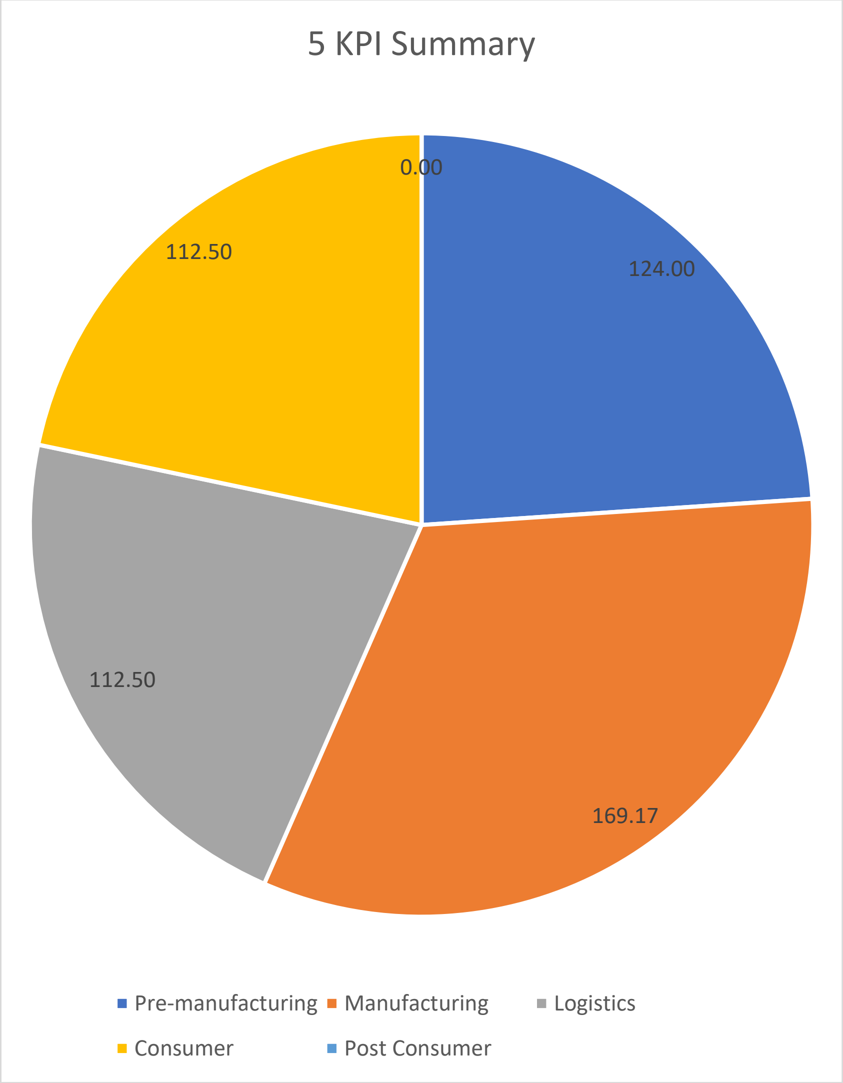


Figure 38: Example five stages' ratings.

From each of these five stage ratings we can construct the absolute rating by adding each of them and then computing a global validation for that absolute rating. However, when testing the model, it becomes apparent quite quickly, that with just an absolute rating and validity, those materials that are in the earlier stages of their development are at a clear disadvantage. With less inputs being known, those materials, not only do they lose out on validity (as they should for lack of information) but they also opt for a much lower amount of points towards their absolute rating. Because of this, a third output was created, to evaluate which sort of potential or projected rating a material would have, basing this projected rating on the weighted average of the inputs that the material brings. This projected rating would be used to evaluate what sort of potential each of the materials has although they lack information have. It should always be analyzed on a case by case basis, since lacking certain information (for instance if availability of the raw materials is 0) would result in an unfeasible product. In other words, for those materials that lack inputs, a projected rating would be used to get a glimpse of that material's potential, and that number would be created by using the weighted average of the known inputs to estimate the unknown inputs (see *Table 4* for output example).

Table 4: Example outputs: Rating, validity and projected rating.

Rating	Validity	Projected rating
518.17	76.5%	677.25

As it can be appreciated from the table above, this example material would have an absolute rating of 518.17 with a validity of 76.5% according to this model. In addition to that, based on the strength of this particular material in the inputs that are known it would have a projected rating of 677.25. The absences responsible for this example having less than 100% validity are "availability", "water footprint", "energy footprint", "collection cost" and "incentives". Some inputs were purposefully missed in order for this example to have a projected rating and to show in this example how the projected rating is calculated using the available information to estimate the material's overall strength and have a complete rating. It should be noted that the previous example is merely included to display how the model works, meaning that the outcome of this example is of course meaningless unless it is being compared to the outcome of using another material in this model.

4.5 Conclusion

As stated throughout this section's introduction, the aims for this particular section were, firstly to lay some common ground so that we can reach the specific inputs that we would want to be used for the model. Then, the aim was to explain how important these inputs are towards giving a rating and finally to show how the model computes a rating based on an example.

5. Quantitative Analysis

5.1 Introduction

Having laid the foundation on which inputs will be available and how they operate towards calculating a rating for a material, this section aims to quantify the previously analyzed materials in order to have a more comparable way to determine which of the materials could be feasible options in this market. Additionally, this section will present results, which will later help in reaching conclusions and in exploring which future applications or further advancements could be made.

5.2 Polyethylene Terephthalate (PET)

5.2.1 PET: Introduction

For the sake of establishing a standard for comparison, the rating for the leader material being used in water bottling should be determined first. This would act as a base rating for the other materials to face off against and see in what aspects of their product lifecycle they differ the most from the material that has led the market for decades. Firstly, each of the inputs for PET will be explained and then finally show what is PET’s resulting rating.

5.2.2 PET: Inputs

Starting off with the “pre-manufacturing” inputs, PET, currently presents the following data:

Table 5: PET pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	77	170	136.88	170
	Origin	Petrochemical	50	0.00	50
	Availability	Standard	100	50.00	100

According to the American plastic brokers that were consulted, raw material costs for PET range from 75 cents to 80 cents per pound, and at the current day of checking, costs were 77 cents per pound. This corresponds to 136.88 points being awarded. Like mentioned in the previous section of the paper, when constructing the model, the objective inputs are designed in such a manner that when introducing PET's data, the amount of points awarded was close to the weight value as to leverage the margin for improvement down the line. The resulting formula for raw material costs' rating sum is:

$$Rating\ sum\ for\ raw\ material\ costs = \frac{62 * 170}{raw\ material\ cost\ \left(\frac{cents}{lb}\right)}$$

Formula 1: rating sum, raw material costs.

Additionally, as it is known, PET comes from a petrochemical source which awards no points in that particular category. Finally, its availability when compared to other materials is known to be "standard", awarding 50 points (out of 100) for that particular category.

Table 6: PET manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	High	80	60.00	80
	Processing cost (cents/lb)	80	150	97.50	150
	Carbon footprint (kg CO_2 / kg produced)	2	50	6.25	50
	Water footprint (liters)	17.4	50	32.60	50
	Energy footprint (MJ/liter)	7	90	76.00	90
	Adaption cost	Very low	60	60.00	60

As it can be seen on *Table 6*, these are the inputs that correspond to PET's manufacturing stage, where PET clearly struggles in the carbon footprint generated as can be seen by the low rating it obtains for that particular input. In this particular general department, PET proves to be quite strong, particularly in its high throughput speed and its non-existent adaptation costs, seeing as no changes would need to be made to manufacture this particular material.

Table 7: PET logistic inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	Very high	65	65.00	65

From the logistics stage for PET it is displayed on *Table 7* that both feasibility and transportation costs are standard, whereas shelf-life is awarded with the maximum amount of points due to the physical properties that PET possesses. It is one of the best materials for maintaining its composition and contents in their initial condition.

Table 8: PET consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	Standard	150	75.00	150
	Adaptability	Standard	75	37.50	75

From a consumer standpoint, customers are tending to shift towards "greener" alternatives but are still willing to keep on consuming these types of bottles as has been shown by the fact that water bottle consumption maintains its growth. For how customers would adapt to this kind of bottle, the "standard" option has been chosen since consumers would still need to be weary and mindful in order to recycle.

Table 9: PET post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	No	90	0.00	90
	Recyclability	Standard	40	20.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

Finally comes the last set of inputs for the final product lifecycle stage, "post-consumer". For this particular section, it is known that PET is not biodegradable, with "standard" recyclability (since it does lose some of its properties in the process and cannot be infinitely recycled). For this particular market, no collection costs are added (and hence "very low" is awarded to even these materials) and incentives are non-existent for this material.

5.2.3 PET: Outputs and Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 10: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 39*).

Table 10: 5 KPI summary, PET.

Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	186.88	100.0%
Manufacturing	332.35	100.0%
Logistics	145	100.0%
Consumer	112.5	100.0%
Post Consumer	80	100.0%

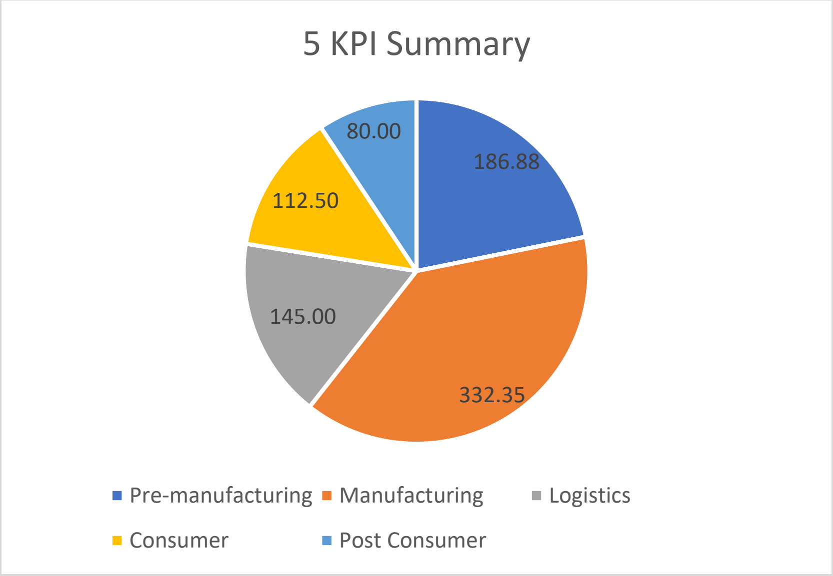


Figure 39: 5 KPI summary, PET.

As *Table 10* displays, under this particular model, PET would have 100% validity for each of the five lifecycle stages. As a consequence, PET would obtain an absolute rating of 856.73 with 100% overall validity (*Table 11*), making PET's projected rating the same as its absolute rating.

Table 11: Model outputs, PET.

Rating	**Validity**	**Projected rating**
856.73	100.0%	856.73

Now that the information for PET has been entered and a rating has been obtained for the leading material in the market, we can now enter data for the rest of the alternatives and see how they stack up with today's standard.

5.3 Recycled Polyethylene Terephthalate (rPET)

5.3.1 rPET: Introduction

Having obtained the outcomes and results for PET, this subsection will focus on the inputs that are to be entered for recycled PET (rPET) and the outcomes of the model.

5.3.2 rPET: Inputs

As common sense would suggest, rPET shares most of the properties that PET has, and therefore, most of the inputs will be the same as PET's. With that being said, below are the first set of inputs (pre-manufacturing) for rPET:

Table 12: rPET pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	82	170	128.54	170
	Origin	Petrochemical	50	0.00	50
	Availability	Low	100	25.00	100

It is no surprise that raw material costs would be slightly larger since rPET is still not as available as "virgin" PET since recycling facilities in the US are oversaturated and overloaded.

Table 13: rPET manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	Standard	80	40.00	80
	Processing cost (cents/lb)	80	150	97.50	150
	Carbon footprint (kg CO_2 / kg produced)	2	50	6.25	50
	Water footprint (liters)	17.8	50	32.20	50
	Energy footprint (MJ/liter)	7.5	90	75.00	90
	Adaption cost	Very low	60	60.00	60

Since the recycling rates slow down the throughput speed, rPET would be introduced as a "standard" speed as opposed to a "high" throughput speed. Also, since additional cleaning would be needed for the rPET flake (or resin) the footprints would be slightly higher than for PET. Other than that, since the machinery used for the process would be identical to the machinery being used to manufacture PET bottles, adaptation costs would remain as "very low".

Table 14: rPET logistics inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	Very high	65	65.00	65

For this particular stage of the product lifecycle, rPET would be identical to PET, and hence the same inputs would be entered for this particular section.

Table 15: rPET consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	High	150	112.50	150
	Adaptability	Standard	75	37.50	75

The "consumer" stage brings a slight difference in that consumers searching for a "greener" alternative to traditional PET would choose rPET. Recycling PET would incite consumers to be more willing to shift towards this option and how they adapt to the way the bottle is consumed would remain as "standard" due to the fact that consumers would still need to be weary of recycling and proper disposing of the bottle.

Table 16: rPET post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	No	90	0.00	90
	Recyclability	Low	40	10.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

The main difference between these inputs and PET's is that rPET loses part of its ability to be once again recycled which is why for that particular input, the value entered was "Low".

5.3.3 rPET: Outputs & Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 17: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 40*).

Table 17: 5 KPI summary, rPET.

Lifecycle stage	**5 KPI summary**	**Validation by lifecycle stages**
Pre-manufacturing	153.54	100.0%
Manufacturing	310.95	100.0%
Logistics	145	100.0%
Consumer	150	100.0%
Post Consumer	70	100.0%

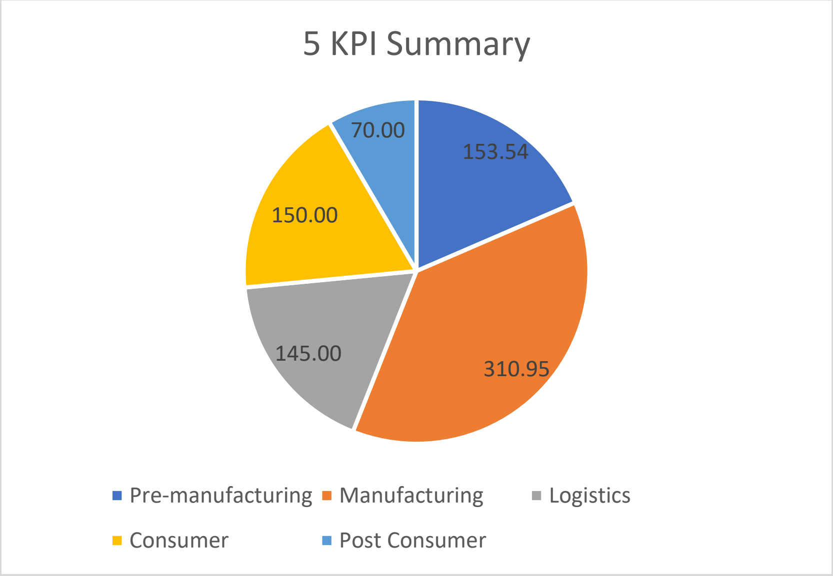


Figure 40: 5 KPI summary, rPET.

As *Table 17* displays, under this particular model, rPET would have 100% validity for each of the five lifecycle stages. As a consequence, rPET would obtain an absolute rating of 829.49 with 100% overall validity (*Table 18*), making rPET's projected rating the same as its absolute rating.

Table 18: Model outputs, rPET.

Rating	**Validity**	**Projected rating**
829.49	100.0%	829.49

As it was to be expected rPET presents a rating that is close to PET's (856.73). rPET proved to overcome PET in the consumer department, but failed to keep up in the pre-manufacturing, manufacturing and post-consumer. In a scenario where rPET was more easily available (either, via more efficient procedures or more recycling facilities) this would push this material up to a rating of 854.49 which is extremely close to PET's absolute rating.

5.4 Bio-based Polyethylene Terephthalate (BioPET)

5.4.1 BioPET: Introduction

To complete the PET group of materials, this subsection will first show and explain BioPET's inputs to then analyze the outcomes from the model and compare to the previous materials.

5.4.2 BioPET: Inputs

As with the previous two materials, this subsection will begin by displaying BioPET's inputs for the first of the lifecycle stages (*Table 19*).

Table 19:BioPET pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	95	170	110.95	170
	Origin	Bio/Petrochemical	50	12.50	50
	Availability	Standard	100	50.00	100

BioPET is still predominantly a petrochemical-based plastic (as of today). However, as its name implies, BioPET is a blend of PET obtained through petrochemical sources (usually 70% of the bottle) and PET obtained through biological sources, such as crops, which usually make up as much as 30% of the water bottle. Due to this reason, in the "origin" category, BioPET receives more points that both PET and rPET but compensates by having a higher raw material cost, due to crops being a more costly source for plastics.

Table 20: BioPET manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	Standard	80	40.00	80
	Processing cost (cents/lb)	80	150	97.50	150
	Carbon footprint (kg CO2 / kg produced)	1.85	50	6.76	50
	Water footprint (liters)	Unknown	50	0.00	0
	Energy footprint (MJ/liter)	Unknown	90	0.00	0
	Adaption cost	Very low	60	60.00	60

BioPET's availability means that its throughput speed is not compromised (as it was with rPET). Its processing cost would be identical to rPET and PET since their properties are the same, and the carbon footprint would be slightly less due to the fact that a percentage of each bottle would not be made from petrochemical sources. Water footprint and energy footprint is likely to be higher than PET's but no objective information was available for this particular material. Finally, since their properties are the same, BioPET also obtains the highest amount of points possible for the category of "adaptation cost" (as no adaptations would need to be made for this material).

Table 21: BioPET logistics inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	Very high	65	65.00	65

As with PET and rPET, BioPET shares identical conditions and therefore inputs for the logistics stage of the product lifecycle.

Table 22: BioPET consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	High	150	112.50	150
	Adaptability	Standard	75	37.50	75

In the same manner as rPET, BioPET would have consumers more willing to switch to this type of bottle due to the fact that it has a lower carbon footprint and is not entirely from a petrochemical source. With that being said, although it is a "greener" alternative it is still a non-biodegradable material and consumers would therefore still need to be careful of its disposal. This means that in adaptability for consumers in terms of disposal would still have a "standard" value.

Table 23: BioPET post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	No	90	0.00	90
	Recyclability	Standard	40	20.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

As it has just been mentioned, BioPET, despite its name, is not a biodegradable option, so it will have the same inputs for the "post-consumer" stage as PET given that it has not yet been recycled and thus, has a "standard" recyclability.

5.4.3 BioPET: Outputs & Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 24: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 41*).

Table 24: 5 KPI summary, BioPET.

Lifecycle stage	**5 KPI summary**	**Validation by lifecycle stages**
Pre-manufacturing	173.45	100.0%
Manufacturing	204.26	70.8%
Logistics	145	100.0%
Consumer	150	100.0%
Post Consumer	80	100.0%

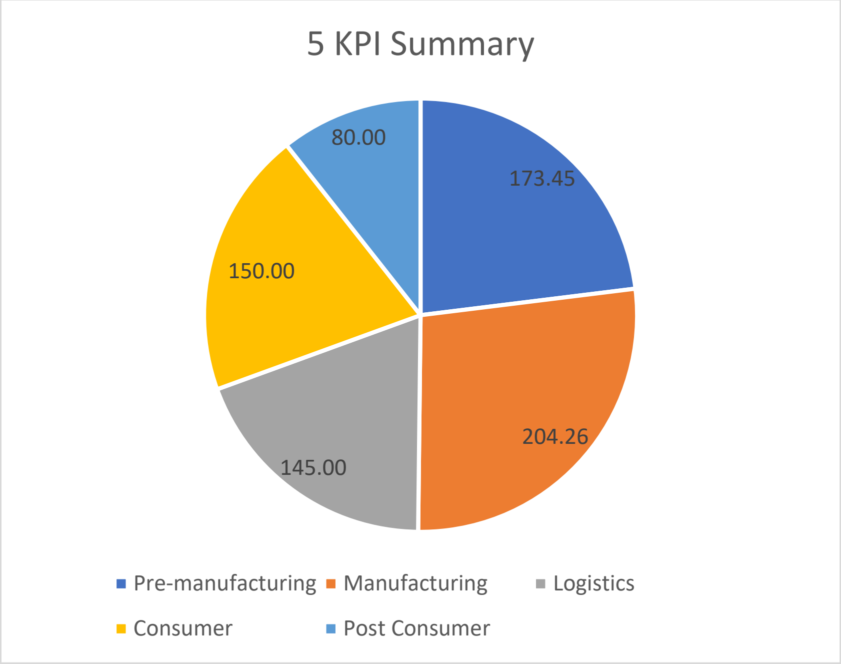


Figure 41: 5 KPI summary, BioPET.

As *Table 24* displays, under this particular model, BioPET would not have 100% validity for all of the five lifecycle stages. As a consequence, BioPET would obtain an absolute rating of 752.70 with 90.6% overall validity (*Table 25*), making BioPET's projected rating 830.76.

Table 25: Model outcomes, BioPET.

Rating	Validity	Projected rating
752.70	90.6%	830.76

As it was to be expected BioPET brings a lower rating to PET's (856.73). Although, BioPET proved to overcome PET in the consumer department and managed to tie PET in the logistics and post-consumer stages, BioPET failed to keep up in the pre-manufacturing and manufacturing, especially considering the lack of reliable information that is available for the manufacturing stage. The projected rating was designed to make up for the lack of information in some of the less established materials but we should be careful in comparing absolute ratings to projected ratings.

For this particular case, BioPET has a projected rating that is much closer to PET's rating. This projected rating supports the hypothesis that although we do not know the energy and water footprints exactly, they are presumably bigger footprints than those of PET, and thus, giving BioPET a lower overall score or rating that traditional PET.

5.5 Polylactic Acid (PLA)

5.5.1 PLA: Introduction

Having already completed the PET group of materials, this subsection will revolve around the first of the biodegradable materials, PLA. The aim is to first show and explain its inputs to then analyze the outcomes from the model and compare to the previous materials.

5.5.2 PLA: Inputs

As with the rest of the materials this subsection will begin by analyzing the inputs that correspond to the first stage of the product lifecycle, pre-manufacturing.

Table 26: PLA pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	99	170	106.46	170
	Origin	Crops	50	33.33	50
	Availability	Standard	100	50.00	100

According to the American plastic brokers that were consulted, raw material costs for PLA range from 90 cents to 105 cents per pound, at the current day of checking, costs were 99 cents per pound. This corresponds to 106.46 points awarded (see *Formula 1*). As explained in previous sections, PLA comes from biologically-based sources (crops) which awards 33.33 points in that particular category (out of 50 possible points). Finally, its availability when compared to other materials is known to be "standard", awarding 50 points (out of 100) for availability.

Table 27:PLA manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	Low	80	20.00	80
	Processing cost (cents/lb)	70	150	111.43	150
	Carbon footprint (kg CO_2 / kg produced)	0.3	50	41.67	50
	Water footprint (liters)	Unknown	50	0.00	0
	Energy footprint (MJ/liter)	Unknown	90	0.00	0
	Adaption cost	High	60	15.00	60

As PLA is still quite a recent material some of the objective data is still difficult to come across. With that being said, its nature in both sources and physical properties make it a more viscous plastic than PET and therefore a slower one to produce in terms of throughput. This is why throughput speed is considered to be slow. However, it has a lower melting point than PET making it easier to mold and therefore cheaper to melt which drops processing cost. It also brings a far lower carbon footprint when compared to PET and is estimated to continue to lower it in the coming years. From an adaptation point of view, PLA would require high costs to make proper use of the equipment available for PET bottling.

Table 28: PLA logistics inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	High	65	48.75	65

The main difference that this material holds when being compared to the previously mentioned materials is that since it is biodegradable, we cannot expect for this material to have the same shelf-life as a material that could potentially hold its composition for hundreds or even thousands of years. It is because of this reason that PLA would have a “High” shelf-life as opposed to PET’s “Very high” shelf-life.

Table 29: PLA consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	High	150	112.50	150
	Adaptability	High	75	56.25	75

From a consumer standpoint a biodegradable water bottle would be highly desirable and so would their willingness to consume it. From a convenience point of view, having a consumer know that a PLA bottle biodegrades in compost environments (hot, humid, with bacteria) means that they will have an easier adaptation since they could dispose of it without being extremely worried of its destination.

Table 30: PLA post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	Compost	90	40.00	90
	Recyclability	None	40	0.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

As has been the theme for PLA's section, its main difference is the fact that this bottle biodegrades. This information is also relevant here as it can be seen on *Table 30*. This property means that since this material biodegrades in compost (it is very slow to biodegrade in marine water) this material is awarded 40 points (out of the 90) for this particular category and 0 points from the recyclability and incentives categories (in other markets this sort of initiative could be enhanced by means of incentives).

5.5.3 PLA: Outputs & Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 31: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 42*).

Table 31: 5 KPI summary, PLA.

Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	189.80	100.0%
Manufacturing	188.10	70.8%
Logistics	128.75	100.0%
Consumer	168.75	100.0%
Post Consumer	100	100.0%

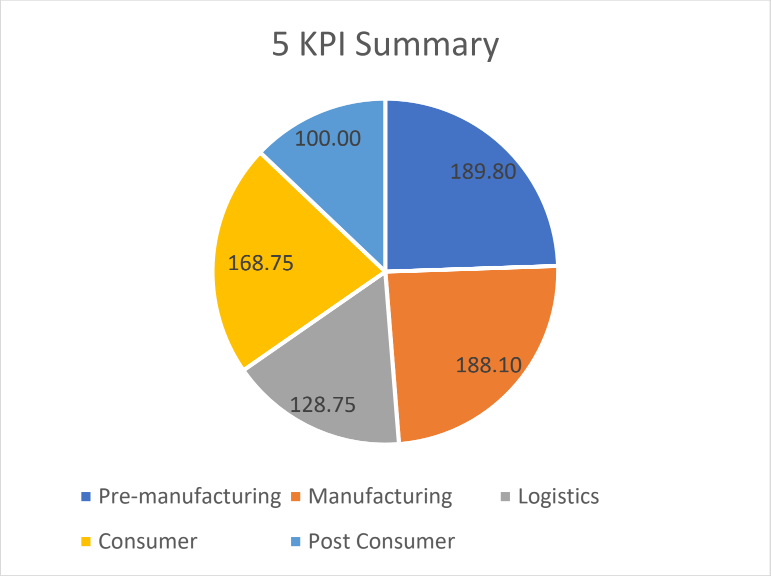


Figure 42: 5 KPI summary, PLA.

With PLA not being as “mature” as other materials, as *Table 31* displays, under this particular model, PLA would not have 100% validity for all of the five lifecycle stages. As a consequence, PLA would obtain an absolute rating of 775.39 with 90.6% overall validity (*Table 32*), making PLA’s projected rating 855.80.

Table 32: Model outcomes, PLA.

Rating	Validity	Projected rating
775.39	90.6%	855.80

The lack of information available means that PLA opts for a lower absolute rating than those materials with more widely known data. With that being said, it comes as no surprise that PLA has a lower rating than PET (856.73) or even rPET (829.49). When compared to BioPET, however, with both having the same validity (they both had the same inputs entered), PLA makes up for the manufacturing and logistic stages with its points in pre-manufacturing, consumer and post-consumer stages. When looking at the projected rating, one can see that PLA is less than 1 point away from PET’s absolute rating. With all things considered, although this shines some hope on PLA for this particular market, it should be noted that in terms of objective (numeric data) PET is clearly the more feasible material. Nonetheless, considering that PLA’s initial raw material costs were as high as $3 and have severely and consistently dropped, there is certainly some hope that this material will play some role in the future market for water bottles.

5.6 Spherification

5.6.1 Spherification: Introduction

Continuing the trend of analyzing the biodegradable materials, this section will aim to quantify and analyze, what would be the most revolutionary of the materials that have been discussed, water spherification. This will be done by first explaining the inputs for this material and then the outcomes received from the model.

5.6.2 Spherification: Inputs

In the same manner that the previous materials' inputs have been explained, this subsection will start by showing the inputs that spherification brings for the first stage of the product lifecycle, the pre-manufacturing stage.

Table 33: Spherification pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	Unknown	170	0.00	0
	Origin	Algae	50	50.00	50
	Availability	Very high	100	100.00	100

Since spherification is primarily made from algae it is awarded the most amount of points for the "origin" category (since it is from biological sources that are not competing with feeding people as crops would). This type of source also means that it is the most available out of the options that are being presented in this project. With spherification being the most recent and innovative alternative option for water bottling, a lot of the crucial information for determining this materials feasibility is not available. This means that the raw material cost would be determined as "unknown".

Table 34: Spherification manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	Very Low	80	10.00	80
	Processing cost (cents/lb)	Unknown	150	0.00	0
	Carbon footprint (kg CO_2 / kg produced)	Unknown	50	0.00	0
	Water footprint (liters)	Unknown	50	0.00	0
	Energy footprint (MJ/liter)	Unknown	90	0.00	0
	Adaption cost	Very high	60	7.50	60

As it was to be expected, there are a lot of inputs for this specific method of "bottling" that are unknown. As a result of its current production techniques and how hard it would be to adapt current available systems to fit this material, it comes to no surprise that this particular section receives a very low feasibility score.

Table 35: Spherification logistics inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Very high	70	8.75	70
	Transportation feasibility	Very Low	90	11.25	90
	Shelf-life	Very Low	65	8.13	65

Spherification properties make for the logistics stage of the product life-cycle quite difficult as can be seen by the inputs. For the spheres to make it in good conditions to the supermarket, they would need to be very carefully packaged and kept at a temperature that would maintain the structure and the integrity of the sphere. In addition to that, these spheres would have the lowest shelf life by far.

Table 36: Spherification consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	Low	150	37.50	150
	Adaptability	Very low	75	9.38	75

From a consumer standpoint, a lot of consumers would be willing to try this technique but not many would switch over permanently for this type of water consumption due to its limitations in carrying. Additionally, the taste of these spheres is not yet tasteless and could make customers shy away from this type of product.

Table 37: Spherification post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	Yes	90	90.00	90
	Recyclability	None	40	0.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

Spherification's strengths lie in its biodegrading nature, where it can degrade in just weeks in nearly every environment.

5.6.3 Spherification: Outputs & Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 38: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 43*).

Table 38: 5 KPI summary, Spherification.

Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	150.00	46.9%
Manufacturing	17.5	29.2%
Logistics	28.13	100.0%
Consumer	46.88	100.0%
Post Consumer	150	100.0%

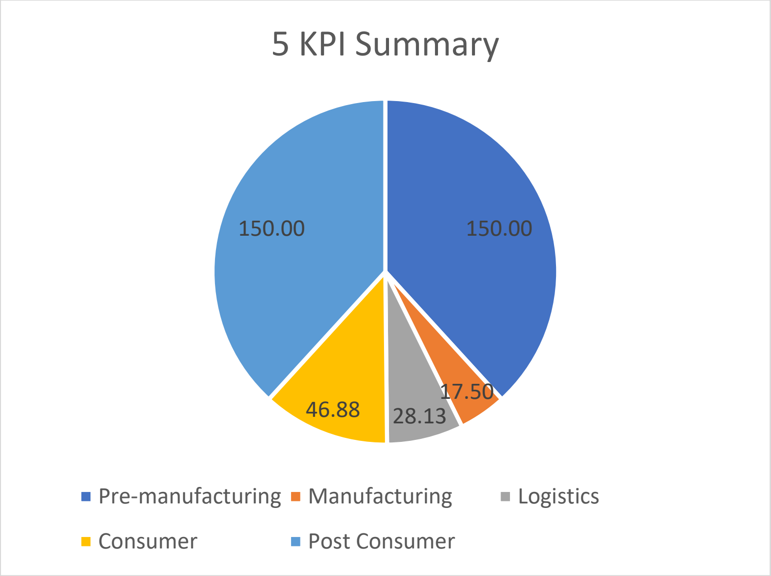


Figure 43: 5 KPI summary, Spherification.

As spherification is the least "mature" material (as it has been shown throughout this section) a lot of information was simply not available. This means that as *Figure 43* shows the majority of Spherification's absolute rating comes from the pre-manufacturing and post-consumer stages. As a result, *Table 39* displays, the outputs of Spherification's inputs, resulting in an absolute rating of 392.50 with 65.8% overall validity, making Spherification's projected rating 596.76.

Table 39: Model outcomes, Spherification.

Rating	Validity	Projected rating
392.50	65.8%	596.76

It comes as no surprise that spherification brings not only the lowest absolute rating but also the lowest projected rating. This technique brings too many differences to compete with the already standardized bottles which makes it nearly impossible for it to compete with them. The fact that this method would require both a manufacturing revolution, but also a consuming revolution (in terms of how the general public consumes water on the go) makes this option very difficult to call feasible on a large scale. It should also be noted that even if the projected ratings came to be high, the user should look carefully at what type of information is missing from the inputs because it seems highly improbable that we can call a material feasible without knowing either the raw material costs or the processing costs (without these it would be hard to trust the model).

5.7 Polyhydroxyalkanoates (PHA)

5.7.1 PHA: Introduction

Finally, to conclude the quantification phase of this project, PHA (the last biodegradable plastic to be introduced) will be entered in the model and compared to the rest of the materials.

5.7.2 PHA: Inputs

Staying consistent with the rest of the materials, the first of the inputs that will be explained are those corresponding to PHA's pre-manufacturing phase.

Table 40: PHA pre-manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Pre-manufacturing	raw material cost (cents / lb)	225	170	46.84	170
	Origin	Crops	50	33.33	50
	Availability	Standard	100	50.00	100

According to the American plastic brokers that were consulted, raw material costs for PHA range from 200 cents to 245 cents per pound, at the current day of checking, costs were 225 cents per pound. This corresponds to 46.84 points awarded (see *Formula 1*). As explained in previous sections, PhA comes from biologically-based sources (crops) which awards 33.33 points in that particular category (out of 50 possible points). Finally, its availability when compared to other materials is known to be "standard", awarding 50 points (out of 100) for availability.

Table 41: PHA manufacturing inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Manufacturing	Throughput speed	Very low	80	10.00	80
	Processing cost (cents/lb)	70	150	111.43	150
	Carbon footprint (kg CO_2 / kg produced)	0.2	50	62.50	50
	Water footprint (liters)	Unknown	50	0.00	0
	Energy footprint (MJ/liter)	Unknown	90	0.00	0
	Adaption cost	High	60	15.00	60

As PHA is still quite a recent material some of the objective data is still difficult to come across (it is even more recent than PLA). With that being said, its nature in both sources and physical properties make it a more viscous plastic than PET and therefore a slower one to produce in terms of throughput. In addition to that, due to its method of manufacturing being slower than PLA's, PHA is considered to have a "very low" throughput speed. However, it has a lower melting point than PET making it easier to mold and therefore cheaper to melt which drops processing cost. It also brings a far lower carbon footprint when compared to PET, and even PLA. As it is still in its early stages, PHA is expected to continue to lower its footprints (as well as its raw material costs) in the coming years. From an adaptation point of view, PHA would require high costs to make proper use of the equipment available for PET bottling.

Table 42: PHA logistics inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Logistics	Transportation costs	Standard	70	35.00	70
	Transportation feasibility	Standard	90	45.00	90
	Shelf-life	High	65	48.75	65

In the same manner as PLA, we cannot expect for PHA to have the same shelf-life as a material that could potentially hold its composition for hundreds or even thousands of years. It is because of this reason that PHA would have a "High" shelf-life as opposed to PET's "Very high" shelf-life. Other than that, PHA, would not bring any changes to transportation, which is why both transportation feasibility and costs remain as "Standard".

Table 43: PHA consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Consumer	Willingness	High	150	112.50	150
	Adaptability	High	75	56.25	75

From a consumer standpoint a biodegradable water bottle would be highly desirable and so would their willingness to consume it. From a convenience point of view, having a consumer know that a PHA bottle biodegrades in both compost environments (hot, humid, with bacteria) or in marine water, means that they will have an easier adaptation since they could dispose of it without being extremely worried of its destination.

Table 44: PHA post-consumer inputs.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum
Post Consumer	Biodegradability (type)	Marine	90	90.00	90
	Recyclability	None	40	0.00	40
	Collection cost	Very low	60	60.00	60
	Incentives	None	50	0.00	50

PHA's ability to also degrade in marine water means that this material would not contribute to the massive amounts of plastic that have been building up for the last decades. As a result, this material is the full 90 points for this particular category and 0 points from the recyclability and incentives categories (in other markets this sort of initiative could be enhanced by means of incentives).

5.7.3 PHA: Outputs & Conclusion

For the first part of this subsection, the ratings for each of the five lifecycle stages will be shown (*Table 45: 5 KPI Summary*) along with a visual representation for the absolute rating (*Figure 44*).

Table 45: 5 KPI summary, PHA.

Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	130.18	100.0%
Manufacturing	198.93	70.8%
Logistics	128.75	100.0%
Consumer	168.75	100.0%
Post Consumer	150	100.0%

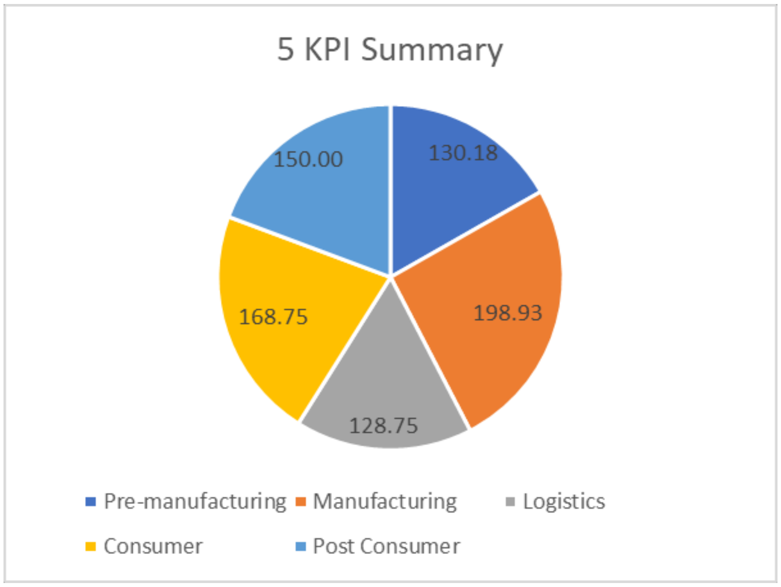


Figure 44: 5 KPI summary, PHA.

When analyzing the five stage ratings, it can be said that from all of the materials that have been explored throughout this project, PHA has the most balanced contribution from each of the stages. This becomes quite apparent by just comparing the *5 KPI summary* pie charts for all of the evaluated materials. As a result of PHA not being as "mature" as other materials, under this particular model, PHA would not have 100% validity for all of the five lifecycle stages. As a consequence, PHA would miss out on some of the available points and obtain an absolute rating of 776.61 with 90.6% overall validity (*Table 46*), making PHA's projected rating 857.14.

Table 46: Model outcomes, PHA.

Rating	Validity	Projected rating
776.61	90.6%	857.14

As with other materials, the lack of information available translates in PHA opting for a lower absolute rating than those materials with more widely known data. This of course means that PHA has a lower rating than PET (856.73) or even rPET (829.49). However, PHA's absolute rating exceeds the ratings obtained by BioPET, PLA and spherification. When compared to BioPET, with both having the same validity (they both had the same inputs entered), PHA makes up for the pre-manufacturing, manufacturing and logistic stages with its points in consumer and post-consumer stages. The fact that PHA relies more on its subjective data supports the idea that PHA is a product that is still in its early stages when compared to the rest. Since the stages in which BioPET exceeds PHA are more objective, it should be noted that although it has a lower rating, BioPET is more probable to have a successful market presence as of today. This is also the case when we are comparing PLA and PHA, where PLA's superiority in pre-manufacturing demonstrates that it has been further developed (better pre-manufacturing conditions such as drop of raw material costs as previously mentioned). This should also bring optimism that in a few years to come, PHA raw material costs might also drop in a similar manner as PLA's (keeping in mind that they are different materials with different properties of course). When looking at the projected rating, it can be seen that PHA less than 1 point ahead of PET's absolute rating. This should be carefully analyzed seeing as when comparing an absolute rating to a projected rating we are comparing more objective data to an estimation based on the strength of both objective and subjective data. With all things considered, we cannot assume from this model that PHA is a more feasible alternative than PET but it surely is interesting to see that it could potentially compete, given these sorts of circumstances. Nonetheless, considering that other biodegradable materials' raw material costs have severely and consistently dropped (area where PHA is struggling the most for this particular model), there is certainly some hope that this material will start to get involved in the future market for water bottles, in fact, Nestlé has announced a collaboration to develop biodegradable water bottles using Danimer Scientific's Nodax PHA.

5.8 Conclusion

This section's goal was to calculate and group the results for each of the materials. In order to summarize all of the information displayed throughout this section the following table and bar charts have been constructed:

Table 47: Results summary for all 6 materials.

		Material					
		PET	rPET	BioPET	PLA	Spherification	PHA
Results	Pre-manufacturing	186.88	153.54	173.45	189.80	150.00	130.18
	Manufacturing	332.35	310.95	204.26	188.0952	17.50	198.93
	Logistics	145.00	145.00	145.00	128.75	28.13	128.75
	Consumer	112.50	150.00	150.00	168.75	46.88	168.75
	Post-consumer	80.00	70.00	80.00	100.00	150.00	150.00
	Absolute rating	856.73	829.49	752.70	775.39	392.50	776.61
	Projected rating	856.73	829.49	830.76	855.80	596.76	857.14

Figure 45: Absolute ratings for all 6 materials

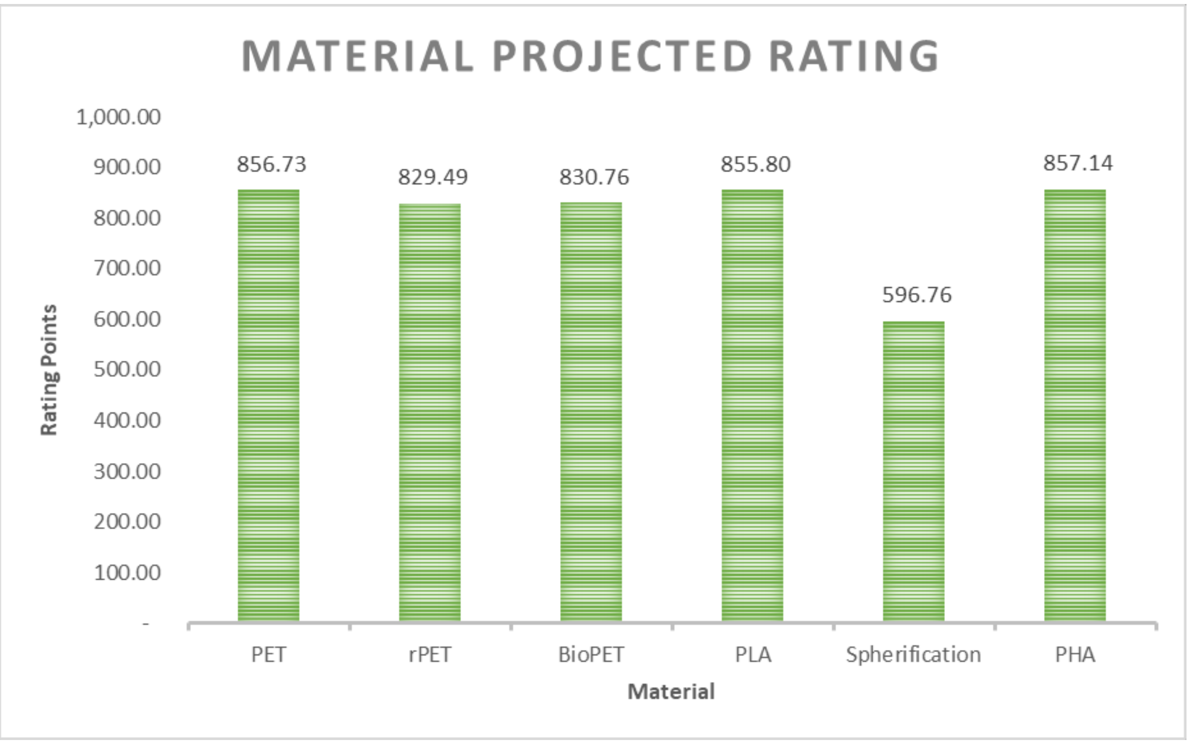


Figure 46: Projected ratings for all 6 materials.

6. Future applications & Conclusions

6.1 Introduction

The sixth and final section of the project has several objectives. Firstly, it is to look back and analyze what this project really means and what the results support. In addition to that it is to reflect on the project and see what sort of other future applications it may have, as well as further developments that could be introduced in the future.

6.2 Future applications & further developments

As mentioned in other parts of this report, this tool could potentially be used as a sensitivity analysis tool towards helping us reach a better understanding of material comparison. For instance, with the information that is available, we could use this tool to answer the question: What raw material costs would be necessary, for PHA to overtake PET in absolute rating? As it turns out, once PHA reaches a raw material cost of 83 cents per pound, it would narrowly overtake PET in absolute rating (meaning we would still have missing information in the same inputs as before) as can be seen on *Table 47* and *Table 48.*

Table 48: Sensitivity analysis example.

Lifecycle stage	KPI Input	Material Inputs	KPI Input weight	Rating sum	Validity sum	Lifecycle stage	5 KPI summary	Validation by lifecycle stages
Pre-manufacturing	raw material cost (cents / lb)	83	170	126.99	170	**Pre-manufacturing**	210.32	100.0%
	Origin	Crops	50	33.33	50			
	Availability	Standard	100	50.00	100			
Manufacturing	Throughput speed	Very low	80	10.00	80	**Manufacturing**	198.93	70.8%
	Processing cost (cents/lb)	70	150	111.43	150			
	Carbon footprint (kg CO_2 / kg produced)	0.2	50	62.50	50			
	Water footprint (liters)	Unknown	50	0.00	0			
	Energy footprint (MJ/liter)	Unknown	90	0.00	0			
	Adaption cost	High	60	15.00	60			
Logistics	Transportation costs	Standard	70	35.00	70	**Logistics**	128.75	100.0%
	Transportation feasibility	Standard	90	45.00	90			
	Shelf-life	High	65	48.75	65			
Consumer	Willingness	High	150	112.50	150	**Consumer**	168.75	100.0%
	Adaptability	High	75	56.25	75			
Post Consumer	Biodegradability (type)	Marine	90	90.00	90	**Post Consumer**	150	100.0%
	Recyclability	None	40	0.00	40			
	Collection cost	Very low	60	60.00	60			
	Incentives	None	50	0.00	50			

Table 49: Sensitivity analysis example ratings and validity.

Rating	Validity	Projected rating
856.75	90.6%	945.60

Additionally, and to make up for the fluctuations in price that might occur in a day to day basis, and advancement that could be made on this model would be for it to be given a certain range or a deviation to use for the model to calculate an average price that accounts for that deviation.

In terms of future applications, this project is meant to be the beginning for this sort of analysis. It would be especially interesting to try and use it in a number of years once the situation has experienced changes and could include future ratings by estimating new material trends. For example, if a new material is discovered in five years-time with similar properties to PLA and PHA, a more advanced model of this sort could be used to use previous and current PLA and PHA ratings to estimate what future ratings for that new material.

6.3 Conclusions

The main goal of this research project was to see if there were alternative materials that could potentially be a feasible solution to the water bottle situation that has been reached through so many years of extensively using PET as the main material for water bottling. There are serious consequences to using this type of material in the way that it has been used throughout our history and those consequences might soon reach an irrevocable point.

In order to set up why other alternatives need to be considered, we needed to establish how we have reached the current situation in terms of bottled water consumption. Knowing we got where we are today and the sorts of repercussions this way of consumption has makes us realize that something needs to change. Once we understood that our current way of operating is not sustainable, and seeking out the market for alternatives we wanted to analyze very different materials. Through our qualitative analysis we managed to understand what each material could bring to the table and provide towards a more sustainable future, however, the differences in the materials' maturity resulted in very different pools of information for each of them. As a result, the qualitative analysis was too inconclusive due to its lack of objectivity. It was then, that inspired by businesses being obsessed in quantifying their proximity towards an objective, we came to the realization that we could translate that to this situation. As mentioned, our objective was to compare these materials and to see how close other alternatives were to the already fully established material, PET. Through this model we have been capable of quantifying different material properties and although these results are not 100% objective or certain, this model helps us reach a conclusion that is more rational and objective. The results from the model led us to a conclusion that was to be expected when this project started. As of today, and the way things stand in this country, no material can fully overtake PET. However, there are signs that suggest that there are alternatives to PET that are less harmful and that have true potential to coexist with PET. Particularly PLA and PHA are supported by this model. Nevertheless, since our true objective is to see how we can make bottled water consumption more sustainable, and keeping in mind the results that have been retrieved, the only true effective solution would be to transition PET's "monopoly" in this market into a market with various options. A mix of PET (merging into BioPET and rPET) along with PLA and PHA given the right conditions, would lead human bottled water consumption into a far more sustainable and stable situation.

Additionally, this model proved to not only be useful in comparing materials but also in performing sensitivity analysis in determining the sort of situations that would be required for one material to overtake another. Finally, this model is likely to be useful in the coming years once more information is available especially if trend analysis can be added to it.

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