Universiteit Utrecht

BIO-BASED POLYAMIDES

Environmental impact and applicability in soccer shoe outsoles

Abstract

This thesis proposes a methodology to assess commercial and lab-scale materials for any specific application on the aggregate of technical performance, environmental impact and economic impact where fragmented, uncertain and incomplete data is available. The methodology combines a material decision-making framework for technical performance and economic impact with early-stage chemical assessment methods for environmental impact using publically available data. The methodology is applied to a comparative case study where injection-molded bio- and petro-based polyamides are tested for application in soccer shoe outsoles. The results show that partially bio-based PA6.10 performs better than bio-based PA11 and petro-based PA12 using the proposed methodology. In addition, the case study shows that bio-based polyamides are better for the environment and do not necessarily have higher cost or compromise technical performance. Additionally, the sensitivity analysis performed on the case study results shows that the outcome does not change when changing the weighting factors, which have the largest effect on the end results. This shows that the proposed methodology provides a correct indication that PA6.10 is the best material for use in soccer shoe outsoles.

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Research partners

EIT Climate KIC master label

Climate-KIC is a knowledge and innovation community founded by the European institute of Innovation and Technology that focuses on entrepreneurship and sustainability. This research fits into two of the themes that are important within the program. The first is Industrial Symbiosis, which looks specifically into understanding the flows of materials and energy and increase resource efficiency. The second theme is developing a Bio-economy, where the greatest fit with this research is found. This lies in the development of sustainable and optimal feedstock production, in addition to the creation of biorenewable products.

Adidas

This company is known for its position in the footwear and apparel markets. It is one of the leading firms with regard to promoting social and environmental awareness within the industry. The company is ambitious and sets specific goals with regard to recycling, sustainable sourcing and improving working conditions. Adidas aims to reduce its dependence on petrochemical inputs and is specifically looking into bio-based materials for application in apparel and footwear. The role for Adidas is to aid in data collection, connecting with suppliers and providing information on technical performance metrics.

Education details

Master program Energy Science

The two-year (120ECTS) Energy Science master program is focused on calculating on and the managing of energy flows, processes and energy efficiency for the transition towards a more sustainable energy supply. More specifically, it provides courses on energy analysis, energy conversions (high focus on renewable energy production, thermodynamics), energy systems modelling (well to wheel, macro-economic, technology-oriented, static, dynamic, simulation and optimization models) and models of technological change.

Motivation Annotation Sustainable Entrepreneurship and Innovation

For this university-wide master track, the research component of the Master thesis should meet specific requirements. This research qualifies for the annotation because it (1) studies the state-of-art for bio-based polyamides, which will be used for the production of sustainable footwear. Adidas is already familiar with petro-based polyamides but bio-based polyamides are not yet widely used because of uncertain environmental and functional benefits. Therefore the material can be considered (2) new to the business. (3) Data will be collected on the application of polyamides in footwear to accommodate new business activities and reach a holistic verdict on the positive or negative influence of the material. (4) This research constitutes 30 ECTS in the Master's program, which exceeds the required credits for eligibility.

Contents

1. Introduction

1.1 Background and problem definition

Materials have been produced as long as humanity has existed. Each era has built upon the next and mankind has figured out how to produce a wider variety of materials and how to produce all materials faster. The greatest advances have been made in the industrial and petrochemical revolution, where machines powered by crude oil, gas and coal have exponentially enhanced the production capacity of materials (Bennett and Pearson, 2009). This fossil-fuel based economy has also significantly increased economic growth because it enabled refining of resources into a wide variety of value-enhancing products (Unruh, 2000; Unruh 2002). However, growing dependence on petrochemicals is causing a lock-in into resources that are finite and expected to be economically depleted in 40, 70 and 200 years respectively for crude oil, gas and coal (Shafiee and Topal, 2009). Petrochemicals are characterized by highly variable prices caused by strong fluctuations and mismatches in supply and demand (Kantchev, 2015). In addition, associated negative externalities such as air, water and land pollution and global warming are causing a shift towards sustainable and renewable alternatives in all fossil-fuel dependent sectors (Brown, 2001; Nkwachukwu et al., 2013). This shift is driven by regulatory, competitive and stakeholder pressures in addition to risks in supply chain disruption (O'Shea et al., 2012; Dauvergne and Lister, 2012).

The polymer and plastics industry is a sector that is heavily dependent on petrochemical input. Polymers and plastics are macromolecules that consist of repeating units called monomers, which are bonded in long chains. Various types exist, of which Polypropylene (PP), Low Density Polyethylene (LDPE), Polyvinyl Chloride (PVC) and High Density Polyethylene (HDPE) are the most widely used polymers (Plasticseurope, 2015). A broad range of applications (i.e. packaging, insulation, kitchen utensils, pipes, cars, telephones) have made polymers and plastics essential to everyday life (CIEC, 2015). The industry makes all its products using oil, coal or gas. In 2009, this sector accounted for an economic activity of roughly €200 billion for Europe (Eurostat, 2009). In light of the negative externalities related to the petrochemical industry, the polymers and plastics sector is expressing increasing interest in materials that require more environmentally friendly inputs (Patel and Crank, 2007; Marchildon, 2010) which also has implications for its related industries such as the footwear industry.

The footwear industry is very dependent on polymers for the production of footwear (Riber et al., 2009). This indicates that reduction of dependence on synthetic polymers is essential for long-term survival of companies in the footwear industry which has led to interest for bio-based[1] polymers (Patel and Crank, 2005; Berezina and Martelli, 2014; Weiss et al., 2012). Bio-based polymers are derived from natural feedstocks that are subjected to specific processing steps such as the PET bottle partly made from plants (Coca-Cola, 2016). Of particular interest is the family of bio-based polyamides (PA), because it can be made entirely from renewable inputs such as plant oils or fibers and it can potentially replace synthetic polyamides (Ibid.). In 2013, polyamides accounted for roughly 2% of the plastics trade volume in Europe with a consumption of 1 Mt (Plasticseurope, 2015).

[1] Bio-based products are products that are fully or partially made from biogenic sources such as plants and animals.

1.2 Scientific background and previous related studies

Bio-based PA is promising for footwear applications as shown in numerous studies (Pilla, 2011; Isikgor and Becer, 2015; Drobny, 2007). Polyamides are already used in shoe soles, and are generally interesting for shoes as indicated by DPMA, (2013) and Arkema (2012). Shen et al. (2009) also give an overview of the material properties for various types of polyamide. However, studies on what the required technical performance characteristics are for specific applications in footwear are necessary to study the application of polyamides in shoes.

For commercial attractiveness, many studies have been done on the cost-side of bio-based polyamides. Bienmuller et al. (2013) mention that bio-based PA is not yet priced competitively due to higher complexity of the processes. Patel et al. (2006) mention that bio-based adipic acid, the monomer for PA66 requires favorable to very favorable market conditions to achieve market potential, which indicates that it is performing worse when compared to petro-based adipic acid. Costs are the aspect on which bio-based polyamides and other bio-based polymers generally perform worst. However, the negative externalities mentioned are not reflected in the price which distorts the cost benefit of petro- versus bio-based polyamides (Helbling, 2012).

Environmental impact has also been researched. Patel et al. (2005) found that production of petrochemical polyamides is two to three times more energy intensive than manufacture of petrochemical bulk polymers (i.e. PE, PET, PS), but it does not compare between bio-based and petro-based polyamides. Weiss et al. (2012) performed a meta-analysis on 44 life cycle assessment (LCA) studies. LCAs are a useful tool for determining the environmental impacts of materials throughout the life cycle of a material (EEA, 1997). Weiss et al. (2012) found that, as a result of bio-based polyamides, greenhouse gas emissions potentially decrease and eutrophication potential increases. Monomers for bio-based PA have been investigated specifically, but the results contain uncertainties that range from negative climate impact to positive climate impact for various climate impact indicators. Many studies with relation to the source and type of the feedstocks, the chemical processes, land use, water usage, greenhouse gas emissions and energy use remain fragmented (Muthu, 2014). This shows that environmental impact studies remain inconclusive due to uncertain and fragmented data. In addition, the uncertainties found in literature provide no conclusive evidence that bio-based polyamides provide lower environmental impact than petro-based polymers.

1.3 Literature gap

Data on life cycle assessment for PAs is essential to indicate that moving from synthetic PAs towards bio-based PAs actually has environmental benefits, however data is currently not always adequate or publically available. Quantitative cost comparisons between petro- and bio-based PAs are necessary to make investment decisions for companies but these are also missing. In addition, harmonizing material properties of bio-based PAs with the technical performance required in footwear products is missing. This is essential in deciding whether the material is already able to substitute the materials that are currently being utilized in the industry.

Decision-making for investments in an environmentally friendly product requires more information than just the environmental impact. Investments also require information on the costs and the technical performance of a product to make a decision that accounts for the most important aspects in decision-making (Perrini and Trencati, 2006; Broeren et al., 2016). In addition, polyamides should be easy to monitor throughout its product lifecycle development. This requires an analysis tool that can distinguish between lab-stage and commercialized polyamides and that can handle the information intensiveness and uncertainties that are associated with different phases of the product life cycle (Kiker et al., 2005). This report builds a framework that helps in decision-making for injection-molded[2] bio-based polyamides investments and insight into the state-of-art for polyamides. This framework is used to make a modelling tool and a case study is done on soccer shoe outsoles using this model. This has led to the following research aim:

1.4 Main aim and research questions

> The aim of this research is to develop and apply a material selection tool that enables comparative analysis of biobased and petro-based materials on the aggregate of technical performance, environmental impact and economic impact.

To guide this aim, a case study was done on injection-molded polyamides for application in soccer shoe outsoles. This has led to the following research questions:

1. Which injection-molded polyamides have adequate technical performance for application in soccer shoe outsoles?
2. What is the environmental impact of this selection of polyamides?
3. What is the economic impact of this selection of polyamides?
4. Which injection-molded polyamides in the selection are most suitable for use in soccer shoe outsoles based on the aggregate of technical performance, environmental impact and economic impact?

By applying the decision-making framework to a tool, companies can assess materials on the core impacts relevant for its business. In the case study, core impacts are covered in the first three research questions. Research question 1 covers technical performance which has been included because it directly reflects the quality of a material for use in soccer shoe soles. Answering this question provides a selection of materials that are used for the next steps of the case study and an overview of the best materials for soccer shoe outsoles. Research question 2 covers the environmental impact of the selected materials, which has been included because it directly relates to the environmental benefits or drawbacks in switching from biobased to petro-based materials. Research question 3 covers economic impact of the selected materials which has been included since it directly relates to the price for a product which is a key component in making investment decisions. Research question 4 combines the other research questions through weighting and provides the best material for use in soccer shoe outsoles based on technical performance, environmental impact and economic impact.

1.5 Scientific, social and practical relevance

Data on technical performance and economic impact are generally available for a company. However, this is not the case for environmental impact. This is therefore the focus point of this research. The tool that is created serves as an easy to use ex ante or ex post analysis method for combining the complex aspects that are present in determining material suitability for specific applications. The tool can be used by scientists, retail companies, chemical companies and policy makers to assess a selection of materials for a specific application. Within this research, the aim is to develop and apply a material selection tool that is specific to sportswear. However, the scope of the tool is broader since it can be used for many applications besides sportswear. The tool can be adapted for assessing other application areas, ranging from batteries, furniture, and construction materials to food.

This research attempts to solve important issues faced by research on environmental impacts which is the speed at which data is available and data availability. The methodology proposed will enable environmental analysis for materials, applications and complete products without the need to wait

[2] This is a method for producing plastics. Pellets are injected into a mold and a combination of heat and pressure gives the plastic the shape needed.

until complete environmental data is published. Especially in light of the speed at which environmentally sound decision-making should take place to prevent global climate issues that disrupt society at all levels, having a model that can make a preliminary environmental assessment becomes crucial.

The tool becomes more relevant for its users because it not only evaluates environmental impact but also technical performance and economic impact. This holistic approach enables bridging of the gap between the scientific nature of environmental analyses and the corporate nature of technical and economic aspects.

In the next chapter, the general research methods will be elaborated and details are given for the research steps used. This is followed by an operationalization of the method in a case study. After this, the results of the case study are given and these results are then put into perspective with the discussion. The last chapter will conclude with the answer to the research question and conclusion of the main aim stated in the introduction.

2. Methodology

This chapter provides an overview of the methodology that is followed in this research. The methodology starts off with the scientific background for the model, followed by the general description of steps taken in the research after which the steps are elaborated on.

This research method will lay the foundation for the inclusion of scientific principles in an applied setting. For this purpose, the chemical process design decision-making framework proposed by Sugiyama et al. (2008) and the early-stage environmental and economic assessment method by Patel et al. (2012) will be combined with the stepwise material decision-making framework proposed by Broeren et al. (2016). These studies are briefly explained before moving on with the methodology proposed in this research.

Broeren et al. (2016) have created a framework that assist in incorporating sustainability assessment in the material selection process. This framework uses a stepwise process to select an application, its requirements and the materials that meet these requirements. This method is used as a backbone for the stepwise methodology used in this research. Instead of starting with the chemical process as is the case in Sugiyama et al. (2008) and Patel et al. (2012), the starting point is an application for which materials are selected and after selection of materials, the chemical processes or life cycle impacts are assessed. This modification makes the method proposed more widely usable by policy-makers, scientists, chemists and companies that want to incorporate sustainability in the material decision-making process for retail products.

Sugiyama et al. (2008) have created and applied a design framework that comprises four stages of process modeling using economical aspects, environmental impacts, health, environment and safety hazards and technical aspects. This design framework is relevant for chemical companies who wish to incorporate early-stage sustainable development of chemicals. The data used in this method is generally not available for companies outside the chemical industry and the goal is to aid in decision-making for creation of novel chemical synthesis routes.

Patel et al. (2012) have adapted the method proposed by Sugiyama et al. (2008) to enable early-stage analysis of emerging laboratory-stage chemical processes on green chemistry principles, techno-economic analysis and life cycle assessment elements. The method enables comparison of new and existing chemical processes to aid chemists and engineers in developing and analyzing sustainable chemistry pathways.

The next section explains the framework and how these studies have been incorporated.

2.1 Steps and methods

In this research, the conceptual model shown in figure 2.1 is applied. This serves as the flow in which the research is done, starting at step 1 and ending at step 6. The stepwise method is adapted to the method used in Broeren et al. (2016), where step 4 and 5 are based on the chemical process analysis proposed by Sugiyama et al. (2008) and Patel et al. (2012). The stepwise process is used for the case study in chapter 3. Step 1 covers the definition of goals and constraints used for a case study. This means that an application is selected, specific goals are set and constraints are put in place to ensure the research focus. Step 2 covers definition of the function that a selected application should provide and this function is translated into measurable indicators of technical performance. In step 3 materials are selected that meet the demands on technical performance after which they can be ranked. Step 4 covers the analysis of environmental impact for the selected materials. This step is composed of Environmental Impact of Raw Materials (EIRM) and Process Costs and Environmental Impacts (PCEI). EIRM is effectively the lifecycle assessment part of this research and this is supplemented by PCEI, which is a chemical process analysis method used when EIRM is unable to account for a material's entire synthesis process. Step 5 covers the analysis of the economic impact for the selected materials. This analysis shows which materials are cheapest and which are the most expensive. The last step, number 6 is the multicriteria analysis where the outcomes of technical performance, environmental impact and economic impact are weighted and ranked. After this, the best material to use in the defined application is acquired.

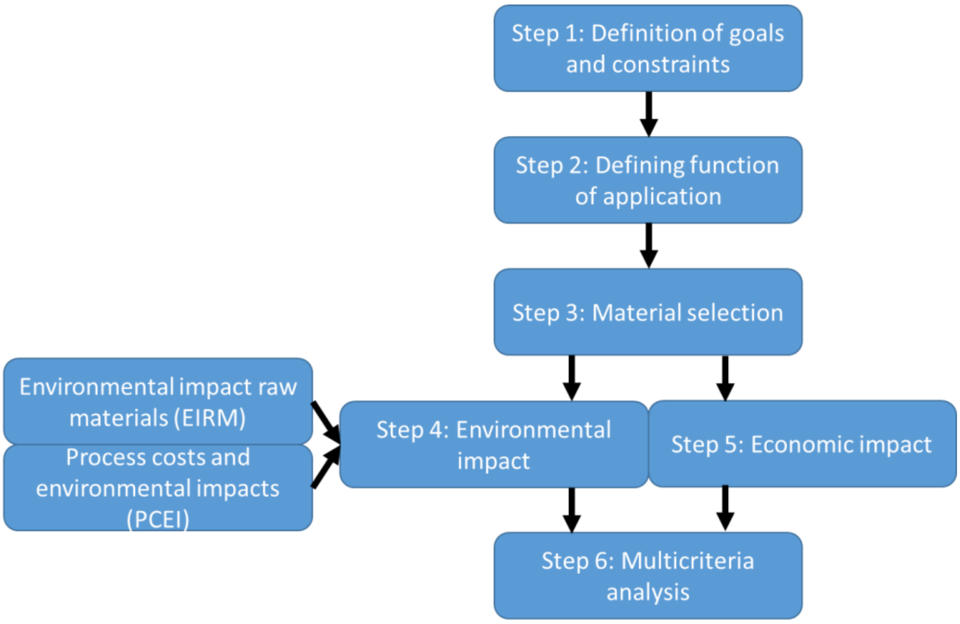

Figure 2.1: Material selection and testing process (adapted from Broeren et al., 2016, Sugiyama et al., 2008 and Patel et al., 2012).

The following sections contain detailed information on the application of the conceptual model. Keep in mind that the text refers to a number of equations and concepts. The equations are summarized in table 2.4, at the end of this chapter. This table is referenced to when equations are used in the text. The most important concepts that need explanation before further reading are the scores and index scores. Scores can take a value of zero and above, without distinction whether this value has a positive or negative contribution to the end result. Scores need to be normalized and are the input for the index calculations. Index scores always have a value between zero and one, where a higher value indicates a better result for a material. Index scores undergo no additional standardization, only weighting. For explanation of abbreviations or other concepts, see appendix A and B.

2.2 Step 1: Defining goals and constraints

The first step is used to determine the scope and depth applied in the decision-making tool. First, goals are defined. Examples are "identifying the benefits of bio-based products compared to petro-based products", "discovering new emerging materials that can fill a specific application", "finding alternatives for current materials" and "analyzing a material that is brought in by a supplier". A wide variety of goals can be stated before starting the analysis and there can be more than one.

Secondly, the application that needs to be studied is determined which is done in collaboration with materials experts. After the application is known, the most important functions of that application should be identified. Functions are concepts such as "increasing durability", "keeping the user dry" or "decreasing weight".

After this has all been identified, constraints need to be set for the case study. Constraints can range from production method (i.e. extrusion-molded plastics), types of materials (i.e. PET, Carbon-reinforced plastics, PP), the depth of analysis which depends on the amount of parameters considered to the number of materials selected for analysis. The selected application is also essentially a constraint in this sense. The output for this step is a list of goals and constraints in addition to the application that is investigated.

The model as it is might not be adequate to achieve all specific goals, thus it can be extended with further impact categories. Possible additions are social impacts, risk assessments and environmental, health and safety impacts (Sugiyama et al., 2008). These additions are out of scope for this research.

2.3 Step 2: Defining function of application

Step 2 goes deeper into the technical performance and function for a specific application. Concepts in the function of the application need to be translated into tangible indicators. This means that concepts such as "decreasing weight" can be measured by density in kg/m^3, "keeping the user dry" by water absorption in m^3 water per unit of time and "increasing durability" by abrasion resistance in kg material lost with a vector of force over a number of cycles. These translations are done in collaboration with a materials expert and the testing methods for the indicators are pre-defined by standardized testing institutions such as ASTM (2016) and ISO (2016). The materials expert should also aid in determining the numerical boundaries for the indicators used which will differ per application and indicator. For the calculation conditions, see appendix C. The output for this step is a selection of technical performance parameters and the numerical boundaries within which the characteristics of the materials need to be.

2.4 Step 3: Material selection

This step is intended to find materials that fit in the technical performance conditions set in step 2. This can be done by physically testing material samples or by consulting supplier datasheets. In both cases it is advised to start with datasheets to find materials that are suitable for the selected application, after which in-company tests can be done to determine whether the datasheets are correct. Suppliers tend to have different testing methods or slightly different interpretations to testing which makes it important to re-test their materials. This enables a higher degree of certainty with respect to the input for technical performance.

The preferred method for consulting datasheets is to use a materials database such as the Campus Database, MatWeb and IDES. The preference is to use the Campus Database since this database contains up-to-date comparable material data measured by material suppliers according to international standards (ASTM, 2016; ISO, 2016). Material search criteria can be set up and a list of materials is acquired that are suitable for further analysis. This list is inserted into the model and the scores are assigned according to the score calculation shown in appendix C. When a technical performance parameter for a material is not available in the database and at the supplier, a score of zero is assigned. The final index calculation for technical performance is dependent on the number of parameters, their boundary conditions and the desired values. These differ per application and should be defined for each research. A score of zero indicates that a material does not meet requirements set or is missing data, whereas a score of one indicates that the material fully meets the requirements for a technical performance parameter. Depending on the scores for each technical performance parameter, the index score is calculated using equation *0.0* in table 2.4 where the score is multiplied with the weighting factor for each parameter. The output for this step is a list of at most 10 materials that are able to fully or partially meet the set technical performance criteria. Depending on the goals defined in step 1, the selection should enable distinction between various materials on their properties. This means that a material in the selection needs to have at least one property that is unique to that material, such as the chemical composition, biobased content, supplier or technical performance parameter properties. This ensures that the analysis is done on a varied selection of materials to enable comparison between various options. The selected materials will be investigated further on their economic and environmental impact in step 4 and 5.

The material databases only contain commercialized materials, thus for lab-scale materials different data sources need to be used. These come from various sources, such as scientific articles, online sources and patents. Materials should only be included when enough technical performance conditions are met or when the expectation is that the material might meet the technical performance conditions in the future. This generally requires more research and more testing. In this case, additional data or updated research should be requested from material suppliers or the authors of publications.

2.5 Step 4: Environmental impact

The environmental impact is determined by the influence that utilization of feedstock and processes exert on the environment, both direct and indirect. The method generally used is the lifecycle analysis. This encompasses the impact of raw materials, acquisition of raw materials, transport of material between sites, processing of raw materials into the desired product, the transport of the product to the customer, the use of the product and the disposal of the product. Depending on the depth of the analysis, more components of the production chain can be included. Environmental impacts range from greenhouse gas emissions to eutrophication potential, energy use, acidification and more.

This research makes use of ecoinvent data to determine the environmental impacts of raw materials (EIRM). The EIRM method analyzes the quantifiable environmental impact that raw materials have on the total environmental impact of a product. Environmental impact for materials is in impact per kg of material. The preference is to use full LCA data when available. However, when quantified environmental impact is not known in LCA software such as SimaPro or GaBi, the process costs and environmental impacts (PCEI) method is used to supplement the environmental data found in the EIRM step. The PCEI method looks specifically at the chemical conversions that take place in the synthesis from raw materials to the end product or final material. The outputs for this step are total scores for indicators in EIRM and if limited LCA data is available, indicators of PCEI. The EIRM and PCEI methods are explained in section 2.5.2 and section 2.5.3, respectively. The next section explains when to use the EIRM and when to use the PCEI method.

2.5.1 Making inventory of production steps and methods to use

For the initial phase of the analysis, an inventory of data is made to decide where to use the EIRM and PCEI methods. First, an inventory of materials for which the entire synthesis process is fully covered by LCA data is made. Materials that are not fully covered by LCA data require more detailed information on the synthesis processes and selection of methods based on available and unavailable LCA data. Table 2.1 illustrates the selection of the methods. For the synthesis process of a material, the starting point is the first synthesis step. This step is where the reactants A and B are combined to make product C. In this case, LCA data is available for product C. This means that the next synthesis step needs to be analyzed where C and C’ are combined to create main product D and byproduct D’. In this case LCA data also is able to cover main product D. In step 3, where D and E are combined, no LCA data is available for F. This means that the available LCA data for D and E is used in the EIRM method. Inherently included in the LCA data for D and E are the life cycle impacts for A, B, C and D’, since these impacts occur in the synthesis process of D and E. This LCA data is the input for the EIRM analysis.

The PCEI method is used for analyzing F, which covers the environmental impact that occurs in the process of converting D and E into F. The PCEI method is then also used for synthesis step 4, where LCA data is not available for both reactants and products. For steps that are covered with the PCEI method, reactants can also be reacted with the main product of the previous step. These do not require new LCA data, since the environmental impacts are already covered with the PCEI method. Incorporating an LCA for these reactants would therefore mean double counting of impacts.

Table 2.1: Selection of method for environmental impact analysis.

Synthesis step	Reactants	Products	LCA data available	Method
1	A+B	C	Yes: for C	EIRM
2	C+C’	D+D’	Yes: for D	EIRM
3[a]	D+E	F	Yes: for D and E, but not F	PCEI
4	F+G	H+I	Not for reactants or products	PCEI

a: This step is referred to as the first stoichiometric reaction further in the research.

The starting points for both PCEI and EIRM are the stoichiometric reaction equations. These are determined primarily by consulting existing literature, such as Ullmann’s encyclopedia of Industrial Chemistry (2007) or Kirk-Othmer Encyclopedia of Chemical Technology (1996). When multiple routes are available from a feedstock to a product, the most commonly used route is taken. When information is unavailable or insufficiently extensive, patents and other literature are consulted.

The focus in the synthesis steps lies on the stoichiometric reaction, which means that data on catalysts, solvents, reaction vessels, non-reactants, reaction time and so forth were not considered. In addition, a stoichiometric reaction assumes that all reactants are fully converted into products. Taking note of the reaction temperature inside the reactor vessel is important, as this can influence the reaction enthalpy.

The following sections go deeper into the application of the EIRM and PCEI methods.

2.5.2 Environmental impact of raw materials

The environmental impact of raw materials method describes the quantitative environmental impact of the raw materials that feed into the first stoichiometric reaction (synthesis step 3 in table 2.1). Impact is defined per mass of raw material from cradle to the first stoichiometric reaction. The output for this method is a score for the used indicators that are combined to acquire an index score between zero and one.

Method for determining EIRM parameter values

For the environmental impact of raw materials, parameters need to be selected. The most important parameters that should be included are cumulative energy demand and greenhouse gas emissions, which are explained in the following sections. For bio-based feedstocks, lack of available data in the entire synthesis chain could occur. In this case assumptions need to be made with regard to their environmental impacts. Research is done on other bio-based feedstocks that are comparable with the selected feedstock in cultivation (soil type, irrigation requirement, processing of the plant, plant type). This means that the other feedstock is used as a proxy for the environmental impact.

More parameters can be selected, such as eutrophication potential, water depletion, and acidification. Some parameters describe a local impact (acidification and eutrophication) whereas other parameters describe a more global impact (cumulative energy demand and greenhouse gas emissions). When selecting more parameters, weighting needs to be changed according to the impact and perceived importance of each parameter.

The preferred data source for EIRM is LCA software since this data is most trustworthy. The most preferred database for LCA software is ecoinvent. Using LCA data for materials from suppliers or other sources is not advisable unless all the selected boundaries, assumptions, calculation methods, software used and other details are given. LCA reporting at this level of detail is generally not provided by suppliers or other sources in which case LCA software should be used. This ensures that the LCA parameters in the model are equal for all the selected materials which is an essential requirement to have comparable data.

Cumulative energy demand

Cumulative energy demand consists of the energy demanded to produce a raw material and the energy content of that raw material, in MJ/kg of feedstock. The cumulative energy demand comes from LCA software such as GaBi or SimaPro. In SimaPro, *Cumulative energy demand* (IPCC, 2007) is used to determine cumulative energy demand after calculating the sum of non-renewable and renewable energy.

Greenhouse gas emissions

Emissions consist of the direct emissions into the atmosphere due to the manufacture of a chemical and the carbon taken up by photosynthesis in the case of a bio-based feedstock, both in kg CO_2eq/kg of feedstock. Data in direct emissions into the atmosphere is extracted from LCA software such as GaBi or SimaPro. In SimaPro, the *ReCiPe midpoint H Europe* (IPCC, 2007) is used. For bio-based feedstocks, the carbon counting method is additionally used to determine the uptake of CO_2 by the organism. This means that the number of carbon molecules in the bio-based raw material are counted and each carbon molecule then accounts for one molecule of CO_2 that is taken from the air. When CO_2 is emitted or used in any of the reaction steps in the synthesis process of a material, the CO_2 that is sequestered needs to be corrected. Each mole of CO_2 that is used counts as 1 more molecule of CO_2 sequestered, CO_2 that is emitted counts as 1 molecule of CO_2 that is sequestered less.

Calculation of total feedstock environmental impact

After the cumulative energy demand and greenhouse gas emissions are calculated, a second calculation needs to be done using the stoichiometric equations. The first stoichiometric reaction equation towards making the main material is used for this. With multiple reactants, it is important to determine the allocated mass of each reactant to calculate its relative contribution to the total environmental impact of reactants. The calculation of allocated mass is shown in equation *1.0*. After this calculation is done, the allocated mass for each reactant is multiplied with its environmental impact to determine the relative environmental impact for that reactant. This is shown in equation *1.1* for cumulative energy demand and equation *1.2* for greenhouse gas emissions.

These calculations need to be done for all the stoichiometric reactions of materials that have been selected in the technical performance part of the model. After this, the method for scoring is determined. Calculations can be done by either comparing the impacts of each set of reactants with the highest negative impact within the selection or by comparing the impacts with a benchmark for environmental impacts. The first method will give a score of zero to the worst performing set of reactants (equation *1.4* and *1.6*), whereas the second method will enable analysis based on a desirable value (equation *1.3* and *1.5*). The first method is desirable when comparing materials of the same family (i.e. polyamides) and the second becomes relevant when populating a database where <u>all</u> materials should meet a certain environmental standard.

The last step is to determine the final index score for EIRM, which combines the impact categories used. For this step, weighting factors for each impact category need to be determined and multiplied with the value for that impact category. This is done for all impact categories, the sum of which is the final EIRM index score. This index score indicates the total environment impact for the materials of which the LCA impacts are known. This is shown in equation *1.7*.

2.5.3 Process costs and environmental impacts

The PCEI method describes environmental impacts indirectly, by looking specifically at the process chemistry of the first stoichiometric reaction (synthesis step 3 in table 2.1) to the final material that is selected in the material selection step of the method. This method is used because materials that are in an early stage of development or are not widely used, are generally not fully analyzed with life cycle assessments. This method is based on the notion that energy losses in the reaction and separation of products and byproducts can be used as an indicator for the expected environmental impacts. This method is used as an indication of reality with respect to environmental impacts during processing. Due to the nature of available data, this means that scores are assigned based on process conditions and reaction chemistry. This will therefore not fully show the full impacts of a chemical process but in a scenario of a complete lack of knowledge, it should be seen as an educated guess by including parameters that are known to contribute to environmental impacts.

Product concentration at reactor outlet (PCO)

As a proxy to the efficiency of the chemical reaction, the product concentration at reactor outlet is used. If a source provides product concentration after distillation and not product concentration at outlet, the concentration after distillation is used. This parameter indicates the efficiency of the reaction, a higher value is preferred because it requires less energy and effort to separate the main product from the byproducts.

Water content (WC)

The amount of water present at the reactor outlet is rarely mentioned in literature or patents, however the presence of water is generally indicated. This can be explicitly mentioned as water at the reactor outlet, but also implicit when the main product is distilled to remove impurities. In both cases, water is assumed to be present. A score of zero is applied when there is no water present, which means that no energy needs to be used to remove water and the distillation step is excluded from the process. A score of 1 is applied when water does need to be removed by distillation, since this requires energy and additional processing.

Minimum boiling point difference (MBP)

The MBP is calculated with respect to the main product of the reaction equation. The minimum boiling point for materials that are unable to reach a boiling point is assumed to be the sublimation, transformation or dissociation point of the material. Boiling points of byproducts in the stoichiometric reaction are included, in addition to the presence of other substances. This can be water or products that are present in the reaction while not being included in the stoichiometric reaction. The latter would be a product that is converted into the main product through an extra process. A low boiling point difference increases the amount of energy and time that is required to separate the main product from the by-products, when the boiling point difference is higher, the main product and byproducts can be separated more easily. The calculation is shown in equation *2.0*.

Mass loss index (MLI)

To calculate the MLI, the total mass of reactants was divided by the total mass of the main product. A very low MLI indicates that very little byproducts are formed, which means that less mass needs to be removed from the production process. A high MLI indicates that a high mass of byproducts is formed, which needs to be disposed of in the waste treatment process which consumes energy. The calculation is shown in equation *2.1*.

Reaction enthalpy (RE)

The reaction enthalpy has been calculated using AspenPlus. When a substance is unknown to AspenPlus, reaction enthalpy is calculated manually under assumption of standard atmospheric and temperature conditions. A higher heat of reaction requires more utilities to ensure constant reaction conditions. When the enthalpy of reaction has a negative value, the reaction is exothermic and releases energy. In this case, cooling is required to maintain a steady reaction temperature. Likewise, a positive enthalpy of reaction indicates an endothermic reaction which absorbs energy and needs a heat source to maintain a steady reaction temperature. Both heating and cooling require energy which means that a higher absolute value for reaction enthalpy requires more energy. This is calculated by taking the total enthalpy of the reaction products and subtracting the total enthalpy of the reactants which is shown in equation *2.2*.

Number of co-products (CP)

The co-products after the reaction are counted. This includes water or products that are present in the reaction while not being included in the stoichiometric reaction. The latter would be a product that is converted into the main product through an additional process. More co-products means more waste products that need separation and disposal, thus having a negative impact on the environment.

Pre-treatment (PT)

For some reactions to occur efficiently, feedstocks need to be pre-treated. In this case, additional efforts such as grinding, washing or cutting of feedstock needs to happen to prepare the feedstock for reaction. Pre-treatment requires energy and resources, therefore when pre-treatment is required, a score of 1 is applied. If pre-treatment is not necessary, the applied score is zero.

PCEI score calculation

After the data has been found for all the reactions in the analysis, scores need to be assigned for each synthesis step. This means that 7 scores eventually come out of every synthesis step required to create a monomer. Following the article by Patel et al. (2012), scores are assigned according to table 2.2 below.

Table 2.2: Numerical boundaries and assigned scores to the PCEI parameters (from Patel et al., 2012).

[Score]	PCO [%]	WC [Condition]	MBP [K]	MLI [value]	RE [kJ/mol]	CP [#]	PT [condition]
0	25%	No	20	0,1	100	1	No
0,5	5%	-	10	1	200	3	-
1	1%	Yes	5	10	300	7	Yes

Method for determining scoring:

Due to non-linear relationships between some of the parameters used in the PCEI method and the assigned score, formulas needed to be determined. This was done for product concentration at reactor outlet, minimum boiling point difference, mass loss index and number of co-products at reactor outlet. Relationships for the other parameters were either dichotomous or conditional and linear, which does not make it necessary to determine the relationship between parameter values and the associated scores. A scatterplot was made for each of these parameters with the score (0 to 1) on the y-axis and the parameter values on the x-axis. The three score points at 0, 0.5 and 1 given by Patel et al. (2012) were plotted and a trend-line was added to determine the relationship. The calculated y-values are the scores for the parameters. The results are shown in table 2.3 below.

Table 2.3: Formula for mathematical relation between parameter values and parameter scores.

Parameter (x)	Formula	Relationship
Product concentration outlet	$Y=-0{,}311\ln(x)-0{,}431$ ($R^2=1{,}00$)	Logarithmic
Boiling point difference	$Y=-0{,}721\ln(x)+2{,}161$ ($R^2=1{,}00$)	Logarithmic
Mass loss index	$Y=0{,}217\ln(x)+0{,}500$ ($R^2=1{,}00$)	Logarithmic
Number of co-products	$Y=-0{,}021x^2+0{,}333x-0{,}313$ ($R^2=1{,}00$)	Polynomial

These formulas are then translated to the equations which calculate the scores. In addition, equations for water content, reaction enthalpy and pretreatment are made. The score calculation for each parameter is done for each reaction step in the synthesis process and the scores of each parameter are summed. This is shown in equations *2.3* (PCO), *2.4* (WC), *2.5* (MBP), *2.6* (MLI), *2.7* (RE), *2.8* (NCP) and *2.9* (PT). For each material, the sum of these seven parameters is taken

After the final score for PCEI is known, the data is translated into index scores. This is done by either using equal weighting factors or by comparing the PCEI value of one material with the highest PCEI value of the selected materials. The first method can be used when the total score for PCEI is below 7 since this will enable index scores between zero and one (equation *2.10*). The second method can be used when the PCEI becomes higher than 7 and will then also allow index scores between zero and one. The last method ignores weighting factors and assigns the worst performing main product an index score of zero and everything that performs better will receive a relatively higher index score (equation *2.11*).

2.6 Step 5: Economic impact

The economic analysis is included to identify the costs of the used materials. For any material to be applied in a product, the material should be priced competitively to ensure proper sales of the product. For this reason, bulk price data needs to be collected in €/kg for the materials that are used in the stoichiometric reactions and the end products with a brand name. Data can be gathered from ICIS, materials suppliers, prices for similar materials used internally and commodity trading markets such as Alibaba. The outputs for this step are index scores of the selected materials, where the most expensive material receives the lowest index score and the cheapest material will receive the highest index score.

When prices are internally available for similar materials but not for the exact selected material, uncertainty occurs with respect to the price for the selected material. In this case, the score for the lowest and highest known prices for materials of similar compounds with similar additives (i.e. glass or carbon fibers) needs to be calculated and the average of these scores needs to be taken to acquire the index score. This is covered by the brand price comparison method.

Depending on the availability of data, different calculation methods need to be applied. The preference is to use data that directly relates to brand material prices since these are more relevant and easy to use for companies since they represent the purchase price for the company. These are not always available because they are simply unknown, a new material is investigated or branded materials do not exist for a certain compound. If this is the case, prices for all the materials used in the stoichiometric reactions need to be found. High data uncertainties occur here due to the necessity to consult multiple sources to fill in the data blanks and due to the type of sources consulted. In addition, uncertainty occurs due to a lack of bulk data which is most relevant for a company. This means that assumptions need to be made with translating unit prices to the possible bulk price. This method is covered with the price constraint method.

Price constraint method

This method is used when branded material prices are not available. In this case, the stoichiometric equations need to be used to determine how expensive the final material will be. First, the mass of the reactants that enter the first stoichiometric reaction needs to be determined. This is also done for the subsequent stoichiometric reactions. In addition, determine the mass of the main product.
This is done for all reactants needed for the selected stoichiometric reactions. Each reactant's mass will then be multiplied by the price of the reactant to acquire its costs.

For each main product, the cost of reactants is summed to acquire the total costs over the synthesis processes for that main product. The mass of reactants is also summed to acquire the total mass input of reactants. This is done to acquire the average price per kg for the reactants. The same calculations are done for the main product of the reaction. This will normally give the price per kg of the main product as found on the market, but in some cases multiple main products are acquired in a single reaction. The possibility also exists that multiple main products are needed for a single material, which requires calculation of the allocated price based on the allocated mass for each main product. After these prices have been calculated, the final score is calculated by dividing the average price of inputs with the average price of the products or price of material. This is shown in equation *3.0*. This score should be used as the index score when the price constraint method is used next to the brand price comparison method. In addition, the index score provides an indication of price. A higher score than materials for which brand prices are available does not necessarily mean that the final branded material will be cheaper. Instead, it gives an indication that the material is interesting for future use but only after additional bulk data of the selected material becomes available. This data should be requested at the supplier of the material before selecting a material based on the price constraint method.

When the selection exclusively contains materials that need to be investigated using the price constraint method, an additional step can be taken to calculate the index. In this case, the score of one material is compared with the highest score in the selection, which sets the highest score as one. This is shown in equation *3.3*. This method gives an index value that can't be generalized for multiple models, only within a single model. In addition, this method will have a large influence on the end result and is therefore not preferred.

Brand price comparison method

This method can be used to compare a price in the selection of branded materials with a benchmark price or with the highest price in the selection. When using a benchmark price, a preferred price for a material is set and prices of branded materials are compared to that price. This will give negative index scores for materials that are more expensive and index scores from zero to 1 for materials that are cheaper than the benchmark. This is shown in equation *3.1*. When a material has a negative index score, it should be removed from the selection since it does not meet the required brand price. Comparison with the highest price enables analysis of materials compared to the most expensive material in the selection, which gives the most expensive material an index score of zero. This is shown in equation *3.2*.

2.7 Step 6: Multicriteria analysis

This step is where all components are incorporated into a single model. The MCA is used to combine the outcomes of the technical performance, environmental impact and economic impact. Each of these aspects is scored and a ranking is provided.

The MCA is needed to combine all the calculated scores and their contribution to the end result. This step is intended to incorporate weighting into the scores, which can change depending on the priorities set forth in the model. When no priority is assigned, all factors are weighted equally.

Determining weighting factors can be done by interviewing stakeholders that determine organizational goals. These goals will have a long-term strategy attached which should be reflected by the weighting factors. After doing this, a ranking can be made with the selected products. The highest score will provide the best material to use in the selected application based on all the aspects that have been incorporated into the model. When the best material is known, a decision needs to be made whether to incorporate the material into the application

Overview of equations

For technical performance, environmental impact and economic impact, calculations have been done to determine the values, scores and indicators. These are summarized in table 2.4 on the next page. The numbers in brackets indicate the equation number that is referred to in the text. The index calculation gives an index score of zero (bad) to one (good) for a material's performance on technical performance, environmental impact and economic impact and this will be incorporated in the end result.

Table 2.4: calculation methods for indicators, scores and indices. For technical performance and environmental impact formulas used in Excel, see appendix C. Explanation of abbreviations and notations are given at the bottom of this table.

Step	Indicator calculation	Score calculation	Index score calculation
1, 2, 3 (TP) Technical performance	-	-	$TP_W = \sum_{t=1}^{TPc} WF_t * TP_t$ (0.0)
4 (EIRM) Environmental impact	$AM_i^{RM} = \frac{M_i^{RM}}{\sum_{j=1}^{r} M_j^{RM}}$ (1.0)	-	-
	$CED_n = \sum_{i=1}^{r} (AM_i^{RM} * CED_i^{RM})$ (1.1)	$EIRM_{CED,BM} = 1 - \frac{CED_n}{CED_{BM}}$ (1.3), OR $EIRM_{CED,RH} = 1 - \frac{CED_n}{CED_{HS}}$ (1.4)	$EIRM_W = \sum_{i=1}^{EIRMc} WF_i * EIRM_i$ (1.7)
	$GHG_n = \sum_{i=1}^{r} (AM_i^{RM} * (GHG_i^{RM} + GHGO_i^{RM}))$ (1.2)	$EIRM_{GHG,BM} = 1 - \frac{GHG_n}{GHG_{BM}}$ (1.5), OR $EIRM_{GHG,RH} = 1 - \frac{GHG_n}{GHG_{HS}}$ (1.6)	
4 (PCEI) Environmental impact	-	$PCEI_{PCO} = \sum_{r=1}^{rs} -0{,}311 * \ln(PCO_n^F) - 0{,}431$ (2.3)	$PCEI_W = 1 - \sum_{i=1}^{PCEIc} WF_i * PCEI_i$ (2.10) OR $PCEI_{HS} = 1 - \frac{\sum_{i=1}^{PCEIc} PCEI_i}{(\sum_{i=1}^{PCEIc} PCEI_i)_{HS}}$ (2.11)
	-	$PCEI_{WC} = \sum_{r=1}^{rs} \begin{cases} 0{,}0: \textit{no water present} \\ 1{,}0: \textit{water is distilled} \end{cases}$ (2.4)	
	$MBP_n^F = MIN(BP_n^F - BP_i^F)$ (2.0)	$PCEI_{MBP} = \sum_{r=1}^{rs} -0{,}721 * \ln(MBP_n^F) + 2{,}161$ (2.5)	
	$MLI_n^F = \frac{(\sum_{i=1}^{r} M_i^{RM}) - M_n^P}{M_n^P}$ (2.1)	$PCEI_{MLI} = \sum_{r=1}^{rs} 0{,}217 * \ln(MLI_n^F) + 0.5$ (2.6)	
	$\Delta H_{RE}^F = \left(\sum_{n=1}^{p} Hf_n^{PS}\right) - \left(\sum_{i=1}^{r} Hf_i^{RM}\right)$ (2.2)	$PCEI_{\Delta H} = \sum_{r=1}^{rs} 1 - \left\lvert \frac{300 - \Delta H_{RE}^F}{200} \right\rvert$ (2.7)	
	-	$PCEI_{NCP} = \sum_{r=1}^{rs} -0{,}021 * NCP_n^{F^2} + 0{,}333 * NCP_n^F - 0.313$ (2.8)	
	-	$PCEI_{PT} = \sum_{r=1}^{rs} \begin{cases} 0{,}0: \textit{no pretreatment} \\ 1{,}0: \textit{pretreatment needed} \end{cases}$ (2.9)	
5 (EI) Economic impact	-	-	$EI_{n,PR,BM} = 1 - \frac{P_n}{P_{BM}}$ (3.1), OR $EI_{n,PR,RH} = 1 - \frac{P_n}{P_{HS}}$ (3.2)
	-	$EI_{n,PC} = \frac{\sum_{i=1}^{r} M_i^{RM} C_i^{RM}}{\sum_{j=1}^{p} M_j^P C_j^P}$ (3.0)	$EI_{n,PC,RH} = 1 - \frac{EI_n}{EI_{HS}}$ (3.3)

Concepts: AM=allocated mass, M=mass, GHG=greenhouse gas emissions, GHGO=greenhouse gas emissions offset, CED=cumulative energy demand, EIRM=environmental impact raw materials, WF=weighting factor, MBP=minimum boiling point difference, BP=boiling point, MLI=mass loss index, ΔH=enthalpy change, Hf=enthalpy of formation, PCEI=process costs and environmental impacts, NCP=number of co-products, EI=economic impact, C=substance costs, P=end product brand price. *Subscripts:* t=technical performance indicator, i,j=species i or j, n=main product, BM=benchmark, RH=relative to highest in selection, W=weighted, r=reactions step, RE=reaction enthalpy, PCO=product concentration at outlet, WC=water content, PT=pre-treatment, PC=price constraint, PR=price. *Superscripts:* TPc=number of indicators for TP, RM=raw materials, r=number of raw materials, EIRMc=number of indicators for EIRM, F=a single internal reaction within the synthesis process of a main product, P=main stream leaving an internal reaction containing only the main product of that reaction, rs=number of reaction steps in the synthesis process of a main product, PCEIc=number of indicators for PCEI, PS=all products after reaction, p=number of products.

2.8 Relevance of the method

Multi-criteria analyses are important tools that are widely used for communication purposes in various settings. They contain a selection of the most important aspects. Each aspect is measured, weighted and added to the aggregated outcome. The final outcome is a number between zero and one that can easily be interpreted by engineers, managers and scientists. The main benefit is the ability to compare options, rank them and make a decision on which options are the most important.

The main problems with existing MCAs are information intensiveness, time intensiveness and the lack of quantitative data. Quantitative and qualitative methods exist that assess a specific product or process attribute. E-factor is a lifecycle analysis method that compares kg of waste with the kg of pure end product, which gives an indication of the quantitative impact of production. Although useful for communicating waste production and understanding process attributes, the method is very time intensive as it looks at all the chemical processes taking place. The waste that is produced ranges from harmless sodium chloride to toxic chromium salt and excludes water, but the resulting influence of this waste on the environment is left out (Sheldon, 2007). Global material economy (GME) is another method that describes the ratio between the mass of a produced product and the total mass used in synthesis. It is easy to use when a single process is analyzed but grows exponentially in complexity as more processes are included. (Augé and Scherrmann, 2012). What is needed is a method that can reduce information and time intensiveness while being able to handle qualitative data.

This method is a means to provide a quick but informative assessment that can aid in key decision-making at the laboratory and commercialized stage of process and product development. It is a means to keep track of important material developments and to make a selection of existing materials and materials that are worth purchasing when put on the market.

2.9 Data sources used

To acquire the necessary data on product characteristics, material and processing costs and environmental impact, exploratory interviews will be conducted and confidential data will be gathered in Germany at Adidas and their suppliers. Data that is available online will also be used for the analyses that will be done during the research. This includes scholarly articles, patents, scientific journal publications, publically available company publications and other internet sources.

3. Case study

This research has applied the methodology in chapter 2 to a specific case study. The goal of this case study is (1) to build the model and (2) to test the methodology and find solutions to problems that might arise in applying the method to practice. The stepwise structure of the methodology will be applied and for each step the intermediary results are shown. The operationalization of the case study is given in table 3.1 below. This shows the data needs for all the steps, categories and the indicators. The sources are also provided to give a quick overview of where to find data. The next sections explain the case study in more detail.

Table 3.1: Operationalization of the case study.

Step	Category	Aspect		Indicators	Unit	Sources
1, 2 and 3	Technical performance	Characteristics for application		Density	[kg/m3]	Materials engineer, campus database, material property sheets, suppliers
				Tensile modulus	[MPa]	
				Strain at break	[%]	
4	Environmental impact	EIRM	Highest known level of LCA data	Cumulative energy demand	[MJ/kg]	SimaPro, GaBi, literature, suppliers
				Emissions	[kg CO2eq/kg]	
		PCEI	Synthesis steps	Reactants and products	-	Ullmann, Kirk-Othmer, patents, literature
				Reaction conditions: pressure and temperature	[atm] [K]	
				Co-products	[#]	
				Product concentration	[%]	
				Pre-treatment	[#]	
				Water presence	[yes/no]	
			Properties chemicals used	Molar mass	[g/mol]	Ullmann, Kirk-Othmer, patents, literature, internet, AspenPlus
				Boiling point	[K]	
				Enthalpy of formation	[kJ/mol]	
			Make-up of end product	Single monomer	[100%]	Ullmann, Kirk-Othmer, patents, literature
				Multiple monomers	[%monomer1] + [%monomer2]	
5	Economic impact	Product prices		Bulk price polyamide	[€/kg]	ICIS, suppliers, literature, prices similar materials used in organization, Alibaba
		Reactant and product prices		Price constraint	[€/kg] feedstocks	ICIS, suppliers, literature, Alibaba
6	Weighting	All aspects, categories and indicators	Determine weighting method	Equal weighting	[%]	-
				Priority weighting[1]	[%]	Interviews in organization
	Ranking	All materials		Score	[rank]	Model outcome

1: Priority weighting was not used in the case study.

3.1 Step 1: Defining goals and constraints

The investigated materials are injection-molded polyamides for application in soccer shoe outsoles. A soccer shoe outsole is the part of a soccer shoe that has studs and that makes contact with the ground. Polyamides are known for their durability and strength which is why they are ideal for the high performance that is required in soccer shoe soles. Polyamides are currently already widely used in soccer shoes, where PA11 and PA12 are most common.

Injection-molded polyamides belong to the family of long-chain polyamide thermoplastics with recurring amide groups [-CONH-] in the polymer chain. Polyamides are characterized by high toughness, high fatigue and abrasion resistance, high stability at elevated temperatures, processability and resistance to oils and solvents (Kohan et al., 2003). The most commonly used polyamides such as PA6, PA6.6 and PA12 are manufactured with crude oil derivatives. Less commonly used petro-based polyamides are PA4.6 and PA6.12 (Plasticseurope, 2016). Polyamides that are (partially) biobased are also available, such as PA4.10, PA6.10 and PA11 (Shen et al., 2009).

The goals of this case study are to identify the benefits and drawbacks of replacing petro-based polyamides with bio-based polyamides and selecting the best polyamide type for application in soccer shoe outsoles. In addition, the case study aids in selecting a material that performs best on the combination of technical performance, environmental impact and economic impact. The research will provide an assessment on a selection of polyamides, with a larger focus on bio-based polyamides. Additionally, the research will only cover polyamides that are injection-molded since this is the production method for polyamides in soccer shoe soles.

3.2 Step 2: Defining function of application

When looking specifically at the requirements for soccer shoe outsoles, the most important characteristics and desirable values for technical performance were determined. This was done in collaboration with an engineer at Adidas' futures department. The three most important characteristics were decided to be the density, tensile modulus and strain at break of the material. Density should not become too high because a soccer shoe needs to be light and strong, keeping weight as low as possible therefore is very important for technical performance. Tensile modulus (E-modulus) is important because the material should be bendable to aid in the running motion of an athlete, but not too bendable because it can cause injuries to the foot. Strain at break is important because the material should not fracture when it is bended, which will lower the lifetime of the shoe and deteriorate other functions of the soccer shoe.

Desirable values were determined to be at most 1100kg/m3 for density, 50 to 5000 MPa for tensile modulus with 1500 MPa as the desirable value and strain at break should be between 50 to 1000%. This has been summarized in table 3.2, below.

Table 3.2: Performance requirements and desirable values for soccer shoe outsoles.

Technical performance characteristic	Unit	Desirable value
Density	[kg/m^3]	1100 kg/m3
Tensile Modulus	[MPa]	50-1500-5000 MPa
Strain at break	[%]	50-1000%

3.3 Step 3: Testing and calculating technical performance scores

In this step, physical testing is optional and within this case study out of scope because of the time needed to receive samples from suppliers and the time needed to test materials. For further refining of technical performance characteristics, this step can be included during the process or after step 7 when the most desirable materials have been determined.

Technical performance testing data was instead extracted from the Campus materials database, which maintains a large database for plastics. A search profile was used to look for materials that fit the technical performance characteristics and a selection was made of various polyamides. In this research, two fictitious instances were considered. The first is when Adidas is looking for existing materials that are available on the Campus database that suit their needs and the second instance is a lab-scale material that could suit Adidas' needs. The latter material was added to simulate the instance where a supplier approaches Adidas with a novel material, which needs to be analyzed. For the lab-scale material, a desktop research was done and the inventor of the material was contacted for more information on technical performance.

The materials selected by Adidas are brand-named and available at chemical companies, whereas the lab-scale material will not have a brand name and needs a more extensive data search to discover whether it has added value for application in soccer shoe outsoles.

The end selection of materials is given in table 3.3 below. The selected materials need to cover the possible types of material. These are materials that are fully biobased, partly biobased and fully petro-based. The materials come from various suppliers and have different characteristics. The weight% biobased is based on the relative weight of biobased monomers versus the total weight of monomers. In addition, co-polymers have been included to show how to analyze materials that are made of multiple monomers. Here, the brand names indicate commercialized products and the lab-scale PA5.10 does not have a brand name since it has not been commercialized yet.

Table 3.3: Selected materials.

Material	Polyamide	Weight% biobased
EcoPaXX Q-E7300	PA4.10	70%
EcoPaXX Q-150D	PA4.10	70%
Lab-scale PA5.10+30%GF	PA5.10	100%
Ultramid S3K Balance	PA6.10	64%
Grilamid 2S20nat	PA6.10	64%
Grilamid XE3959Black9992	PA6.10	64%
Rilsan BECN OTL	PA11	100%
Rilsamid AESN OTL	PA12	0%
Grilamid L25A NZ	PA12	0%
Vestamid X7373 nc	PA12	0%

From the Campus database, 9 materials were selected that perform adequately on the technical performance characteristics that have been selected for application in soccer shoe soles. Tensile modulus contains values for dry and wet conditions that accounts for weather influences. Calculations were done on the value that is least ideal, which gives worst-case weather condition scores for each material. One lab-scale material was additionally selected and its characteristics were extracted from Wittmann et al., (2014) and von Abendroth (2010). The values for density and tensile modulus for PA5.10 are on the basis of 30% glass fiber mixed in which essentially raises the tensile modulus. No data has been found for pure PA5.10, therefore these values have been used. For all materials, no data was available on the strain at break which means testing should be done to ensure the material performs adequately.

The selected materials are EcoPaXX (PA4.10), Ultramid (PA6.10), Grilamid (PA6.10), Rilsan (PA11), Rilsamid (PA12), Grilamid (PA12) and Vestamid (PA12). In addition, lab-scale PA5.10 was included. The characteristics are shown in table 3.4 below. The weighting factors for density, tensile modulus and strain at break are 33%, as shown in table 3.9 at the end of the case study chapter.

Table 3.4: Technical performance characteristic data for the selected materials

		Technical performance characteristic			
		Density	Tensile Modulus		Strain at break
			Dry	Wet	
Material	Compound	[kg/m3]	[MPa]	[MPa]	[%]
EcoPaXX Q-E7300	PA4.10	1050(1)	900(2)	1800²	n/a
EcoPaXX Q-150D	PA4.10	1090(1)	1700(2)	3100²	n/a
Labscale PA5.10+30%GF	PA5.10	1070(3)	8310(4)	7927⁴	n/a
Ultramid S3K Balance	PA6.10	1080(1)	1300(2)	2400²	n/a
Grilamid 2S20nat	PA6.10	1080(1)	1300(2)	2200²	n/a
Grilamid XE3959Black9992	PA6.10	1070(1)	1200(2)	2200²	n/a
Rilsan BECN OTL	PA11	1030(1)	1330(2)	1470²	n/a
Rilsamid AESN OTL	PA12	1010(1)	1440(2)	1500²	n/a
Grilamid L25A NZ	PA12	980(1)	750(2)	1000²	n/a
Vestamid X7373 nc	PA12	1010(1)	1500(2)	1500²	n/a

Source and testing method. (1): From Campus database, ISO 1183, (2): From Campus database, ISO 527 -1/-2, (3): From Kind et al., 2014, test method not provided, (4): From Kind et al., 2014, ISO 527 -2

3.4 Step 4: PCEI and EIRM

In this case study, the feedstock of the bio-based polyamides comes from living organisms, whereas the petro-based PA will be essentially based on petrochemical sources such as crude oil, gas and coal.

The selection of polyamides were analyzed on their impact of the environment. When analyzing a co-polymer, the material needs to be split to enable the analysis. This is the case for PA4.10, PA5.10 and PA6.10, where the separate numbers (4, 5, 6 and 10) indicate different monomers. For PA11 and PA12, only a single monomer is required to make the polymer.

For the environmental impacts and raw materials analysis, the lifecycle impact categories of cumulative energy demand and greenhouse gas emissions have been included. For this, it is also relevant to mention that PA5.y, PAx.10 and PA11 are made from bio-based feedstocks, which means that CO_2-emissions are offset in the cultivation phase. The weighting factors for EIRM and PCEI are 50%, as listed in table 3.9.

EIRM

None of the selected materials can be fully covered by LCA which means that the first main product covered by LCA data was analyzed on environmental impact. Co-polyamides were split into their monomers. This was done for PA4.10, which consists of PA4.y and PAx.10, PA5.10, consisting of PA5.y and PAx.10 and PA6.10, which consists of PA6.y and PAx.10. Table 3.5 shows the main feedstocks for which LCA data is available.

Table 3.5 Materials fully covered by LCA:

Monomer	Primary feedstock	Secondary feedstock
PA4.y	Acrylonitrile	Hydrogen cyanide
PA5.y	Glucose	Ammonium
PA6.y	Acrylonitrile	Hydrogen
PAx.10	Ricinoleic acid	Sodium carbonate
PA11	Ricinoleic acid	Methanol
PA12	Butadiene	

With respect to EIRM, no data was available for castor oil (ricinoleic acid). This meant that an LCA was done on the production of Jatropha oil as proxy for the castor oil. The Jatropha plant is suitable as a proxy because it is also grown in depleted soils with little irrigation and in the same areas as the castor plant. In addition, the seeds are very similar in size, have a similar oil content and require the same mechanism for oil extraction. The included components were cultivation of the plant in India, truck transport of the seeds to a processing site 300km away in a harbor to extract oil, extraction of oil from the seeds, 13500km transport overseas to Europe and truck transport to a chemical processing plant 300km away. When comparing the calculated values of greenhouse gas emissions and cumulative energy demand for ricinoleic acid in table 3.6 with other sources, the emissions and energy demand were within reasonable bounds. Danisco (2011) acquired a value of 1.95 $kgCO_2eq/kg$ for a product based on castor oil, which contains ricinoleic acid. Liang et al. (2013) have also compared the castor plant to the Jatropha plant due the similarities between the plants. They acquired a value of 2.60 $kgCO_2eq/kg$ for the production of biodiesel. This also includes burning of the diesel. In addition, the energy demand was calculated to be 36.90 MJ/kg which is very similar to the cumulative energy demand determined in this research (36.63 MJ/kg). Helling and Russell (2009) acquire a different value for gross energy consumption with values ranging from 70 to 92 MJ/kg and greenhouse gas emissions of -0.1 $kgCO_2eq/kg$. These figures are based on 1 kg of polymer that uses ricinoleic acid and not on 1 kg of ricinoleic acid and are based on data acquired in Texas, whereas the data used here is based on India. The greenhouse gas emissions and the gross energy demand are quite close to the values calculated in this research.

The offset emissions for the biological production of glucose and ricinoleic acid were calculated with the carbon counting method as -1.22 $kgCO_2eq/kg$ and -2.65 $kgCO_2eq/kg$ respectively. In the second stoichiometric reaction for production of PA5.y, 1 mole of CO_2 is emitted, which lowers the offset emissions for glucose.

Data for EIRM was available in ecoinvent databases for the other inputs and no further steps were needed to triangulate the results. The intermediate results for feedstock cumulative energy demand and emissions are shown in table 3.6 below.

Table 3.6: Environmental impact of raw materials.

Environmental impact raw materials					
Input [formula]	Input [name]	Cumulative energy demand [MJ/kg]	Emissions [kgCO_2eq/kg]	Offset emissions [kgCO_2eq/kg]	Corrected emissions [kgCO_2eq/kg]
C_3H_3N	Acrylonitrile[1]	88.37	3.04	n/a: not biological	3.04
CHN	Hydrogen cyanide[2]	88.37	3.04	n/a: not biological	3.04
$C_6H_{12}O_6$	Glucose[3]	10.10	0.86	-1.22	-0.36
NH_3	Ammonia[4]	34.33	1.75	n/a: not biological	1.75
H_2	Hydrogen[5]	75.60	2.07	n/a: not biological	2.07
$C_{18}H_{34}O_3$	Ricinoleic acid[6]	36.63	2.28	-2.65	-0.38
NA_2CO_3	Sodium carbonate[7]	19.70	1.05	n/a: not biological	1.05
CH_4O	Methanol[8]	39.44	0.74	n/a: not biological	0.74
C_4H_6	Butadiene[9]	67.05	1.17	n/a: not biological	1.17

1: 1 kg Acrylonitrile from Sohio process, at plant/RER S.
2: 1 kg Hydrogen cyanide from Sohio process, at plant/RER S.
3: 1 kg Sugar, from sugar beets.
4: 1 kg Ammonia, as 100% NH3 (NPK 82-0-0), at plant/RER Mass (of project Agri-footprint - mass allocation).
5: 1 kg Hydrogen, liquid {RER} Market for Alloc Def. S.
6: 1 kg Jatropha seed {GLO}| market for | Alloc Rec, U. Including transport farm to oil mill, pressing at oil mill, transport overseas to Europe from India and transport from EU port to a processing site. No data for ricinoleic acid available, therefore assumed to be equal to Jatropha process. See text.
7: 1 kg Sodium carbonate from ammonium chloride production, at plant/GLO S.
8: 1 kg Methanol, at plant/GLO S.
9: 1 kg Butadiene, at plant/RER S.

Table 3.7 shows the energy demand and corrected emissions for the selected monomers after mass allocation of the reactants that are listed in table 3.6. The mass allocation is based on the mass distribution of inputs for the first stoichiometric reaction. The table shows that PA4.y and PA6.y have very high greenhouse gas emissions, in combination with a very high cumulative energy demand. This is because acrylonitrile and hydrogen cyanide have a significant contribution to these monomers. Cumulative energy demand is also high for the monomer of PA12, which is mainly due to the input of butadiene which comes from crude oil cracking. The emissions are not as high as those of acrylonitrile and hydrogen cyanide. The cumulative energy demand for PA5.y is lowest and the emissions are slightly negative, which is due to the large contribution of glucose to the monomer and the emissions that are offset in the production of glucose. The use of ammonia also has a negative impact on emissions for PA5.y. Having PAx.10 as co-polymer has a relatively large impact on environmental impact, as the cumulative energy demand is the second lowest and the emissions are almost zero. PA11 also has a low cumulative energy demand and the lowest corrected emissions of the selected materials.

Table 3.7: Mass allocated cumulative energy demand and corrected emissions for the selected monomers.

	Input 1 [Name]	**Input 2 [Name]**	**Input 1 [kg/kg total]**	**Input 2 [kg/kg total]**	**Cumulative energy demand [MJ/kg]**	**Corrected emissions [kg CO_2eq/kg]**
PA4.y	Acrylonitrile	Hydrogen Cyanide	66%	34%	88.37	3.04
PA5.y	Glucose	Ammonia	84%	16%	13.95	-0.03
PA6.y	Acrylonitrile	Hydrogen	98%	2%	88.14	3.03
PAx.10	Ricinoleic acid	Sodium carbonate	70%	30%	31.62	0.05
PA11	Ricinoleic acid	Methanol	98%	2%	36.69	-0.36
PA12	Butadiene		100%		67.05	1.17

PCEI

Table 3.8 shows the stoichiometric reactions for which the main products were not fully covered by LCA data. A large amount of steps are required in the production of PA11 and PA12, whereas monomers that make up the co-polymers all need less steps. For PA4.y, PA5.y PA6.y and PA12 more synthesis steps occur before the first stoichiometric reaction. These formulas were used for determining the parameters that make up the PCEI impact category. For the properties of the substances shown, refer to appendix table D8.

Table 3.8: Stoichiometric reactions used for environmental impact.

Monomer	Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
PA4.y	$C_3H_3N+CHN \rightarrow C_4H_4N_2$ (1)	$C_4H_4N_2+4H_2 \rightarrow C_4H_{12}N_2$ (2)			
PA5.y	$C_6H_{12}O_6+2NH_3 \rightarrow C_6H_{14}N_2O_2+2H_2O+O_2$ (3)	$C_6H_{14}N_2O_2 \rightarrow C_5H_{14}N_2+CO_2$ (3)			
PA6.y	$2C_3H_3N+H_2 \rightarrow C_6H_8N_2$ (4)	$C_6H_8N_2+4H_2 \rightarrow C_6H_{16}N_2$ (5)			
PAx.10	$49C_{18}H_{34}O_3+58Na_2CO_3 \rightarrow 16C_{10}H_{18}O_4+25C_8H_{18}O+58C_{10}H_{16}Na_2O_4$ (6)				
PA11	$16C_{18}H_{34}O_3+3CH_4O \rightarrow 15C_{19}H_{36}O_3+2C_3H_8O_3$ (7)	$C_{19}H_{36}O_3 \rightarrow C_{12}H_{22}O_2+C_7H_{14}O$ (8)	$C_{12}H_{22}O_2+H_2O \rightarrow C_{11}H_{20}O_2+CH_4O$ (7)	$C_{11}H_{20}O_2+HBr \rightarrow C_{11}H_{21}BrO_2$ (9)	$C_{11}H_{21}BrO_2+NH_3 \rightarrow C_{11}H_{23}NO_2+HBr$ (10)
PA12	$3C_4H_6 \rightarrow C_{12}H_{18}$ (11)	$C_{12}H_{18}+3H_2 \rightarrow C_{12}H_{24}$ (12)	$2C_{12}H_{24}+O_2 \rightarrow 2C_{12}H_{22}O+2H_2$ (13)	$2C_{12}H_{22}O+H_8N_2O_6S \rightarrow 2C_{12}H_{23}NO+H_2SO_4+2H_2O$ (13)	$C_{12}H_{23}NO \rightarrow C_{12}H_{22}NOH$ (13)

1: US2481580 2: US5254738 3: Kind et al., 2014 4: Smiley, 2005 5: US3758584(A) 6: US2674608(A) 7: WO2013079888(A) 8: CN103113224(A) 9: CN101289379(A) 10: CN101289409(B) 11: US3723553 12: US3513208 13: Schiffer and Oenbrink, 2005

3.5 Step 5: Economic impact

Many of the polyamides that are being analyzed are already being used by Adidas. This is the case for PA6.10, PA11 and PA12. For these materials the brand price comparison method can be used. For PA5.10 and PA4.10 no price data is available, which means that for both materials the indicative price constraint method is applied for the economic costs.

3.6 Step 6: Multicriteria analysis

For the purpose of building the framework and testing the model, equal weighting has been assumed for every component and no interviews were done. This gives a 33% weight for technical performance, environmental impact and economic impact. Within the impact category, equal weighting was also assumed for subcategories and again equal weighting is assumed for indicators that comprise the sub categories. These weighting factors are summarized in table 3.9 below.

Table 3.9: weighting factors used in the case study. Equal weighting assumed for each (sub) category and indicator.

Weight	Impact category	Weight	Subcategory	Weight	Indicators
33%	Technical performance	-	-	33%	Density
		-	-	33%	Tensile modulus
		-	-	33%	Strain at break
33%	Environmental impact	50%	Environmental impact raw materials	50%	CO_2-equivalent Emissions
				50%	Cumulative energy demand
		50%	Process costs and environmental impacts	14.3%	Product concentration
				14.3%	Water content
				14.3%	Minimum boiling point difference
				14.3%	Mass loss index
				14.3%	Reaction enthalpy
				14.3%	Co-products
				14.3%	Pre-treatment
33%	Economic impact	-	-	100%	Market price end product

4. Results

This section shows the results that follow from the case study and the research questions. The first section shows the results for research question 1, which covers the technical performance. The second section shows the results for research question 2, which covers environmental impact. This is subdivided into EIRM and PCEI. The third section shows the results for research question 3, which covers the economic impact. The last section shows the results for research question 4, where the outcomes of research question 1, 2 and 3 are weighted and the best material is selected.

4.1 Technical performance

Scores were calculated for each of the materials. Due to the lack of data for strain at break all materials have received a score of zero for this parameter. For tensile modulus, the lowest calculated score for either dry or wet conditions was used for the final score calculation. The lab-scale PA5.10 performs poorly on tensile modulus, which is based on the only known data for this parameter. The expectation is that PA5.10 might provide a better score on tensile modulus as a pure compound without mixing of glass fiber. This material also has the lowest final score for technical performance but it might remain interesting to monitor PA5.10 development.

The most used materials at Adidas for soccer shoe soles (PA11 and PA12) also give the highest scores for technical performance (see table 4.1). Vestamid X7373nc has the highest score, closely followed by Rilsamid AESN OTL and Rilsan BECN OTL. This means that for high-end shoes these materials are preferred. For in-line products[3], the Ultramid and Grilamid PA6.10 materials are usable which is deducted from their above average scores. Interestingly, EcoPaXX is one of the worst performers, which is due to their large variability in tensile modulus under either dry or wet conditions. An unknown compound of this material has also been tested by Adidas but due to a mismatch between requirements and EcoPaXX performance, this material is no longer relevant (DSM, 2016). Apart from the low score for technical performance, this is an additional reason to not further investigate the EcoPaXX materials in this selection. All materials lack data for strain at break, which gives a score of zero for this parameter and artificially lowers the scores for all selected materials.

Table 4.1: Technical performance scores and index scores for the selected materials.

Brand material name	Compound	Density	Tensile Modulus		Strain at break	Final score
		[Score]	Dry [Score]	Wet [Score]	[Score]	[Index]
EcoPaXX Q-E7300	PA4.10	1.00	**0.59**	0.91	n/a:Test Needed	0.53
EcoPaXX Q-150D	PA4.10	1.00	0.94	**0.54**	n/a:Test Needed	0.51
Labscale PA5,10+30%GF	PA5.10	1.00	**0.00**	0.00	n/a:Test Needed	0.33
Ultramid S3K Balance	PA6.10	1.00	0.86	**0.74**	n/a:Test Needed	0.58
Grilamid 2S20nat	PA6.10	1.00	0.86	**0.80**	n/a:Test Needed	0.60
Grilamid XE3959Black9992	PA6.10	1.00	**0.79**	0.80	n/a:Test Needed	0.60
Rilsan BECN OTL	PA11	1.00	**0.88**	0.98	n/a:Test Needed	0.63
Rilsamid AESN OTL	PA12	1.00	**0.96**	1.00	n/a:Test Needed	0.65
Grilamid L25A NZ	PA12	1.00	**0.48**	0.66	n/a:Test Needed	0.49
Vestamid X7373 nc	PA12	1.00	**1.00**	1.00	n/a:Test Needed	0.67

[3] In-line products are sold to regular consumers, which means that price need to be balanced with quality of the product and thus requires use of less expensive materials.

4.2 Environmental impact

This section shows the results for both the environmental impact of raw materials and the process costs and environmental impacts. After the results of the two categories, the results are combined to show the total environmental impact.

Environmental impact of raw materials

The final scores for environmental impact of raw materials for the monomers present in the selection are listed in table 4.2. The scores were calculated by comparison with the highest value for each impact category. This yields a score of zero for the worst performing monomer for cumulative energy demand and corrected emissions. Scores higher than 1 occur for the corrected emissions for PA5.y and PA11, which is the result of the negative value for corrected emissions. In the selection, monomers for PA5.y, PAx.10 and PA11 perform best, whereas the PA4.y, PA6.y and PA12 monomers perform worst.

Table 4.2: EIRM scores and index scores for monomers.

Monomer	EIRM parameter score		EIRM weighted score [Index]
	Cumulative energy demand [Score]	Corrected emissions [Score]	
PA4,y	0.00	0.00	0.00
PA5,y	0.84	1.01	0.93
PA6,y	0.00	0.01	0.00
PAx,10	0.64	0.99	0.81
PA11	0.58	1.12	0.85
PA12	0.24	0.62	0.43

Process costs and environmental impacts

The scores for the seven parameters in table 4.3 below are the total scores over all reaction steps for each monomer. The contribution of each reaction step to the monomer score is documented in appendix table D1 through D7. Scores are not limited as zero to one, since these are the totals for all synthesis steps, thus scores higher than 1 occur.

In table 4.3, a higher total score indicates greater negative environmental impact and a lower total score means more negative environmental impact. When looking at the weighted index scores for the selected monomers, it is visible that PA12 has the lowest index score, whereas PA4.y and PA6.y have the highest indices. For all monomers, the largest contribution to the total score comes from water content and distillation. Reaction enthalpy also has a significant impact on the total score for PA4.y, PAx.10, and PA12. All monomers except PA12 have a score of zero for boiling point difference and product concentration. Pre-treatment scores also impact the total scores for the bio-based monomers PA5.y, PAx.10, PA11.

Table 4.3: PCEI scores and index scores for monomers.

Monomer	Mass loss index [Score]	Reaction Enthalpy [Score]	Boiling point diff [Score]	Co-products [Score]	Water content, distill [Score]	Product conc [Score]	Pre-treatment [Score]	Total score [Score]	Weighted index score[1] [Index]
PA4,y	0.00	0.88	0.00	0.27	2.00	0.00	0.00	3.15	0.55
PA5,y	0.65	0.47	0.00	0.54	2.00	0.00	1.00	4.67	0.33
PA6,y	0.00	0.02	0.00	0.54	2.00	0.00	0.00	2.57	0.63
PAx,10	0.87	1.00	0.00	0.27	1.00	0.00	1.00	4.14	0.41
PA11	0.80	0.00	0.00	0.27	2.00	0.00	1.00	4.07	0.42
PA12	0.31	1.33	0.50	0.81	2.00	0.35	1.00	6.31	0.10

1: Index calculation based on equal weighting for each parameter

Combining PCEI and EIRM

In table 4.4, the weighted scores for EIRM and PCEI were combined for each monomer. The best performing monomers on environmental impact are those based on bio-based feedstocks, whereas the worst performance comes from the petro-based feedstocks.

Table 4.4: Environmental impact scores and index score for monomers.

Monomer		TOTAL [Index]	PCEI [Score]	EIRM [Score]
PA4,y	Petro	0.27	0.55	0.00
PA5,y	Bio	0.63	0.33	0.93
PA6,y	Petro	0.32	0.63	0.00
PAx,10	Bio	0.61	0.41	0.81
PA11	Bio	0.63	0.42	0.85
PA12	Petro	0.26	0.10	0.43

The results from the table above are the index scores for each monomer. Since this report looks at both co-polymers and pure polymers, an extra step needs to be taken. This is shown in table 4.5 below, where the co-polymers are split into the monomers that comprise them. The allocated weight of each monomer that makes up a kg of polymer has been calculated or taken from literature. The total scores indicate the low contribution by weight of the petro-based monomers PA4.y and PA6.y and the high contribution by weight of PAx.10 has resulted in a reasonable score. It is also visible that the 100% bio-based polymers PA5.10 and PA11 outperform the polymers that contain petro-based monomers on environmental impact.

Table 4.5: Environmental impact scores and index scores for monomers and their polymers.

Material	Polymer type	X-Component [Notation]	Y-Component [Notation]	X [%weight]	Y [%weight]	X Score [Index]	Y Score [Index]	X,Y Total Score [Index]
PA4,10	Co-polymer	PA4.y	PAx.10	30%	70%	0.27	0.61	0.51
PA5,10	Co-polymer	PA5.y	PAx.10	34%	66%	0.63	0.61	0.62
PA6,10	Co-polymer	PA6.y	PAx.10	38%	62%	0.32	0.61	0.50
PA11	Pure polymer	PA11		100%		0.63		0.63
PA12	Pure polymer	PA12		100%		0.26		0.26

4.3 Economic impact

Table 4.6 shows the economic impact index scores for the materials in the selection. Prices for PA6.10, PA11 and PA12 are known within Adidas and an uncertainty range for prices has been included. The exact prices can be found in confidential appendix F. For these materials the calculated scores are relative to the highest market price in the selection. The price constraint method was used for PA4.10 and PA5.10 because there was no price data for these compounds known at Adidas. The various used methods make it impossible to compare the undefined materials with PA6.10, PA11 and PA12. PA4.10 receives a relatively good score for economic impact, but with the use of the price constraint method this score should preferably be above 0.6 to become interesting. For PA6.10 it becomes apparent that prices can be low which gives a higher score than for the other materials. Prices can also come close to those of PA11 and PA12 which means that there is a high uncertainty with respect to PA6.10 prices.

Table 4.6: Economic impact scores and index scores for the selected materials.

Material	Compound	Market price end product		
		Low [Score]	High [Score]	Average [Index]
Undefined	PA4,10	0.25[1]		0.25
Undefined	PA5,10	0.03[1]		0.03
Ultramid S3K Balance	PA6,10	0.48[2]	0.04[2]	0.26
Grilamid 2S20nat	PA6,10	0.48[2]	0.04[2]	0.26
Grilamid XE3959Black9992	PA6,10	0.48[2]	0.04[2]	0.26
Rilsan BECN OTL	PA11	0.00[2]	0.03[2]	0.01
Rilsamid AESN OTL	PA12	0.01[2]	0.04[2]	0.03
Grilamid L25A NZ	PA12	0.06[2]	0.03[2]	0.04
Vestamid X7373 nc	PA12	0.10[2]	0.00[2]	0.05

1: Price constraint method used. 2: Score calculated relative to highest in selection.

4.4 Ranking of materials

Table 4.7 shows the final result for this case study. Included are the category scores calculated for technical performance, environmental impact and economic impact. The weighted score is based on 33% of the category score for each impact category and the higher a score, the more suitable it is for application in soccer shoe outsoles. The final outcome shows the aggregated score for the three impact categories combined. PA4.10 performs quite well, but as mentioned it did not meet performance testing by Adidas and therefore is not interesting for further use. PA11 is very interesting based on its high technical performance and best environmental impact, the largest downside is the price. This is the case for both PA11 and PA12, but since both materials are already being used at Adidas for soccer shoe outsoles it becomes interesting to focus more on PA11 and less on PA12 for this specific application. This will not increase prices, but it will have a positive effect on the environmental impact. PA5.10 might become interesting as a material to use in the future because of its good environmental impact, but the technical performance for the material investigated in this selection is not good enough. This might improve when data becomes available on a pure compound of PA5.10 instead of the 30% glass fiber compound used here and the material could additionally be used for different applications. Lastly, significant improvements need to be made on costs for the material before it becomes interesting. The best material to use is PA6.10, which performs best over the three categories. It has above average technical performance, reasonable environmental impact and the best economic impact.

Table 4.7: Aggregated results of technical performance, environmental impact and economic impact for the selected materials.

		Technical performance		Environmental impact		Economic impact		Final Outcome
Branded material	Compound (%Bio)	Cat score [Index]	Weighted score [Index]	Cat score [Index]	Weighted score [Index]	Cat score [Index]	Weighted score [Index]	Total Score [Index]
EcoPaXX Q-E7300	PA4.10 (70%)	0.53	0.18	0.51	0.17	0.25	0.08	0.43
EcoPaXX Q-150D	PA4.10 (70%)	0.51	0.17	0.51	0.17	0.25	0.08	0.43
n/a: Lab-scale	PA5.10 (100%)	0.33	0.11	0.62	0.21	0.03	0.01	0.33
Ultramid S3K Balance	PA6.10 (64%)	0.58	0.19	0.50	0.17	0.26	0.09	0.45
Grilamid 2S20nat	PA6.10 (64%)	0.60	0.20	0.50	0.17	0.26	0.09	0.45
Grilamid XE3959Black9992	PA6.10 (64%)	0.60	0.20	0.50	0.17	0.26	0.09	0.45
Rilsan BECN OTL	PA11 (100%)	0.63	0.21	0.63	0.21	0.01	0.00	0.43
Rilsamid AESN OTL	PA12 (0%)	0.65	0.22	0.26	0.09	0.03	0.01	0.31
Grilamid L25A NZ	PA12 (0%)	0.49	0.16	0.26	0.09	0.04	0.01	0.27
Vestamid X7373 nc	PA12 (0%)	0.67	0.22	0.26	0.09	0.05	0.02	0.33

5. Discussion

The greatest scientific contribution of the model comes from the combination of three impact categories and the inclusion of environmental impact in particular. As mentioned in the introduction, assessing environmental impacts has become increasingly important for companies. However, assessing environmental impact is a time-consuming and slow process, if at all successful. This was also the biggest issue faced during this research. Problems occur mainly with gathering data that is representative for environmental impact. The required data often involves knowledge across an entire supply chain, which consists of multiple independently working companies with unique knowledge of a small portion in the supply chain. Most knowledge is protected and cannot be shared since it is part of a company's core business. In addition, the further away a company is in the supply chain from selling their product to a consumer, the less interesting it becomes for it to invest in assessing environmental impact and the higher the perceived risk of sharing knowledge becomes. Therefore, this research has intended to work around the data blockade by using data that is publically available.

The model created in this research has been set up to make sure that an educated guess can be made on a product's environmental impact when data is incomplete or not available at all. When considering the uncertainties that are present in the model, the alternative would be not having any indication on a product's environmental impact.

The components that will be discussed in the next sections are the environmental impact, technical performance and economic impact. This is followed by the model discussion and the discussion ends with an analysis of the model sensitivity.

Discussion environmental impact

The environmental impact category requires a large amount of data and this causes uncertainties in the model. LCA data needs to be gathered from reliable sources, such as LCA software and scientific articles. When not all assumptions are clearly specified, sources that need to be avoided specifically are company LCAs, LCAs in patents or any other type of source where low environmental impacts improve the marketability of a product. Generally, only black box LCA data is available, where the environmental impacts for the production of a substance are aggregated. This prevents the analysis on the contribution of specific steps in the production process, which is important data for scientific work. For corporate policy-making, this kind of data insight might not be relevant.

More specific in this case study is the importance of LCA data for castor oil, which was not available in SimaPro. For this reason, the EIRM analysis for castor oil was assumed to be equal to that of Jatropha oil due to similarities in cultivation. To triangulate the reliability of this outcome, a comparison was made with various sources to ensure that the LCA data is within reasonable bounds. Further research needs to be done on the exact environmental impacts for castor oil that is area-specific. In addition, data needs to become available on the amount of irrigation and fertilizer use for maximum yields, waste disposal methods, ricin neutralization and CO_2-sequestration during growth. This data will aid in understanding the actual environmental impact of castor oil production.

Additional components can be included in the environmental impact that move beyond the production of the material. Recyclability and biodegradability need to be considered when assessing the full life cycle of a material, since these account for the re-usage of materials after they are past their lifetime or the prevention of hazardous waste.

With regard to PCEI, scientific literature and encyclopedia frequently did not cover all the relevant synthesis steps in enough detail or only covered a part of the synthesis steps. In this case, patents had to be consulted which are slightly less reliable than literature but still subject to a peer-reviewing process. Some of these patents date back more than fifty years which means that newer production processes might be available that are more efficient. However, most efficiency improvements come from incremental improvements such as changing solvent, changing machinery, increasing stirring, changing catalyst, and so on. These are out of scope since they do not change the basic chemistry that is taking place in the stoichiometric conversion from one substance to another. Thus, old patents can still be used. More recent patents were only used when the efficiency was improved due to a new synthesis process with different reactants and when this process has also become the industrial standard.

Using both PCEI and EIRM for the environmental impact is essential since it enables a more complete analysis. When LCA data becomes unavailable, the EIRM analysis stops. In a scenario where LCA data covers the first 5 out of 10 synthesis steps for monomer production, it is unwise to neglect processing steps 6 through 10, because emissions and energy usage are still present. For this reason, the PCEI analysis is included. Although it does not fully cover all the environmental impacts, it can determine this from the chemistry in the synthesis processes. In addition, combining EIRM and PCEI will reward materials that require less synthesis steps and penalize materials that require more in the final index score.

Combining PCEI and EIRM enables an analysis that spans across the production chain without neglecting any steps. In a scenario where LCA data is available for 9 out of 10 synthesis steps, the EIRM score will probably show a more negative environmental impact, whereas the PCEI score will show a more positive environmental impact. When considering the fact that these scores are already compared with scores of other materials, the relative contribution for the tenth step is corrected. This enables taking the average of PCEI and EIRM which will then provide a reasonable indication of environmental impacts.

With respect to gathering data on the molar mass, boiling point and enthalpy for substances, uncertainties occur due to the rarity of substances such as hydroxylammonium sulfate, disodium sebacate, ricinoleic acid, 11-aminoundecanoic acid and the cyclododecanone oxime. When a substance was widely used, information was readily available in AspenPlus and on chemical databases. However, the chemical characteristics for a rare material had to be gathered at different sources to fill in the data gaps. This meant that the testing method of chemical characteristics for each source had to be verified for consistency with the other chemical data used in the model.

Discussion technical performance

For technical performance, several causes exist for uncertainty in the data. The first uncertainty occurs when selecting the technical performance parameters. The selected technical performance parameters used do not necessarily cover all the aspects that are relevant for an application, but it is rather a selection of the most crucial aspects. Additional technical performance parameters will enable a more thorough analysis on technical performance, but the weighting of additional parameters will need to be changed according to the parameter's importance for the final product. The second uncertainty occurs when not all technical performance parameters are known as is the case for strain at break. The last uncertainty occurs in the technical performance testing results published by companies, which might focus more on the benefits of a material and neglect the downsides. Monitoring testing methods and performing in-house testing of materials that are adequate for a specific application solves uncertainties in technical performance for a material. In addition, defining the function of the application with a materials expert can minimize uncertainties with respect to determining of technical performance requirements.

Discussion economic impact

For economic impact, causes for uncertainty also come from the data used. The preferred source for data is internal price information on materials that are already being used by the company and for which bulk prices are consequently available. If these were not available the ICIS price database had to be consulted, which contains prices on the most widely used substances. Most materials however, are not covered by ICIS which meant that other sources had to be investigated. For companies that have an unlimited budget, expensive market reports can be bought which will contain relevant price data for substances. This report could not do this which meant that price information had to be gathered from other sources such as publically available literature and Alibaba. The latter source is of questionable scientific quality because it is largely dependent on supply and demand, with large price fluctuations and significant price differences between suppliers. In addition, each day can provide new offers which means that this type of price data is very variable. Although uncertain, this data is intended to provide a notion of how expensive a material might be. When prices are extremely high, the decision can be made to not further investigate a material.

Discussion model

Depending on the application and the goals of research, several aspects of the model can be changed. The first and most important is parameter weighting, which can be adjusted to account for the perceived relevance of each impact category and its parameters. In the case study, equal weighting was assumed because all components were deemed equally important. The second aspect that can be modified is the addition of components. These can be in the form of impact categories such as social impact, health, safety and economic risks. Technical performance can be extended with more impact categories and environmental impact of raw materials can be extended with more LCA indicators. The amount and types of materials investigated can also be increased.

The model attempts to describe reality with as little data input as possible. More data will lead to a more comprehensive result, where the impact of uncertain data on the end result will become lower. However, adding more components will also lead to more complexity, more time needed to fill the data gaps and more data that can be uncertain by itself.

Further validation is needed to confirm that the methodology for assessing environmental impact provides a proper indication of reality. This means that an ex post analysis should be done once full LCA data becomes available for the materials investigated in this case study. In addition, further case studies should be done for materials for which full LCA data is available. This would mean that an analysis is done using the material selection framework, where the EIRM method covers the environmental impacts up to a random pre-defined point in the synthesis process and the PCEI method is then used to supplement the EIRM data. This can then be compared to the already known full LCA data.

For the model to become easy to use, it needs to be populated with more data for the impact categories and various indicators. Generalizing multiple materials with the model requires consistency in calculation methods. If this becomes the goal for the model, it is prudent to use the benchmark calculation for EIRM and economic impact. For the technical performance, no changes need to be made and for PCEI, the calculation should be using weighting factors. New LCA data that is able to cover the EIRM components of the model should also continuously be monitored to replace PCEI data. Over time it might be advisable to use software for the model, which makes the model easily transferable and accessible to all relevant people within a company or within a scientific arena.

Model sensitivity

The sensitivity of the model to faulty data is quite limited. This is achieved primarily by translating all the impact categories to index numbers that range from zero to one and limiting scores to this range. Sensitivity is also limited due to the inclusion of weighting and a large number of data points. For the case study, the weighting factors are indicative of the maximum influence each data point will have on the final model as shown in table 3.9 in the case study. In addition, the model is designed in such a way that index scores for materials are compared with other materials. The last way in which the model decreases sensitivity to faulty data is by assigning lower index scores to materials for which data is either missing or very uncertain. This effectively makes materials less interesting for further research when data is hard to obtain, a scenario in which risks will probably also be higher. Higher index scores will indicate that a material is interesting for further use which will result in a decision to invest more in a material, therefore uncertainty should not be able to increase index scores. This is inherent to the calculations done within the model.

The impact category with the highest sensitivity is the economic impact, which can consist exclusively of brand material price. Theoretically the influence of this indicator is limited to the weighting factor adhered to the impact category, which is 33% in the case study. This means that in the most extreme and unlikely scenario where a brand material price is 0 €/kg, the influence of brand material price can contribute an index value of 0.33 to the end result. In reality prices do not become this low, therefore the impact of faulty data will be lower. The odds of having uncertain prices are also quite low, since internally used brand material prices are the actual prices that are being paid by a company. When using the price constraint method, the uncertainty is higher because of several unknowns and uncertainties. The first is the lack of bulk prices, where catalog prices need to be translated into bulk prices using very questionable assumptions. This was also done in the case study which caused extremely high prices. The second uncertainty lies in the fact that economic analysis on the stoichiometric reaction will provide an underestimation of prices since only inputs and outputs to the equation are used. All other aspects that play a role in the synthesis process are either neglected or already inherent to the bulk prices. The last uncertainty occurs because it is unknown what the actual production price of bulk materials are, since the prices used already have profit margins included that inflate the prices. It is also unknown what profit margins are put into place for the final branded product. The lack of bulk prices and the inclusion of profit margins will increase the price for materials in the price constraint method which effectively lowers the index score for economic impact. Prices can also increase or decrease due to the exclusion of other factors in the production process, which means that index scores can respectively decrease or increase.

The sensitivity of the model with respect to technical performance is limited which is due to the selection of materials that suit the application. There is no point selecting a material that is unsuitable for the application and therefore index scores in this impact category are generally high. The highest contribution for technical performance is also limited to the weighting factor adhered to it, which is 33% and at most an index score of 0.33 on the end result in this case study. For the model it is also important to artificially lower scores when data is not available. The amount of indicators in this impact category are however very important. Increasing the number of indicators decreases the influence of faulty data on the end result. The environmental impact and economic impact are important to distinguish between the small differences in the technical performance index scores.

The lowest sensitivity occurs in the environmental impact, because it consists of EIRM and PCEI, which both consist of their own components. The theoretic highest influence of either category is equal to its weighting factor, which is 50% of 33% or an index score of 0.167 in this study. For the case study, indicators within the EIRM component have a higher influence on the end result than indicators in the PCEI. This is mainly because of the number of components and the certainty of the EIRM data. Data for PCEI is less certain and should therefore not be able to inflate or deflate scores as a result.

Although data gathering is important, the model is most sensitive to changes in weighting factors. Decreasing complexity by removing indicators increases the influence of other components on the end result, which should be avoided if possible. For the impact categories, every percent of change equates to a potential final index score change of 0.01 for an impact category with the highest possible index score of 1. Therefore it is very important to thoroughly determine weighting factors for impact categories that represent the values of the company.

For the quantified sensitivity analysis only the impact categories are considered, since these have the largest influence on the end results. The components within each impact category also influence the end result but since they are one of many parts within the impact categories, they have not been included in the sensitivity analysis. For the weighting changes in the sensitivity analysis, refer to table 5.1. The sensitivity to weighting for the final score of impact categories is displayed in table 5.2 below. The latter table shows the material index scores in the case study and the change in material index score relative to the case study after increasing the weighting factor for one of the impact categories. The numbers in red indicate the largest relative increase in index score for a material and the green boxes indicate the three highest index scores of the selection. Total weighting is now 117%, due to weighting increase of 1 impact category to 50% (a 50% increase w.r.t. 33%) and keeping the other parameters constant at 33%. Equal weighting was used in the case study, where all impact categories were assigned weights of 33%, for a total weighting of 100%. The best compound for application in soccer shoe soles stays PA6.10 (each brand material) for every change in weighting factor and only PA11 (Rilsan BECN OTL) receives a score as good as Ultramid S3K Balance in the case of a 50% increase of weighting for environmental impact. This shows the rigidity of the model and the certainty of the results acquired in the case study.

Table 5.1: Sensitivity analysis weighting scenarios.

	Equal weighting (case study)	Technical performance +50%	Environmental impact +50%	Economic impact +50%
Technical performance	33%	50%	33%	33%
Environmental impact	33%	33%	50%	33%
Economic impact	33%	33%	33%	50%
Total	100%	117%	117%	117%

Table 5.2: sensitivity of results to weighting.

Brand Material	Compound	Equal weighting	Technical Performance (+50%)	Environmental impact (+50%)	Economic Impact (+50%)
		Total index score (% change in Index score w.r.t. equal weighting)			
EcoPaXX Q-E7300	PA4.10	0.431 (+0%)	0.519 (+20%)	0.514 (+19%)	0.473 (+10%)
EcoPaXX Q-150D	PA4.10	0.426 (+0%)	0.512 (+20%)	0.510 (+20%)	0.468 (+10%)
Lab-scale PA5,10+30%GF	PA5.10	0.328 (+0%)	0.384 (+17%)	0.430 (+31%)	0.334 (+2%)
Ultramid S3K Balance	PA6.10	0.447 (+0%)	0.544 (+22%)	0.529 (+18%)	0.491 (+10%)
Grilamid 2S20nat	PA6.10	0.454 (+0%)	0.554 (+22%)	0.535 (+18%)	0.497 (+10%)
Grilamid XE3959Black9992	PA6.10	0.453 (+0%)	0.552 (+22%)	0.534 (+18%)	0.496 (+10%)
Rilsan BECN OTL	PA11	0.426 (+0%)	0.530 (+25%)	0.529 (+24%)	0.428 (+1%)
Rilsamid AESN OTL	PA12	0.315 (+0%)	0.423 (+35%)	0.356 (+13%)	0.319 (+1%)
Grilamid L25A NZ	PA12	0.267 (+0%)	0.349 (+31%)	0.309 (+16%)	0.274 (+3%)
Vestamid X7373 nc	PA12	0.327 (+0%)	0.438 (+34%)	0.368 (+13%)	0.335 (+3%)

To minimize subjectivity, all weighting was done equally. The material that has proven to be best for the application in the case study is not what was expected and this result will be elaborated on in the next chapter.

Other findings

This research started off with trying to acquire data from other companies and suppliers at Adidas. This was not successful and although out of scope, appendix E will provide an explanation of why this was the case.

6. Conclusion

This chapter will briefly conclude with the answer to the fourth research question that summarizes the results of the other research questions, after which the report ends with concluding remarks on the main aim of this research.

Ranking materials

"Research question 4: Which injection-molded polyamides in the selection are most suitable for use in soccer shoe outsoles based on the aggregate of technical performance, environmental impact and economic impact?"

The answer to research question 4 is summarized in table 6.1, where the aggregate performance of the selected injection-molded polyamides for application in soccer shoe outsoles is shown. A higher index score means that a material performs better in the impact category. The final outcome shows the aggregated score for the three impact categories combined. PA4.10 performs quite well but after tests done prior to this research it was rejected on technical performance. PA11 is very interesting based on its high technical performance and best environmental impact, the largest downside is the price. This is the case for both PA11 and PA12, but since both materials are already being used at Adidas for soccer shoe outsoles it becomes interesting to focus more on PA11 and less on PA12 for this specific application. This will not increase prices, but it will have a positive effect on the environmental impact. PA5.10 might become interesting as a material to use in the future because of its good environmental impact, but the technical performance for the material investigated in this selection is not good enough. This might improve when data becomes available on a pure compound of PA5.10 instead of the 30% glass fiber compound used here. Lastly, significant improvements need to be made on costs for the material before it becomes interesting. Within the boundaries of the case study, the best material to use in soccer shoe outsoles is PA6.10, which performs best over the three categories. More specifically, the highest index scores occur for Grilamid 2AS20nat (0.454), followed by Grilamid XE3959Black9992 (0.453) and Ultramid S2K Balance (0.447). They all have above average technical performance, reasonable environmental impact and the best economic impact.

Table 6.1: Aggregated category and weighted index scores in all impact categories for the selected materials.

		Technical performance		Environmental impact		Economic impact		Final Outcome
Branded material	Compound (%Bio)	Cat score [Index]	Weighted score [Index]	Cat score [Index]	Weighted score [Index]	Cat score [Index]	Weighted score [Index]	Total Score [Index]
EcoPaXX Q-E7300	PA4.10 (70%)	0.53	0.18	0.51	0.17	0.25	0.08	0.43
EcoPaXX Q-150D	PA4.10 (70%)	0.51	0.17	0.51	0.17	0.25	0.08	0.43
n/a: Lab-scale	PA5.10 (100%)	0.33	0.11	0.62	0.21	0.03	0.01	0.33
Ultramid S3K Balance	PA6.10 (64%)	0.58	0.19	0.50	0.17	0.26	0.09	0.45
Grilamid 2S20nat	PA6.10 (64%)	0.60	0.20	0.50	0.17	0.26	0.09	0.45
Grilamid XE3959Black9992	PA6.10 (64%)	0.60	0.20	0.50	0.17	0.26	0.09	0.45
Rilsan BECN OTL	PA11 (100%)	0.63	0.21	0.63	0.21	0.01	0.00	0.43
Rilsamid AESN OTL	PA12 (0%)	0.65	0.22	0.26	0.09	0.03	0.01	0.31
Grilamid L25A NZ	PA12 (0%)	0.49	0.16	0.26	0.09	0.04	0.01	0.27
Vestamid X7373 nc	PA12 (0%)	0.67	0.22	0.26	0.09	0.05	0.02	0.33

Model conclusion

This section provides the final analysis of the main aim that was set forth in this research.

> *"The aim of this research is to develop and apply a material selection tool that enables comparative analysis of biobased and petro-based materials on the aggregate of technical performance, environmental impact and economic impact."*

Following the main aim, this research has developed and applied a material selection tool that incorporates the scientific principles of chemical process design and sustainable chemistry in addition to the applied principles of material selection. This framework was applied successfully and the case study result shows a holistic conclusion that includes technical performance, environmental impact and economic impact.

Comparisons were made to identify whether replacing petro-based materials with biobased materials has environmental benefits. The final results show that biobased materials indeed have environmental benefits compared to petro-based materials, as reflected by the higher index scores. The higher the biobased content, the better the environmental impact. For the top 3 materials that follow from the case study, better environmental impact does not necessarily compromise technical performance or economic impact.

The sensitivity analysis of the tool has also shown that, due to the combination of scoring, indexation and weighting, the outcome of the case study is robust. A significant increase in weighting for either technical performance, environmental impact or economic impact does not provide a different result. This means that the final result of the case study, as represented by the acquired final index scores for the materials, is highly certain.

This research has successfully developed and applied the material selection tool, but further validation is needed to confirm that the methodology for assessing environmental impact provides a proper indication of reality. This means that an ex post analysis should be done once full LCA data becomes available for the materials investigated in this case study. In addition, new case studies should be done on materials for which full LCA data is available. This would mean that an ex post analysis is done using the material selection framework, where the EIRM method covers the environmental impacts up to a pre-defined point in the synthesis process and the PCEI method is used to supplement the EIRM data. This can then be compared with the already known full LCA data.

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Appendices

Appendix A: List of abbreviations

PP: Polypropylene
LDPE: Low density polyethylene
HDPE: High density polyethylene
PVC: Polyvinyl chloride
PA: Polyamide
PET: Polyethylene terephthalate
PE: Polyethylene
PS: Polystyrene

MCA: Multicriteria analysis
LCA: Lifecycle analysis
EI: Economic impact
EIRM: Environmental impact of raw materials
PCEI: Process costs and environmental impacts
PCO: Product concentration at reactor outlet
WC: Water content
MBP: Minimum difference in boiling point
MLI: Mass loss index
RE: Reaction enthalpy
CP: Co-products
PT: Pre-treatment
GME: Global material economy

Appendix B: List of concepts used

Branded products or materials:	A material or product that has been commercialized by a company and is being sold under a brand name.
First stoichiometric reaction:	The first reaction where no LCA data exists for the main product of the reaction.
Monomer:	A single molecule that binds to other molecules in long chains to form polymers. It is generally the precursor for many types of plastics.
Biobased:	A material or product based on a biological source such as plants or animals.
Score:	Dimensionless value that precedes Index calculation
Index score:	Dimensionless value that undergoes no additional standardization, only weighting
Petrobased:	A material or product based on a fossil/petrochemical source such as crude oil, natural gas or coal.

Appendix C: Excel formulas used in the model.

The numerical boundaries will yield conditions that relate to the best fit of technical performance with the application. Conditions will then serve as the basis of the model's score calculation with a score of 1 as the best fit with the application. Table C1 shows a list of possible conditions.

Table C1: Boundary and score conditions for application in Excel model.

Numerical boundary Value is: …	Score condition	Formula in Excel
…Between x and z	In range = 1 Outside range = 0	=IF((AND((Value>=x);(Value<=z)));1;0)
…Lower than y	Below y = 1 Above y = 0	=IF(Value<=y;1;0)
…Higher than y	Above y = 1 Below y = 0	=IF(Value>=y;1;0)
…Ideal y between x and z	x = 0 z = 0 y = 1	=(IF((AND((Value<=y);(Value>=x)));((Value-x)/(y-x));0))+ (1-(IF((AND((Value<=z);(Value>=y)));((Value-y)/(z-y));1)))+ (IF(AND(Value=y);-1;0))
…equal to y	y = 1 If not y, score = 0	=IF(Value=y;1;0)

Table C2 below summarizes the formulas used in Excel. The model condition for the highest score for density is "below value=1", for tensile modulus "middle value =1" and for strain at break "in range=1". For tensile modulus, values exist for dry and wet conditions, both values were considered and the lowest score was used for the final score for this parameter, to account for worst-case conditions. When data is not available, a score of zero is applied. This last condition is inserted before the formula for each technical performance characteristic. A value of zero is returned when a characteristic is N/A (not available) and if this condition is false (value is available), the normal formula for a characteristic will be applied.

Table C2: Technical performance characteristics used in the case study with conditions and translation into the Excel model.

Technical performance characteristic (TPC)	Abbre viation	Unit	Desirable value	Condition	Formula in excel
Density	D	[kg/m³]	1100 kg/m3	Below value=1, Above value=0	=IF(D<=1100;1;0)
Tensile Modulus	TM	[MPa]	50-1500-5000 MPa	Middle value=1, Min=0, Max=0	=(IF((AND((TM<=1500);(TM>=50)));((TM-50)/(1500-50));0))+ (1-(IF((AND((TM<=5000);(TM>=1500)));((TM-1500)/(5000-1500));1)))+ (IF(AND(TM=1500);-1;0))
Strain at break	SB	[%]	50-1000%	In range=1, Outside range=0	=IF((AND((SB>=50);(SB<=1000)));1;0)
Missing value				(TPC=N/A)	=IF(TPC="N/A";"N/A: Test Needed";(TPC formula))

These formulas are a component in the calculations done with Excel. Table C3 below summarizes the Excel formulas for each of these parameters in addition to the linear and conditional parameters.

Table C3: Score calculation in the Excel model for the PCEI parameters.

Parameter	Abbreviation	Formula score calculation
Product concentration outlet	PCO	=(IF**((AND(PCO>=1%;PCO<=25%))**;(-0,311*LN(PCO)-0,4307);0))
Water content	WC	=(IF(WC=YES;1;0))
Minimum boiling point difference	MBP	=((IF**((AND(MBP>=5;MBP<=20))**;(-0,72135*LN(MBP)+2,161);1))-(IF**((AND(MBP>20))**;1;0)))
Mass loss index	MLI	=(IF**((AND(MLI>=0,1;MLI<=10))**;(0,2171*LN(MLI)+0,5);1))-(IF**((AND(MLI<0,1))**;1;0))
Reaction enthalpy	RE	=((1-(IF**((AND(ABS(RE)>=100;ABS(RE)<=300))**;((300-ABS(RE))/(300-100));1)))+(IF**(AND(ABS((RE))>300)**;1;0)))
Number of co-products	NCP	=(IF**((AND(NCP>=1;NCP<=7))**;(((-0,02083*NCP^2)+(0,33333*NCP)-0,3125));1))-(IF**((AND(NCP<1))**;1;0))
Pre-treatment	PT	=(IF(PT=YES;1;0))

Appendix D: Additional data

Tables D1 through D7 show the scores for the monomers considered in this research. Each reaction number contributes to the total score for that monomer. The first number in each reaction number cell indicates the calculated score which is determined by the number in brackets. The number in brackets indicates the value that is taken from literature or calculated based on the stoichiometric reaction. Refer to table 3.8 for the reaction conditions of the case study. Table D8 shows the molar mass, boiling point, enthalpy of formation and price of all the substances considered in this research. Table D9 shows how the index scores for PA4.10 and PA5.10 have been calculated using the price constraint method.

Table D1: Mass loss index

Monomer	Total Score	Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (MLI [Score])				
PA4.y	0.00	0.00 (0.00)	0.00 (0.00)			
PA5.y	0.65	0.33 (0.47)	0.32 (0.43)			
PA6.y	0.00	0.00 (0.00)	0.00 (0.00)			
PAx.10	0.87	0.87 (5.42)				
PA11	0.80	0.00 (0.04)	0.38 (0.58)	0.12 (0.17)	0.00 (0.00)	0.30 (0.40)
PA12	0.31	0.00 (0.00)	0.00 (0.00)	0.00 (0.01)	0.31 (0.42)	0.00 (0.00)

Table D2: Enthalpy

Monomer	Total Score	Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (Enthalpy [kJ/mole])				
PA4.y	0.88	0.03 (-105.14)	0.86 (-271.21)			
PA5.y	0.47	0.47 (-194.78)	0.00 (-12.50)			
PA6.y	0.02	0.02 (-104.95)	0.00 (-62.08)			
PAx.10	1.00	1 (445.22)				
PA11	0.00	0 (-46.78)	0 (41.82)	0 (19.82)	0 (18.56)	0 (-61.44)
PA12	1.33	0 (-76.88)	0 (-57.78)	1 (-395.00)	0 (-19.31)	0.33 (166.00)

Table D3: Minimum boiling point difference

Monomer		Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (Minimum boiling point difference [K])				
PA4.y	0.00	0 (166.0)	0 (58.5)			
PA5.y	0.00	0 (124.0)	0 (257.5)			
PA6.y	0.00	0 (195.0)	0 (105.0)			
PAx.10	0.00	0 (243.3)				
PA11	0.00	0 (122.0)	0 (100.0)	0 (175.0)	0 (n/a)	0 (383.8)
PA12	0.50	0 (n/a)	0 (499.8)	0 (527.6)	0.5 (10.0)	0 (214.9)

Table D4: Number of co-products

Monomer		Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (number of co-products [#])				
PA4.y	0.27	0.00 (1)	0.27 (2)			
PA5.y	0.54	0.27 (2)	0.27 (2)			
PA6.y	0.54	0.27 (2)	0.27 (2)			
PAx.10	0.27	0.27 (2)				
PA11	0.00	0.00 (0)	0.00 (1)	0.27 (2)	0.00 (0)	0.00 (1)
PA12	0.54	0.27 (2)	0.00 (1)	0.27 (2)	0.27 (2)	0.00 (1)

Table D5: Distillation of water

Monomer		Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (Distillation of water [condition])				
PA4.y	2.00	1 (Yes)	1 (Yes)			
PA5.y	2.00	1 (Yes)	1 (Yes)			
PA6.y	2.00	1 (Yes)	1 (Yes)			
PAx.10	1.00	1 (Yes)				
PA11	2.00	0 (No)	1 (Yes)	1 (Yes)	0 (No)	0 (No)
PA12	2.00	0 (No)	0 (No)	1 (Yes)	0 (No)	1 (Yes)

Table D6: Product concentration at reactor outlet

Monomer		Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (Product concentration at outlet [%])				
PA4.y	0.00	0 (100)	0 (99)			
PA5.y	0.00	0 (50)	0 (40)			
PA6.y	0.00	0 (92)	0 (98)			
PAx.10	0.00	0 (99)				
PA11	0.00	0 (100)	0 (46)	0 (100)	0 (100)	0 (99)
PA12	0.35	0 (47)	0 (99)	0.35 (8)	0 (100)	0 (100)

Table D7: Pre-treatment

Monomer		Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
		Score (Pre-treatment [condition])				
PA4.y	0.00	0 (No)	0 (No)			
PA5.y	1.00	1 (Yes)	0 (No)			
PA6.y	0.00	0 (No)	0 (No)			
PAx.10	1.00	1 (Yes)				
PA11	1.00	0 (No)	0 (No)	1 (Yes)	0 (No)	0 (No)
PA12	1.00	1 (Yes)	0 (No)	0 (No)	0 (No)	0 (No)

Table D8: Chemical and physical properties of substances used. For visual reasons, the sources have been provided in the model.

		Molar mass	Boiling point	Enthalpy	Price
			1atm		
Trivial name	Formula	[g/mol]	[K]	Hf [kJ/mol]	[€/kg]
Oxygen	O2	32.00	80.19	0.0	0.18
Water	H2O	18.02	373.124	-241.8	0.02
Carbon Dioxide	CO2	44.01	194.686	-393.5	0.02
L-Lysine	C6H14N2O2	146.19	497.15	-461.0	1.08
Pentamethylenediamine	C5H14N2	102.18	452.15	-80.0	51.04
Ricinoleic acid	C18H34O3	298.46	518.15	-720.0	0.33
Sodium carbonate	Na2CO3	105.99	673.15	-1127.4	0.19
Sebacic acid	C10H18O4	202.25	404.15	-920.1	0.76
2-Octanol	C8H18O	130.23	452.15	-376.2	0.86
Disodium sebacate	C10H16Na2O4	246.21	647.45	-943.5	0.40
Ammonia	NH3	17.03	239.8	-45.9	0.53
Hydroxylammonium sulfate	H8N2O6S	164.14	393.15	-1231.0	
Cyclododecanone	C12H22O	182.30	547.95	-348.8	
Cyclododecanone oxime	C12H23NO	197.32	383.15	-364.5	
Acrylonitrile	C3H3N	53.06	350.45	179.7	0.54
Succinonitrile	C4H4N2	80.09	539.15	209.7	1.32
Glucose	C6H12O6	180.16	426.15	-1089.0	0.47
Ammonium	NH4	18.04	273.15	0.0	
Hydrogen	H2	2.02	20.38	0.0	5.28
Tetramethylenediamine	C4H12N2	88.15	431.65	-61.5	8.8
Adiponitrile	C6H8N2	108.14	568.15	149.5	
Hexamethylenediamine	C6H16N2	116.20	478.15	-98.8	1.76
Methanol	CH4O	32.04	337.85	-200.9	4.03
Methyl ricinoleate	C19H36O3	312.49	685.15	-781.0	
Glycerine	C3H8O3	92.09	563.15	-577.9	0.36
Methyl undecylenate	C12H22O2	198.30	525.95	-470.1	
Heptanal	C7H14O	114.19	425.95	-269.1	
Undecylenic acid	C11H20O2	184.28	548.15	-491.1	
Hydrogen bromide	HBr	80.91	206.35	-36.3	
11-Bromoundecanoic acid	C11H21BrO2	265.19	626.75	-508.9	
11-Aminoundecanoic acid	C11H23NO2	201.31	590.15	-579.9	
Butadiene	C4H6	54.09	269.15	109.2	0.39

1.5.9-cyclododecatriene	C12H18	162.27	513.15	97.1	
Cyclododecane	C12H24	168.32	520.15	-253.3	
w-Laurolactam	C12H22NOH	197.32	588.05	-359.4	
Hydrogen cyanide	CHN	27.03	298.75	135.1	0.19
Sulfuric acid	H2SO4	98.08	610	-735.2	

Table D9: Price constraint analysis for PA4.10 and PA5.10.

	Cost input [€/kg]	Value main product [€/kg]	Value increase [Factor]	Contribution monomer [%]	Aggregated value increase [Factor]	Value increase [Factor]	Score [Index]
						PA4.10	
PA4.y	1.08	8.8	8.12	30%	2.44	3.94	0.25
PAx.10	0.29	0.62	2.15	70%	1.50		
						PA5.10	
PA5.y	0.63	51.04	80.81	34%	27.48	28.89	0.03
PAx.10	0.29	0.62	2.15	66%	1.42		

Appendix E: Explanation for issues with respect to gathering data at suppliers

When contacting companies and suppliers for Adidas, it became apparent how difficult (if not impossible) it is to gather good data and these problems are also faced by Adidas. This stresses the importance of the workaround method proposed in this thesis. In this appendix, difficulties underlying data gathering at suppliers are explained.

The difficulties lie in the lack of data which has a number of reasons. The first is secrecy which occurs due to protection of core business aspects such as inputs, outputs and production processes. This is especially the case for chemical companies where competition is based on synthesis processes which is the kind of data needed for conducting proper lifecycle analyses (Hischier et al., 2010).

The second reason lies in the fact that primary suppliers have their own suppliers which need to provide data, therefore the question arises whether data is even known for the primary suppliers (O'Rourke, 2014). Supplier knowledge generally does not exceed the boundaries of what they put in and get out of their production process. In addition, the time needed for data gathering increases greatly when the supply chain becomes longer (Wolf, 2011).

The third reason lies in the lack of transparency. Where retail firms have a customer base that consists of consumers, supplier firms only have to deal with a limited number of customers that deliver to consumers. Retail firms have a higher interest in transparent practices and the obligation, through consumers, to promote transparency in the supply chain. This is however not the case for supplier firms, who will only become more transparent when enough pressure is exerted by a large portion of their large customers (Ibid.).

The final reason lies in the fact that data requests are generally one-sided, which means that the supplier gets nothing in return for their efforts, whereas they are requested to provide data that puts their business at risk (Schurr and Ozanne, 1985).

Not only do suppliers not want to divulge their core business secrets, they generally know very little on what their suppliers are doing and they are not under the pressure to be transparent. From these reasons it can be concluded that supplier relations become strained when data is requested by the company at its suppliers. This further underlines the importance of having a method that avoids this kind of stress, as proposed in this research.

Appendix F: Confidential bulk prices for plastics used at Adidas.

Excluded from this report version.