THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

Life cycle assessment of renewable-based hydrocarbon plastics

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Göteborg, Sweden 2011

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ESA report 2011:17
ISSN 1404-8167
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Printed in Chalmers
Göteborg, Sweden 2011

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ABSTRACT

Plastics are an important commodity of our daily life. And although their majority is still based on fossil feedstocks, numerous efforts are made to stem the environmental consequences related to their production. One approach is the use of renewable materials (biomass) to produce today's conventional plastics. Though a considerable part of the development linked to this approach is still in an emerging state, there is a need to assess the environmental impact of these plastics in order to increase knowledge about the environmental advantages and disadvantages of conventional biomass-based plastics.

The aims of this thesis are:

1. To investigate the environmental impact of producing conventional plastics from biomass-based monomers - using low density polyethylene (LDPE) as test case.

2. To investigate the potential of using process simulation for life cycle assessments (LCA) of emerging technologies.

3. To develop a framework that facilitates simplified LCAs for the production of conventional, biomass-based plastics from different types of biomass and via different conversion processes.

The results for greenhouse gas emissions from LDPE based on sugarcane ethanol are uncertain due to uncertainties in data and methodology for emissions from land use change, in particular from indirect land use change (ILUC). Sugarcane LDPE can be better than the fossil alternative, as was found when using a low estimate for ILUC emissions. However, its potential global warming impact can become similar to that of the fossil LDPE, when using a high estimate for ILUC emissions. For other environmental impacts (acidification, photochemical ozone creation, eutrophication) the fossil and the sugarcane alternative showed similar values, with transport being a key contributor. The LDPE based on sawmill chips ethanol was found to have, at its current state of development, an in general higher environmental impact than the sugarcane and the fossil alternative. The key contributor is off-site enzyme production.

For the emerging technology part of the renewable life cycles data is scarce. Process simulation was therefore used to verify and supply data (ethylene production step for both assessments respectively ethanol production step for sawmill chips case). It has been shown to complement the life cycle inventory and with this allowed the assessment of the two biomass cases.

The environmental key contributors (dominant life cycle activities) identified in the above work, together with key contributors found during literature screening, were combined to a framework. Its purpose is to enable simplified LCAs, which can be used to guide further investigations.

Viewed from the current state, renewable routes for the production of conventional plastics like LDPE will need technical improvements, as well as careful decisions regarding biomass choices. Simplified assessments can support these needs in the way that they enable a comparably fast supply of data, which is needed at the screening stage of a project.

Keywords:
renewable LDPE; LCA and process simulation; simplified LCA for conventional, biomass-based plastics

Preface

Parts, but far from all, of the contributions presented in this thesis have previously been submitted to journals and been included in the following works.

- ▷ **Liptow, Ch** and Tillman, A-M, "A Comparative LCA Study of Polyethylene Based on Sugarcane and Crude Oil", *Journal of Industrial Ecology*, to appear.
- ▷ **Liptow, Ch**, Tillman, A-M, Wallberg, O and Taylor G A, "Could by-products from Swedish forest industry be a European alternative to Brazilian sugarcane ethanol for production of polyethylene - an environmental comparison", *manuscript*.

Acknowledgments

During the time of writing this thesis, there have been many people helping and supporting me and I would like to thank them here.

Thanks goes to my supervisor Prof. Anne-Marie Tillman (Chalmers University) for her thoughtful guidance through the challenges of LCA and for her commitment to my work. I would also like to thank my co-supervisor Prof. Glenn A. Taylor (University of New Mexico) for the many critical discussions and for keeping up with my "German student syndrome". Another person I would like to thank is my co-supervisor Dr. Mathias Janssen (Chalmers University), who was of great support in writing this thesis.

This work has been financially supported by Formas (the Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning) as well as by Tetra Pak (Lund, Sweden) and Trioplast AB (Smålandsstenar, Sweden), which is gratefully acknowledged.

The two case studies being part of this work were supported by a number of very competent persons from the Swedish industry, whom I would like to thank here. Thanks goes to Dr. Thorbjörn Andersson from Tetra Pak, Dr. Bernt-Åke Sultan and Reine Spetz from Borealis, Anders Spetz and Susanne Thygesson from Trioplast and Christer Forsgren from Stena Metall for the critical discussions and for keeping an open mind. The study on sawmill chips LDPE was accompanied by very valuable discussions with Dr. Sune Wännström from Sekab, whom I would like to thank here, too.

Another group of people that supported me on my way were my colleagues here at ESA, whom I thank for the thought provoking conversations and various funny moments.

A great "thank you" goes to my friends, who supported me on this not always easy path. It was and is priceless to have you around and go for fika or talk about "Gott und die Welt". You know who you are.

Ich möchte meiner Familie danken, die mich immer auf meinem Weg unterstützt hat. Danke, dass ihr für mich da wart, egal wo auf der Welt ich mich mal wieder "rumgetrieben" habe. Danke auch, für "Kümst övern Hund, kümst ok övern Schwanz".

Finally, I would like to thank Georgios for the "WTFs" and the cute zoo babies, of course, but also for supporting and accompanying me in all my ideas and projects.

Christin Liptow
Göteborg, September 2011

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1 Introduction

When hearing DNA sequencing a term that could possibly be heard in the same sentence is “emerging technology”. However, when searching for what exactly this type of technology stands for, definitions range from: “a cutting edge development” to “a technology one step before commercialization” [1]. What seems to be the common element though is the underlying intention to change the current situation; whereas there are different drivers for change e.g. financial or technical intentions but also environmental consideration.

A major driver for the current push of new technologies and their products towards an emerging state and beyond, is the desire to change our current environmental situation towards a better one. This also applies for the development of conventional biomass-based plastics. Being one of the major non-energy related applications of fossil oil [2], the production of conventional plastics like polyethylene (PE) or polypropylene (PP) from biomass would save considerable amounts of fossil resources. Moreover, it could, under the premise that these plastics cause less emissions, have a decisive impact on our current environmental situation. However, how does, for example, a company know that using biomass to produce their plastic or using biomass plastic for their product, will actually improve their environmental impact? A method that can supply the answer to this question is life cycle assessment (LCA). However, like every other method, it needs to be supplied with data, preferable industrial scale data, in order to produce meaningful answers. This though, is the major challenge when assessing conventional biomass-based plastic. Most of its development is still in its infancy, especially the processes that convert the biomass. Which is why, these data are not readily available. A tool that can overcome this gap is process simulation (here used as synonym for chemical process simulation). It can, with the help of already existing lab or literature data, generate an industrial scale model that can supply the required data to the LCA. However, the time and effort required for this approach should not be underestimated and leads to the reasonable goal of re-using the lessons learned from a previous assessment. This is especially true for the beginning of a project, where the only information needed is which direction to proceed for future investigations.

An approach of re-use is the formulation of a framework based on the already gained understandings, in order to enable simplified assessments needed at project beginnings.

Based on the above, this Licenciate thesis aims at:

1. Investigate the environmental impact of producing conventional plastics from biomass-based monomers - using low density polyethylene (LDPE) as test case.

2. Investigate the potential of using process simulation for life cycle assessments (LCA) of emerging technologies.

3. Develop a framework that facilitates simplified LCAs for the production of conventional, biomass-based plastics from different types of biomass and via different conversion processes.

1.1 Background

The purpose of the following background section is to give an insight into the tools (process simulation) and methods (LCA and simplified LCA) used during this work. Moreover, there is a short section on renewable LDPE, which is of special relevance for the case studies, but also for the framework.

1.1.1 Life cycle assessment

Over the years, the increasing environmental awareness in society has lead to the development of various methods in order to assess the environmental performance of a product. One of these methods is life cycle assessment (LCA), which assesses quantitatively and qualitatively the potential environmental impact of a product, starting with the raw material acquisition, followed by the production and use phase and finishing with the disposal (cradle-to-grave perspective) [3]. According to the standard, that describes the methodology of LCA (ISO 14040 and 14044, cf [3, 4]); this type of assessment consists of four phases - see also Figure 1.1.

Phase 1 is the goal and scope definition. During this phase, the purpose and the scope of the assessment are determined. The most important modeling choices set during the scope definition are: the system boundaries, the level of detail, allocation procedures, impact categories, limitations and assumptions. Moreover, the functional unit, which is the basis for all calculations, is chosen [3].

The next phase is the inventory analysis. It starts with the construction of the process flowchart. This is followed by a data collection, including all relevant input (materials and energy) and output (emissions and wastes) data. The final step is to set the collected data in relation to the functional unit (all data are calculated towards the functional unit) [3].

The third phase is the impact assessment, which consists of two mandatory steps. Step 1 is the classification, during which the inventory results are related to the impacts they belong to. Step 2 is the characterization, here all inventory results are multiplied with the equivalence factors of the various impacts and finally summed up into the different impacts [3]. In some cases, the level of aggregation is even further increased by weighting, which results in a single impact score. However, weighting is not a mandatory step.

The final and fourth phase is the interpretation, during which the results of the inventory or the impact assessment are interpreted and conclusions and recommendations with the regard to the goal of the assessment are given [3].

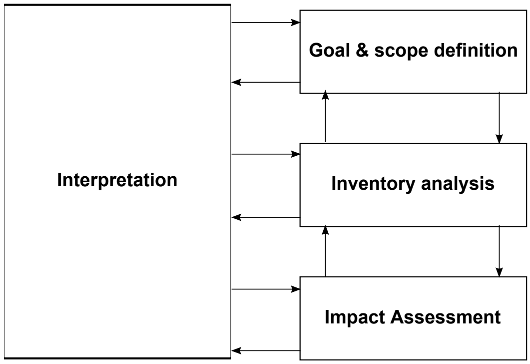


Figure 1.1: *The four phases of an LCA according to ISO 14044 [4]*

1.1.2 Process simulation

In general, process simulation (PS) is a tool that allows the determination of how a process will respond to changes in process conditions, with the help of thermodynamic and physical property based mathematical models [5–7]. In this function, PS is used for various purposes, especially since it can be done at lower cost and faster than real life testing [7]. For example, in industry, PS is used to evaluate optimization and integration possibilities for processes [8, 9] or to evaluate new designs for not yet existing plants [5] and non-industrialized processes. Also in education, the use of PS allows a cost effect learning process on plant design and unit operations [7].

Simulations of chemical processes can be set up in different modes depending on the intended use. According to Gosling [10] evaluation of process economics and resource utilization can be handled with simplified simulations, while process optimization and integration as well as debottlenecking needs detailed simulations. One step further are dynamic simulations, they are used to train operators, evaluate process control options and start up respectively shut down phases of a plant [10].

For LCA purposes the first (simplified) mode that supplies details on resource utilization is of special interest, though also detailed simulations can be relevant when assessing the environmental consequences of optimization measures. However, the use of dynamic simulation appears to be out of scope. This applies particularly for assessments on emerging technologies, since for the latter necessary details for the simulation set up might not even be available.

1.1.3 Combination of life cycle assessment with process simulation

The combination of LCA with process simulation has its beginnings in the mid 1990ies with environmental assessments of already fully commercialized and established processes such as nitric acid production [11] or waste incineration [12]. Since then process simulation has been used for very different LCAs such as on steel production [13] or power generation [14]. However the issue of how to transfer utility (energy, material, water) and also emission data from the simulation to the program used for the life cycle calculations (e.g. dedicated LCA softwares such as SimaPro or spreadsheet softwares like Microsoft Excel) was and still is a major challenge. It has been approached in various ways; for example Kulay et al. [15], Johnson [16] and Herrera [12] used Visual Basic to transfer data into Microsoft Excel; while Alexander et al. [17] use an object link and embedded link (OLE). In addition, there have also been developments within the simulation programs themselves that are intended to ease data transfer - see for example the Workbook in the Aspen programs.

A further approach is to avoid data transfer and instead execute environmental calculations directly in the simulation. This is for example done in the simulation program ChemCad, which uses the WAR (waste-reduction) algorithm for environmental calculations [18]. This algorithm was developed by

Hilaly at the US EPA [19] and further extended by Mallick [20] and Young [21] and combines environmental impacts like e.g. GWP into so-called pollution indices [22].

Over time, the combination of process simulation with environmental assessments has been incorporated into broader contexts such as multi-optimization assessments. The latter aimed at optimizing not only environmental but also economic criteria - see for example [11, 17, 23].

A further, recent extension of this approach is sustainability assessments. They assess, next to environmental and economic, also social impacts (e.g. safety). Studies applying this are e.g. Othman et al. [24] and Fermeglia et al. [25]. They conduct sustainability assessments for the evaluation of chemical process designs. Another trend is the use of process simulation for life cycles that are partly based on emerging technologies. For these life cycles, process simulation supplies industrial scale data for the emerging technology and in this way allows assessments of emerging product and production systems. An area currently making heavy use of this, are assessments on renewable fuels, for which most of the conversion processes are still on lab- or pilot scale (e.g. [26–28].

1.1.4 Simplified LCA

LCA was developed with the ambition of being holistic, that is to assess a product system from its cradle to its grave. However, over time it became clear that, due to reasons like data availability, restrictions in cost, time and product specifications (e.g. at the early phase of product development a product might not be fully specified), this is not always possible. Therefore the investigation of how to simplify LCA methodology started, in order to support cost- and time-effective assessments that could deliver the necessary data required, to support a decision at a certain point in time.

One of the very early approaches towards simplification of LCA was streamlining, which according to Weitz et al. [29] are “approaches to conducting LCAs that reduce the scope, cost and effort required for studies that use an LCA framework" or as later stated by Todd et al. [30] "Streamlining refers to the design of the LCA, particularly decisions concerning what is included in the study and what not". There are various streamlining methods, of which Hunt et al. [31] present a wide range, reaching from removal of up- and/or downstream processes, use of qualitative or less accurate data to exclusion of raw materials based on limits such as comprising less than 10% of the total raw material input.

Another early approach is screening, which Todd et al. [30] describe as "an application of LCA used primarily to determine whether additional study is needed and where that study should focus on". As streamlining, also screening has several methodological variations. They range from qualitative to quantitative methods during which e.g. proxy indicators such as energy or material consumption are used to identify environmental hot spots [32, 33].

Over time streamlining and screening were used together in different ways. For example, Weitz et al. [29] state that streamlined LCA can be applied for screening purposes, though its results are also applicable by itself without further study. In contrast thereto, Jensen et al. [34] state that doing a screening LCA that has already been streamlined undergoes a risk of missing out hot spots, since not the complete life cycle is investigated.

In an effort to settle the issue of simplifying LCA, the Society of environmental toxicology and chemistry [35] Europe proposed a procedure on how to simplify LCA. It consists of the following three steps [35] - also see Figure 1.2:

1. screening - aims at the identification of the life cycle elements that allow the use of generic data and those that may be omitted respectively, without significant effect on the final result

2. simplifying (streamlining) - simplification of the product system model according to the findings from the screening

3. assessing reliability - ensuring that despite simplification the results of the LCA are still reliable and its conclusions are justifiable. Approaches include sensitivity analysis and scenario analysis.

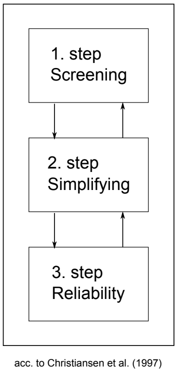


Figure 1.2: *Proposed simplification procedure by SETAC [35]*

However, this proposal is not applied generally when talking about simplified LCA. Although, there are various studies like e.g. [33] and [36] that apply it, there are also studies that develop their own methods of simplification for their assessment; see for example [37]. Another, more recent approach towards simplification is the concept of footprinting [38]. There are several footprinting indicators such as carbon or water footprinting, which can be applied at different levels, reaching from nations to companies and products [38]. However, with regard to the concept of LCA, it is the footprinting of products that can be understood as LCA. For example, the carbon footprint of a product can be compared with the potential impact of global warming, as known in LCA.

1.1.5 Renewable LDPE

One of today's most common plastics is polyethylene (PE). It accounts for approximately 40% [39] of the world's total plastic production and is used for a wide range of applications such as packaging, wiring and piping [40]. In general, PE can be divided into two groups - high and low density polyethylene (HDPE & LDPE) - see Table 1.1 for a short summary of property differences.

The usual feedstocks currently used to produce polyethylenes like LDPE are fossil-based in the form of natural gas or crude oil. Both are processed towards ethylene, the chemical building block of polyethylene. The latter can be done

property	LDPE	HDPE
color	translucent whitish	white opaque
flexibility	fairly flexible	more rigid
density $[m_3/kg]$	924,3	961,0
solubility	do not dissolve at room temperature	

Table 1.1: *Properties of HDPE and LDPE*

in various ways, thought the most common process is via steam cracking as depicted in Figure 1.3 [40].

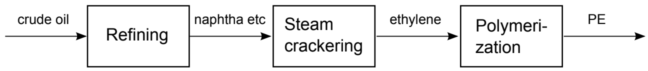


Figure 1.3: *Production of PE from crude oil via steam cracking*

More recently, the production of ethylene and polyethylene came back to its roots (one of the first polyethylene plants operated on ethanol [40]), by using the dehydration of ethanol in order to produce ethylene [41]. In principle, this ethanol could come from various sources. However, in an effort to possibly reduce the environmental impact of the production of polyethylene, ethanol is produced from biomass. More specifically, it is currently commercially produced from Brazilian sugarcane by the Brazilian PE producer Braskem [41] (the Figure 1.4 for production scheme).

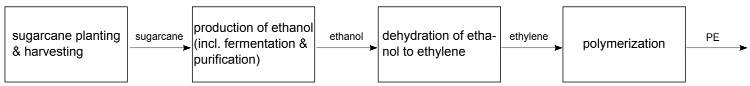


Figure 1.4: *Production of PE from sugarcane*

Nevertheless, despite this already commercialized biomass-based production of PE, the question of what is the environmental impact of such a product is of general societal interest. This does not only apply to sugarcane, but also to other biomass options, that in the future can be under investigation.

1.2 Methodology

1.2.1 Life cycle assessment (LCA)

The environmental assessments in paper I and II mainly followed the methodology of life cycle assessment as described in the ISO standard [4]. However, in contrast to the standard a differentiation between attributional and consequential LCA[1] was made. Moreover, instead of a formal third-party review, a reference group representing different stakeholders along the life cycle of LDPE followed the project and reviewed both studies.

The assessments were conducted from a "cradle-to-grave" perspective. This means they included all life cycle activities from biomass acquisition to disposal of the used plastic. However, the use phase was not included, since it can be assumed to be the same for renewable- and fossil-based LDPE. Furthermore weighting was not part of the assessments.

1.2.2 Process simulation

Process simulation was used for two purposes in this study. For paper I, its purpose was to verify historical data [44] on the production of PE grade ethylene. This was done in the following way:

– Recent patent data [45] on the production of crude grade ethylene (which is not clean enough for PE production) were simulated in the process simulation software Aspen Hysys.

– Subsequently, the output of this simulation was compared to data on crude grade ethylene given in the research paper [44]. The latter also presented data on PE-grade ethylene production.

[1] An attributional (or accounting) LCA accounts for all in- and outputs necessary to produce a certain good at a chosen point in time [42, 43]. In this research average data were used together with partitioning for multi-functional processes under the attributional approach. A consequential (or change-oriented) LCA attempts to assess the environmental consequences of a potential decision [42, 43]. In this research, marginal data were used together with system expansion for multi-functional processes under the consequential approach, if not stated otherwise.

– It was found that both, simulation and paper results are in the same range. Based on this, it was concluded that production data on PE-grade ethylene as stated in Kochar et al. [44] represent current production.

– Therefore, the data for the production of PE-grade ethylene as stated in Kochar et al. [44] were used to assess the process. The data covered material in- and outputs as well as energy consumption.

For paper II, process simulation was used to generate data on the conversion of biomass to ethanol via fermentation. The simulation was done by researchers at Lund University, Lund, Sweden (Ola Wallberg and colleagues). The simulation included the biochemical conversion and all subsequent upgrading processes for the ethanol production and was conducted in the simulation software Aspen Plus. It supplied the data relevant for the life cycle inventory calculations (material in-and outputs, energy consumption, on-site emissions). The model, which is shown in Figure 1.5, was based on data from lab scale experiments conducted at Lund University, Lund, Sweden (see [46–48]).

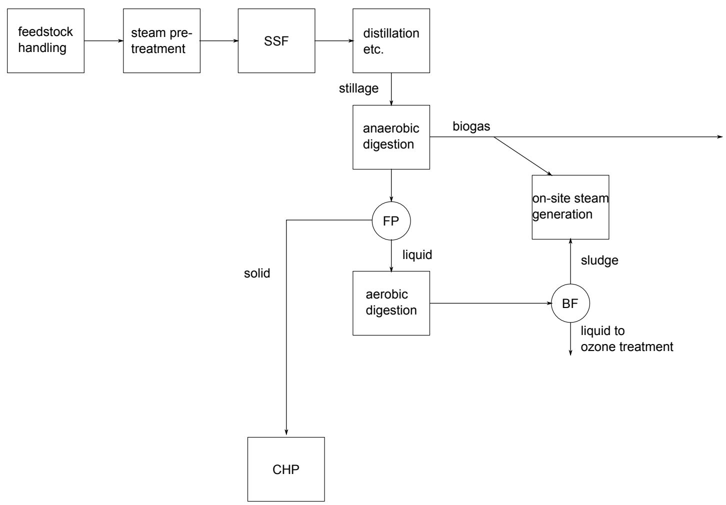


Figure 1.5: *Simplified model of ethanol production*

1.2.3 Framework for simplified LCA on biomass-based plastics

The development of the framework followed in general the procedure as proposed by SETAC [35] (see previous section), though a reliability analysis has not be conducted yet and will be part of future research. The set-up of the framework can be divided into four phases.

1. Carrying out of the two LCA case studies (LDPE based on Brazilian sugarcane and Swedish sawmill chips ethanol), under application of process simulation. This phase included:

    a) The identification of life cycle steps that contribute most significantly to the environmental impact (key contributors) of the LDPE. Key contributors were selected based on their relative share (in comparison to the other life cycle activities) on the total impacts.

    b) The determination of the qualitative information linked to these key contributors (e.g. acquisition of biomass is a key contributor and the qualitative information is that the biomass is a dedicated crop)

2. Setting up a preliminary framework based on the information from phase 1.

3. Literature review in order to confirm and expand the range of key contributors and their qualitative information. Note: Since it was found that the consequences of introducing a new life cycle activity needs to be understood, the review was restricted to hydrocarbon plastics and biomass and conversion options (fermentation and gasification) that can be used to produce these plastics. This was done in order to develop a sound basis for the framework before extending it to more complex plastics.

4. Implementing the results from phase 3 into the preliminary framework set up during phase 2 in order to complete a first version of the framework for hydrocarbon plastics.

1.2.4 Case studies - sugarcane and sawmill chips route

During this work, two case studies were carried out. The first case study assessed the production of LDPE for the use in Europe from Brazilian sugarcane-based ethanol; the second study assessed the same product, however from Swedish wood-based ethanol. The purpose of these two case studies is two-fold:

– Case specific purpose: to assess the environmental impact of producing LDPE from biomass for use in Europe

– Methodology development purpose: to be a starting point for getting an insight into the key contributing life cycle activities for producing biomass-based, conventional plastics

These two cases were chosen, since they represent two ends of the biomass spectrum, as can been seen in Table 1.2 and life cycle flowcharts (Figure 1.6 and Figure 1.7) .

	dedication	material (biomass)	production location
case 1	dedicated agricultural crop	sugarcane	Brazil
case 2	by-product from forestry	sawmill (woody) chips	Sweden
resulting differences		(1) difference in acquisition process, (2) difference in chemical composition - simple sugar vs. lingocellulosic composition; following from that differences in the fermentation process (lingnocellulsic material needs to be hydrolyzed before fermentation)	(1) difference in background conditions e.g. electricity & other energy supply (2) difference in transport distance to use phase (Europe)

Table 1.2: *Presentation of case specific differences*

Next to these case specific differences, there are also methodological differences with regard to the LCA approach and the approach to emissions from

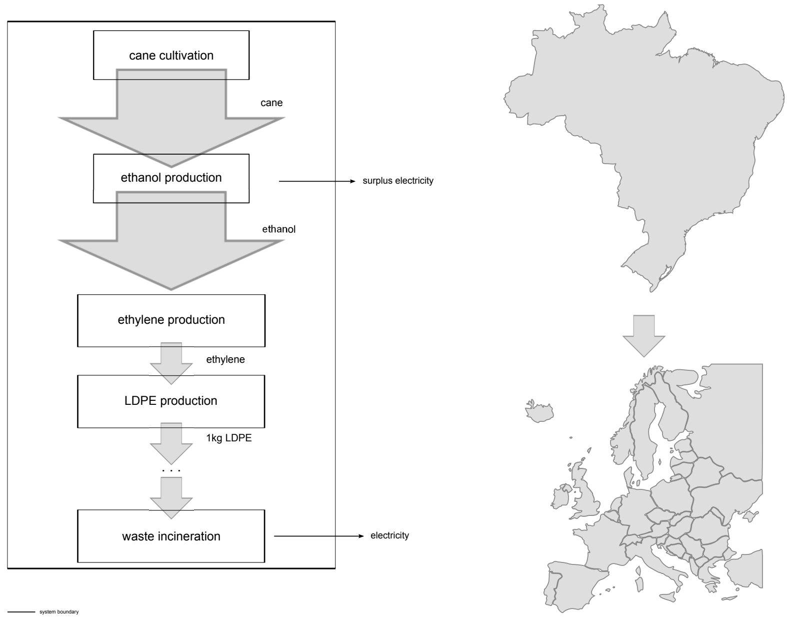


Figure 1.6: *Life cycle flowchart of sugarcane LDPE (attributional approach only; transport omitted from figure for reasons of clarification)*

land use change (LUC). (see Table 1.3)

Similarities with regard to the functional unit and the impacts assessed can be summarized as presented in Table 1.4.

1.3 Results

Case studies The purpose of the case studies is to compare the environmental impact of renewable LDPE based on sugarcane and wood ethanol with the impact of the fossil-oil based alternative. The results of this comparison are presented in Figure 1.8 and described in the following text.

Global warming potential (GWP) As can be seen in Figure 1.8, the wood and the sugarcane LDPE, when assessed under a high estimate for indirect land

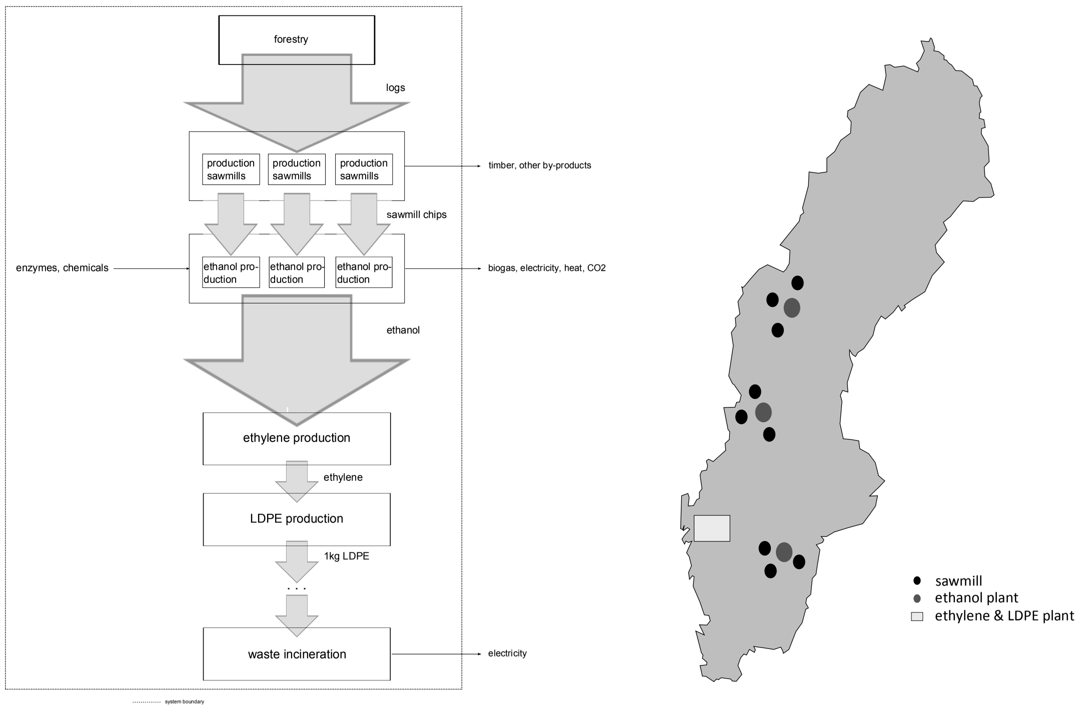


Figure 1.7: *Life cycle flowchart of sawmill chips LDPE (attributional approach; transport omitted from figure for reasons of clarification)*

	LCA approach	approach to emissions from LUC
case 1	attributional & consequential LCA	assessed under attributional & con-sequential LCA; under attributional based on discussion that LUC should be attributed to the product in case of rapid expansion during the past 20 years [49]
case 2	attributional LCA	not assessed, since LUC occurred already centuries ago in Sweden

Table 1.3: *Presentation of methodological differences*

Similarities	
impacts assessed	**functional unit**
global warming (GWP); acidification (ACP); photochemical ozone creation (POCP); eutrophication (EP)	1 kg of LDPE at the gate of the PE production plant

Table 1.4: *Similarities between the two case studies*

use change (ILUC)[2], show no clear advantage over the fossil alternative. Only when using a low ILUC estimate, the GWP of the sugarcane is clearly better than those of the other two routes.

Acidification, Photochemical ozone creation and Eutrophichation potential (ACP, POCP, EP) For the other investigated impacts, the sawmill chips LDPE has the worst environmental performance. Its potential impacts are at least twice the ones of the oil and the sugarcane alternatives. The comparison, between the fossil and the sugarcane LDPE shows, that their ranking depends on which impact is assessed, though overall they are in a comparable range.

For all investigated impacts, off-site enzyme production is the dominant life cycle activity. It causes the low environmental performance of the wood-based LDPE in comparison to the sugarcane- and the fossil oil-based alternative.

1.3.1 Results and findings for the framework

The framework is developed with the purpose of allowing simplified LCAs for the production of conventional, biomass based plastics from different types of biomass and via different conversion processes. Based on this purpose, an investigation into three directions:

- biomass options,
- conversion process options and
- plastic options

was conducted.

The findings and results from this investigation are presented below.

Results and findings from case studies: The results of the case studies with regard to which life cycle activities are the key contributors are presented in Table 1.5 below and can also be seen in Figure 1.8.

[2]The sugarcane results are presented as GWP under a low estimate for emissions from indirect land use change (ILUC) (zero emissions) and GPW under a high ILUC emission estimate (46g CO_2eq/MJ ethanol SOURCE CALIFORNIA EPA).

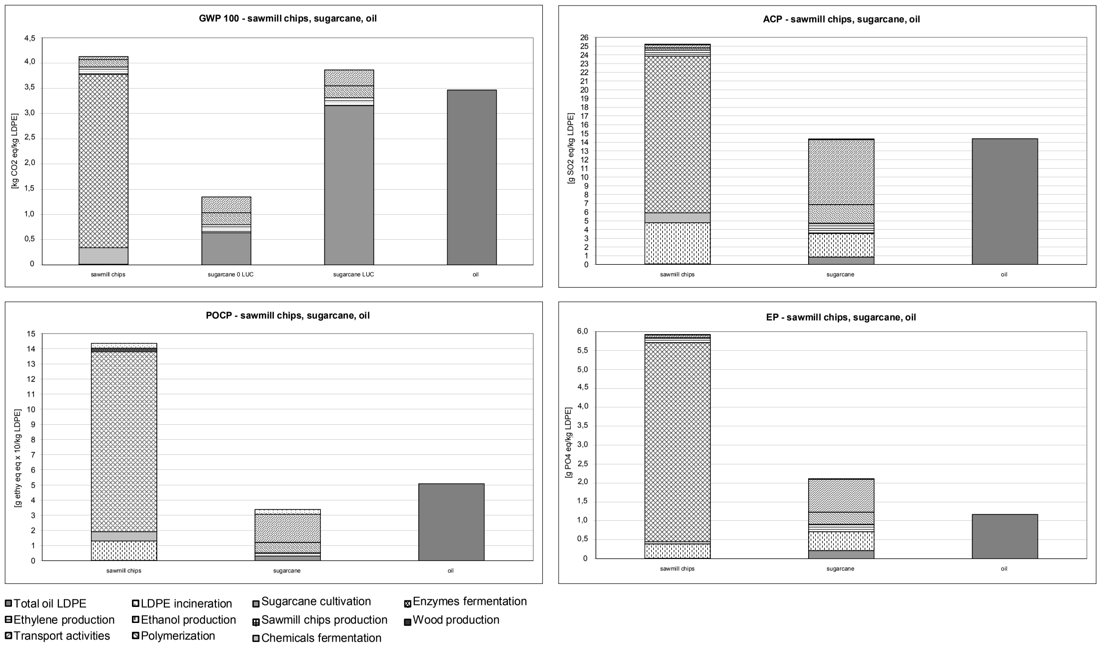


Figure 1.8: *LCA results for sawmill chips- and sugarcane-based LDPE compared to fossil-oil based LDPE (all under attributional approach); GWP = global warming potential; ACP = Acidification potential; EP = eutrophication potential; POCP = photochemical ozone creation potential*

	Key contributors			
	GWP	**ACP**	**POCP**	**EP**
sawmill chips LDPE	- off-site enzyme production - production of chemicals for fermentation	- off-site enzyme production - ethanol production - production of chemicals for fermentation	- off-site enzyme production - ethanol production - production of chemicals for fermentation	- off-site enzyme production - ethanol production
sugarcane LDPE	low LUC estimate - agricultural operations - transport (especially to Europe) - polymerization high LUC estimate - agricultural operations including LUC - transport (especially to Europe) - polymerization	- ethanol production - polymerization - transport (especially to Europe)	- polymerization - transport (especially to Europe)	- ethanol production - polymerization - transport (especially to Europe)

Table 1.5: *Key contributors identified during case studies*

In addition, to the revealed key contributors, there are other findings, though they are not directly related to the framework, worth presenting.

These findings are, with regard to the sugarcane LDPE study:

- Data acquisition for land use change, especially ILUC, was challenging due to the absence of an accepted uniform method on how to account for emissions from LUC and how to implement them into LCA at the time of the study. As a consequence, the range in data was very wide.
- Life cycle data for the production of ethylene from ethanol is very sparse. For this reason, data was acquired combining process simulation and historical research data. This provided a credible estimate for the life cycle data on ethylene production from ethanol.

and with regard to the wood LDPE study:

- Data for off-site enzyme production is very sparse. The data used in this study represent only one specific enzyme product. However, a literature review [50] confirmed that off-site enzyme production is a dominant life cycle activity.

Results and findings from literature review

The literature review served the following purposes:

1. Confirm and extend the key contributors identified in the case studies
2. Identify possible key contributors for a thermochemical route (via gasification) to LDPE
3. Confirm the key contributors identified for LDPE for other hydrocarbon plastics like e.g. PP and if necessary extend the spectrum of key contributors in order to cover other hydrocarbon plastics

To purpose 1 LCA literature on biochemical conversion (fermentation) to ethanol and subsequent processing to ethylene and polyethylene was found to be very sparse. In addition, the studies identified [51, 52] focus on the overall LCA impact of producing PE, with rather limited detail on key contributors. For this reason, the literature review focused on LCAs covering the biochemical production of ethanol, under the assumption that the findings with regard to contribution of ethylene and polyethylene production will not change. This literature was found to be well documented, though publications with very detailed information with regard to key contributors were less well documented. Nevertheless, studies were chosen in an approach to cover a wide spectrum of the currently investigated biomass and process options. The resulting selection allowed a comparison with the findings from the case studies. The overall result was that, the key contributors identified during the case studies were confirmed. Moreover, new key contributors, mainly related to conversion options, were identified - see Tables 1.6, 1.7 and 1.8 for more details.

To purpose 2 Biochemical conversion is not the only option to produce renewable LDPE. Another option is via thermochemical (gasification) conversion. Therefore, this part of the review aimed at identifying key contributors for a possible gasification route. LCA literature on polyethylene production via gasification was found to be very sparse. Because of this, the review was extended towards biomass gasification to ethanol and methanol, under the assumption that the findings with regard to contribution for the ethylene and polyethylene production will stay in accordance with the findings from the studies of [53, 54] that assess the production of PE and PP through gasification - see Tables 1.9, 1.10 and 1.11. However, detailed information with regard to key contributors was still lacking.

To purpose 3 LDPE was used here as the initial plastic for the development of the framework. However, there are various other hydrocarbon plastics, which is why the purpose for this part of the review was to identify whether the key contributors found for LDPE are also valid for these other plastics respectively if the framework needs to be extended. As to be expected, there is little LCA literature about the production of other hydrocarbon plastics from biomass. However, estimates can be made based on current research and development (R&D). One R&D project recently announced by a producer of biomass-based PE, together with a well-known enzyme producer, is the development of biomass-based polypropylene [41]. Following the announcement, the assumption can be made that one route of biomass PP will be via enzymatic fermentation and subsequent dehydration. Since this route is very similar to the one assessed for the wood LDPE, the assumption that key contributors will be similar to the biochemical LDPE seems very reasonable.

Another hydrocarbon plastic that could be produced via fermentation is polybutylene. The monomer of this polymer is 1-butene which can be derived from 1-butanol. The latter is currently investigated for biofuel purposes, however, environmental assessment are still very sparse - see Table 1.12 for examples of LCAs on butanol. Nevertheless, the assumption that the key contributors will be similar to those of the biochemical LDPE seems reasonable.

Both, the results of the case studies and the literature review were used to develop the framework as presented in Figures 1.9 and 1.10. The framework consists of four major blocks (purpose of biomass, conversion of biomass, location of production steps and disposal treatment for plastics) which sequentially lead through the life cycle and result in a simplified LCA. The blocks are further divided into smaller units (rectangle) that distinguish between the different options linked to the main block - for example 'dedicated crop' as an option of the main block 'purpose of biomass'. The smaller units (rectangle) are followed by an 'action' (rhombi) which states whether or not a certain option needs to be assessed for the simplified assessment. Moreover, the 'action' also contains a labeling from 1-4. The latter represent the different life cycle impacts (such as GWP) and are inserted to signal that this specific part of the assessment is of special interest for this impact(s).

1.4 Discussion and conclusion

1.4.1 Case studies

From a case study point of view, the focus of this thesis is on comparing the environmental impact of renewable based LDPE for different biomass options to

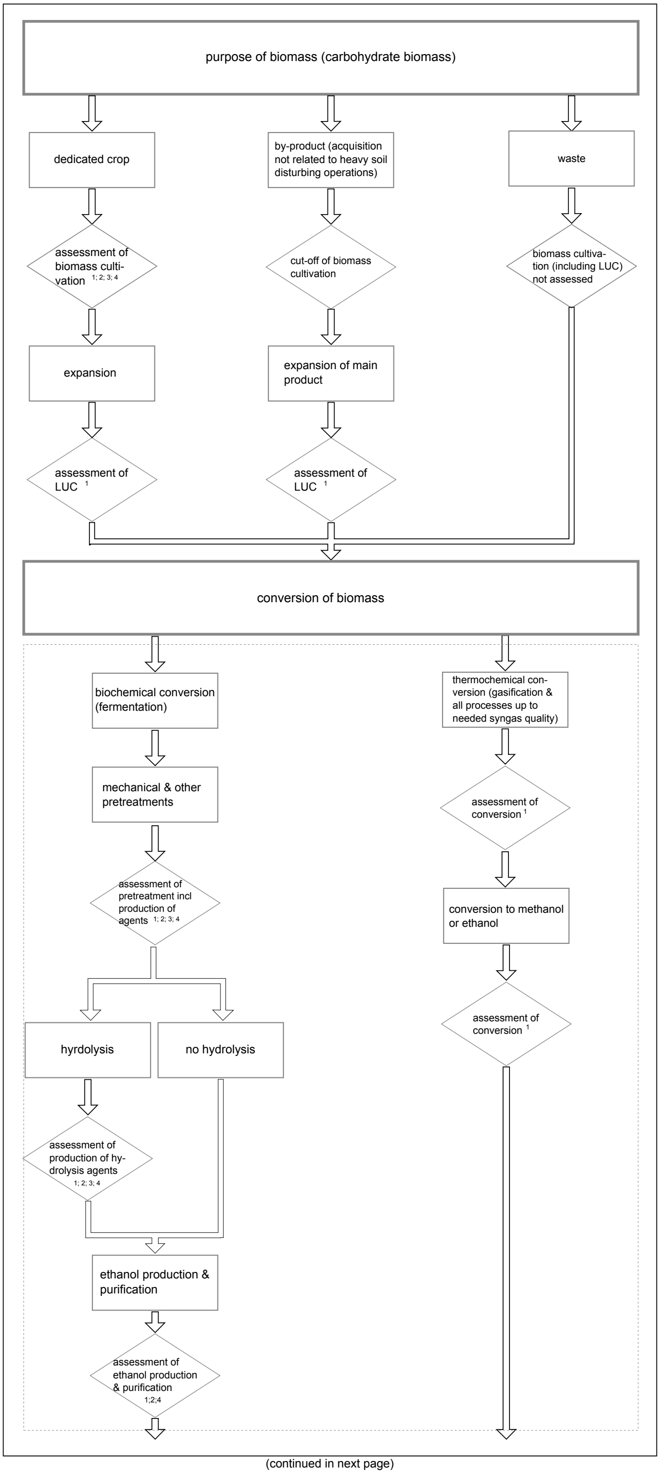
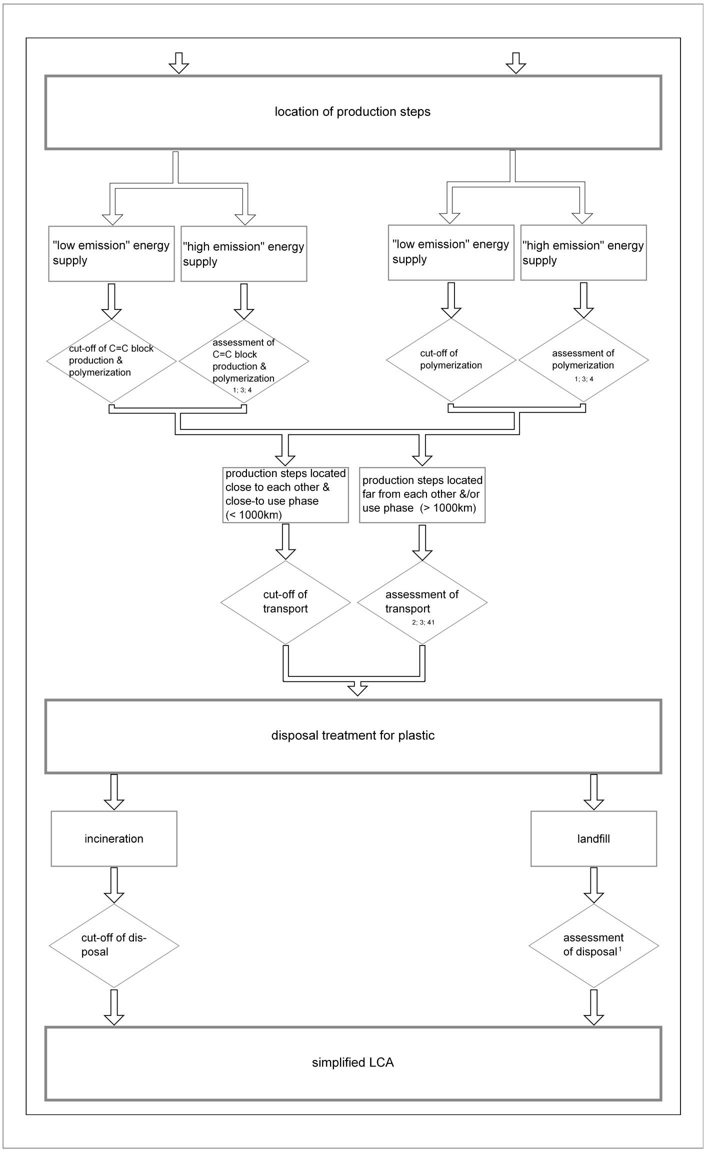


Figure 1.9: *Framework for simplified LCA of hydrocarbon plastics (part 1)*



intended questions for the framework:

What is the environmental impact of producing plastic X from biomass Y via conversion process Z?
e.g. What is the environmental impact of producing PE from straw via a biochemical process route?

➡ attributional approach (see specifications)

for most routes this is the life cycle part that includes emerging technology, a possible way for data acquisition is by the use of process simulation

impacts this part of the assessment is of special relevance for:

1 relevant for GWP
2 relevant for ACP
3 relevant for POPC
4 relevant for EP

note this might not be complete since not all studies assessed all potential impacts

cut-off means that for the simplified assessment this life cycle activity can be omitted

Figure 1.10: *Framework for simplified LCA of hydrocarbon plastics (part 2)*

its fossil based alternative. The biomass options investigated are sugarcane and sawmill chips as a basis for the ethanol used to produce the renewable LDPE. The two renewable LDPEs do not show any clear advantage over the fossil-based LDPE route. Moreover, in comparison to the fossil- and the sugarcane-based product, the sawmill chips-based plastic, is least preferable for all investigated impacts. However, the results for the renewable plastics presented here, should not to be understood as the final answer, but rather as a presentation of the current state of technology development towards a more mature state. This is particularly true for the sawmill chips LDPE, where more development can be expected for the production of enzymes, as well as the biochemical production of the ethanol. In addition, more development can also be expected with regard to cultivation practice and process configuration for the commercialized sugarcane PE.

Since the sugarcane LCA study there has been a lot of discussion and development on how to account for LUC emissions and how to implement them into environmental assessments such as LCA - see for example [55–57]. However, there is still a need for an overall accepted uniform method. The latter is accompanied by a need for reliable data supply for LUC emissions.

Another factor that needs to be considered for biomass-based plastics is production scale. The comparison in this work is between a rather small renewable-based production, and a large commercial fossil-based production of LDPE that is intended to cover the majority of the European production. Scaling up the sugarcane, and the sawmill chips alternatives to such large volume of LDPE could introduce new and/or aggravate already existing environmental drawbacks, such as impact from land use change, and long transport distances. Therefore it is important to not only focus on the overall numerical outcome of the presented comparison, but also on the activities that contribute heavily to it. Comparing the two renewable routes from a key contributor (life cycle activities that contribute dominantly to the environmental impact) point of view, there are clear differences (see paper II) which are mainly based on:

– The varying locations (Brazil vs. Sweden - long vs. short transport, “dirty” vs. “clean” electricity mix)

– The varying feedstock composition and the resulting varying needs in pretreatment before conversion to ethanol via fermentation (easy to ferment glucose vs. more difficult to ferment lignocellulose, which needs more intensive pretreatment)

– The varying "purpose" of the biomass and the resulting allocation of environmental burdens (sugarcane dedicated to the production of ethanol, including large expansion during the recent past vs. sawmill chips a by-product from the timber industry)

All these factors need to be further investigated and considered on the way to an environmentally preferable, renewable LDPE. Further research, however, should not be limited to a certain conversion process or biomass source. Moreover, once a technology has matured enough, investigation into how much biomass LDPE can be produced without superseding the environmental impact of the fossil alternative, is needed. In addition, there is a need for investigations into the overall availability of different biomass options, since there is competition with food, material and energy purposes.

1.4.2 Use of Process simulation

In this thesis, process simulation is used for:

1. **verification of data** on the production of ethylene from ethanol
2. **supply of missing data** on the ethanol production from sawmill chips

Process simulation can be used for different purposes in the context of LCA. However, a process simulation cannot be set up without some knowledge on the process. There has to be a "background information pool" in the form of literature or experimental data. Moreover, there is a need for different knowledge bases, depending on the process to be simulated, in order to use given data in a reasonable way. For this reason, one of the keys to the use of process simulation in the context of LCA is the cooperation with experts from the different fields/knowledge bases. A further key is the understanding that a certain simulation only covers a limited range of process conditions and another set-up might supply a very different result. Therefore, it is critical to document all the assumptions and parameters used in the simulation. However, the ability of developing different set-ups is also one of the advantages of process simulation. It allows an evaluation of a wide range of outputs and can be used to selectively guide the development of an emerging technology towards a low environmental impact.

Another advantage, especially for emerging technologies, is that process simulation can provide data on an industrial scale. Although the data used are based on lab- or pilot-scale experiments, the simulation results still allow a first insight into the environmental impact of industrial scale production when they are used in an LCA. In fact, the simulation results can be used as a first indication of whether or not to proceed into a certain direction of development, whereat development can be looked at from various perspectives. It can, for example, be the development of the process simulated, but it can also be the development of a product, for which the emerging process is only one part of the supply chain. The latter is the case in this thesis and shows that process simulation can be used to bridge the knowledge gap between already established and emerging parts of a life cycle.

1.4.3 Framework

The framework presented in the previous section was developed with the long-term purpose of:

– enabling simplified LCAs that supply reliable data to guide future investigations with regard to:

– biomass and conversion process options for the production of conventional, biomass based plastics.

In this function, the framework is intended to be applicable by industries producing and/or using plastics, in order to support their decision making for further investigations - e.g. with regard to a more detailed investigation for an already assessed option or investigation into other options. Furthermore, the framework can possibly be used by policy as an orientation tool for research and development stirring. Targeting these user groups, the framework not only needs to deliver reliable results, but also needs to be easy to use and understand and to be applicable to more than just one plastic or one type of biomass or process.

With regard to the delivery of reliable results and the ease of use, the framework has not been formally tested yet. Therefore statements for these two factors are based on estimates rather than on experience.

The design of the framework is intended to ease its understanding and use in two ways. First, the sequential guidance through all life cycle activities allows for a systematic walk through the life cycle. Second, the labeling of which life cycle activity is of special importance for which environmental impact, allows a fast overview of which activities need to be assessed for which purpose.

With regard to the delivery of reliable results, from the method used to develop the framework it can be estimated that assessments of similar scenarios (similar to the here investigated scenarios) will result in reliable predictions. 'Similar scenario' is also of relevance for 'being applicable to different plastics, biomass and process options'. Currently, the application of the framework is restricted to hydrocarbon plastics such as polyethylene and polypropylene produced via biochemical (fermentation) or thermochemical (gasification) conversion processes. The restriction in plastics was necessary in order to gain a good understanding of the key contributors of a conventional, though rather simple type of plastic, before extending the scope to more complex products. The necessity of this approach was confirmed, when changing the bioethanol source from sugarcane to sawmill chips for the LDPE. It introduced a new key contributor, in the form of an additional life cycle activity, and illustrated that the consequences of adding new life cycle activities need to be understood in order to develop a reliable framework. The restriction in conversion processes is arbitrary and related to the case study part of this work.

In conclusion, the current framework is applicable for industrial plastic users and producers and possibly policy, though for the restricted spectrum of hydrocarbon plastics. In order to make the framework also usable for other plastics, investigations with regard to such plastics are needed.

1.5 Future work

1.5.1 Future research in the scope of this work

As discussed, reliability of results and applicability to different biomass and conversion options as well as different kinds of plastics are the key features that constitute the framework. In order to further enhance those features and make the framework more reliable, the current scope of investigation needs to be expanded.

A first next step is to test the reliability of results by using the framework for the assessment of a specific case. This case can be, for example, the production of LDPE via fermentation from a biomass such as straw. This will also allow a comparison among the different fermentation routes and the oil route.

Furthermore, the thermochemical (gasification) path in the framework is solely based on very sparse literature. The assessment of a gasification production route will therefore improve the robustness of the path. In addition, the assessment can be used for a direct comparison with the fermentation routes, since model assumptions used for the assessment can be chosen according to the fermentation route - e.g. with regard to production capacity.

Production scale is another factor not yet accounted for in the framework. More investigation into how to consider scale will be needed.

Another important investigation, in order to extend the applicability, is the assessment of additional processes, such as e.g. chlorine production, needed to produce plastics such as polyvinylchloride or polyethyleneterephtalate.

1.5.2 Future research beyond this work

The case study on wood LDPE revealed that off-site enzyme production is an important environmental concern. Therefore, the investigation, both from a process development point of view (e.g. by reducing the consumption of enzymes during the conversion process) and a producer point of view (e.g. by taking emission reducing actions during the enzyme production) are of importance.

Another environmental hot spot found in this work is land use change. Though there is a lively discussion on how to determine and integrate LUC into environmental assessments there is still a need to unify its results into an overachingly accepted method. For this reason, further investigation and development, especially with regard to indirect land use change, are needed.

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	Process & biomass assessed	Location	Impacts assessed	Study question & allocation method	Key contributors relevant for production
Slade et al. 2009	Process: -pretreatment with SO_2 charged steam; SSF process (simultaneous saccharification and fermentation) with enzymatic hydrolysis (FE) - pretreatment with SO_2 charged steam; SSF process (simultaneous saccharification and fermentation) with diluted acid hydrolysis (FA) - with or without C5 fermentation (p or no p) Biomass: - softwood (spruce) - straw	EU (Sweden, UK)	- GWP (per GJ ethanol)	-assessment of bioethanol production from lignocellulosic feedstocks in Europe - allocation via partitioning on energy content	spruce FEp/FE - biomass acquisition - off-site enzyme production - electricity consumed by ethanol production straw FEp/FE - off-site enzyme production - electricity consumed by ethanol production spruce FAp/FA - biomass acquisition - H_2SO_4 production - electricity consumed by ethanol production straw FAp/FA - H_2SO_4 production - electricity consumed by ethanol production
MacLean & Spatari 2009	Process: - dry milling followed by fermentation with enzymatic hydrolysis (for corn ethanol) (DE)	US	- fossil energy (per MJ ethanol) - GWP (per MJ	- develop life cycle model for lignocellulosic	corn - feedstock production - production of process chemicals &

Table 1.6: *Key contributors for ethanol via fermentation literature review (part 1/3) (the table does not represent all the studies reviewed, but the studies with detailed information on key contributors, whereas there is no claim for completeness)*

	- diluted acid pretreatment; SSCF (simultaneous saccharification and co-fermentation) with enzymatic hydrolysis (for switchgrass) (DAE) - ammonia fiber explosion pretreatment; SSCF (simultaneous saccharification and co-fermentation) with enzymatic hydrolysis (for switchgrass) (AFE) Biomass: - corn - switchgrass		ethanol)	ethanol with focus on enzyme & chemical production used in biochemical conversion process - allocation method not specified	enzymes switchgrass - production of process chemicals & enzyme (both for energy & GWP; for DAE, AFE) - feedstock production both for energy & GWP; for DAE, AFE)
Bai et al. 2010	Process: - ammonia fiber explosion; SSCF with enzymatic hydrolysis Biomass: - switchgrass		GWP, ACP, POCP, EP (per power to wheels for 1 km driving middle sized car) – some more impacts were assessed however they are not considered here	- assessment of using switchgrass ethanol as fuel in comparison to the fossil alternative - allocation based on energy content	- fermentation & fossil resource extraction for GWP - fermentation for POCP - agricultural cultivation for EP
Scacchi et al. 2010	Process: - fermentation (not further specified) Biomass: - wheat grain	Italy	GWP, energy use (per fuel required for 1 km distance) LUC not included since carbon soil content was assumed to be stable	- assessment of environmental impact of producing and using bioethanol (attributional LCA) - allocation based on mass	- cultivation and ethanol production for GWP & energy consumption

Table 1.7: *Key contributors for ethanol via fermentation literature review (part 2/3) (the table does not represent all the studies reviewed, but the studies with detailed information on key contributors, whereas there is no claim for completeness)*

	Process & biomass assessed	Location	Impacts assessed	Study question & allocation method	Key contributors relevant for production
Gonzalez-Garcia et al. 2010	Process: - biological conversion according to NREL (Aden) including enzymatic hydrolysis – enzyme production linked to ethanol production Biomass: - poplar as energy crop	Spain	GWP, ACP, POCP, EP (per 1 km driven by a middle sized car)	- assessment of environmental impact of producing and using bioethanol - no need for allocation	- N2O emissions from agricultural phase for GWP (ethanol production, too however, following the approach used here (no accounting for biogenic CO2 ethanol production does not belong to the key contributors) - agricultural activities, ethanol conversion for POCP - agricultural activities for EP - agricultural activities for ACP
Malca & Freire 2006	Process: - yeast fermentation for sugar beet - SSF for wheat Biomass: - sugar beet and wheat	France	primary energy content (per 1 MJ bio-ethanol)	- demonstrate concept of life cycle energy analysis on example of bioethanol - allocation approaches: partitioning by output weight, energy content, economic value , system expansion with replacement value of co-products	- bioethanol production & biomass production for sugar beet and wheat (under mass-based partitioning)

Table 1.8: *Key contributors for ethanol via fermentation literature review (part 3/3) (the table does not represent all the studies reviewed, but the studies with detailed information on key contributors, whereas there is no claim for completeness)*

	Process & biomass assessed	**Location**	**Impacts assessed**	**LCA approach**	**Key contributors**
Mayumi et al. 2010	Process: - gasification to syngas, followed by production of methanol and conversion of methanol to propene Biomass: - waste wood	not specified	GWP (per 1 kg PP)	- demonstration of integration of process simulation into LCA on biomass-based resins - handling of multi-output processes not described	- syngas production - conversion syngas to methanol
Nouri et al. 2006 REPORT	Process: - pressurized fluidized bed gasification, followed by production of methanol and conversion of methanol to propene Material: - wood waste - waste plastics		GWP (per 1kg plastic which consists of 0,68kg HDPE & 0,32 kg PP)	- assessment of whether the use of waste plastics and wood waste to produce resins has an environmental advantage over the fossil alternative (change-oriented)	- syngas production - methanol production - polymerization

Table 1.9: *Key contributors for plastic resins via gasification from literature review*

	Process & biomass assessed	Location	Impacts assessed	Study question & allocation method	Key contributors relevant for production
Bright & Stromman 2009	Process: - allothermal gasification followed by catalytic synthesis to ethanol Biomass: - wood in a mix of surplus from forestry, primary forestry residues, secondary industry residues	Norway	GWP, ACP, EP, HTP (per operation of a flexi-fuel-vehicle over 1km)	- assessment of environmental impact of regional lignocellulosic bioethanol production - physical allocation	worst case scenario (extension of transport distance from forest to biorefinery): - wood chip storage, transport to biorefinery for GWP - forestry operations (coming from surplus forestry operations), transport to biorefinery, ethanol production for HTP - forestry operations (coming from surplus forestry operations), transport to biorefinery, transport of primary forestery residues for ACP - forestry operations (coming from surplus forestry operations), transport to biorefinery, transport of primary forestery residues for EP best case scenario: - wood chip storage, ethanol production, transport to biorefinery for GWP - forestry operations (coming from surplus forestry operations), transport to biorefinery, ethanol production for HTP - forestry operations (coming from surplus forestry operations), transport to biorefinery, transport of primary forestry residues for EP

Table 1.10: *Key contributors for methanol and ethanol via gasification from literature review (part 1/2)*

	Process & biomass assessed	Location	Impacts assessed	Study question & allocation method	Key contributors relevant for production
Hsu et al. 2010	Process: - indirect gasification & mixed alcohol synthesis Biomass: - forestry residues (treated as waste product)	US	GWP , fossil energy input (per 1 km traveled by a light duty passenger car with E 85)	- assessment of GHG emission and Net energy value for ethanol-based transportation fuel in 2022 (attributional approach) - allocation based on "product –purpose" approach	- conversion to ethanol for GWP
Reno et al. 2011	Process: - gasification Biomass: - sugarcane bagasse	Brazil	GWP, HTP, MAE, EP, ACP (1 kg of methanol at facility gate)	- assessment of methanol plant annexed to sugarcane ethanol plant - allocation based on energy content	- conversion to methanol for GWP - syngas production for HTP - sugarcane production for MAE - sugarcane production for ACP - sugarcane production for EP

Table 1.11: *Key contributors for methanol and ethanol via gasification from literature review (part 2/2)*

	Process & biomass assessed	Location	Impacts assessed	Study question & allocation method	Key contributors relevant for production
Wu et al. 2007	Process: - ABE fermentation (acetone, butanol, ethanol) Biomass: - corn	US	- fossil energy consumption, GHG emissions (per mm BTU butanol)	- environmental impact of butanol production - two allocation approaches: system expansion, partitioning on energy content	- conversion to butanol and biomass acquisition (incl. farming and fertilizer production) for fossil energy (under energy content partitioning) - no details for GHG

Table 1.12: *Key contributors butanol via fermentation from literature review*