Life Cycle Assessment In Biorefineries

Case Studies And Methodological Development

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FACULTEIT BIO-INGENIEURSWETENSCHAPPEN

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Life Cycle Assessment in biorefineries: case studies and methodological development

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Levenscyclusanalyse in bioraffinaderijen: toepassingen en methodologische ontwikkeling

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Woord vooraf

Door je jonge jaren heen word je heen en weer geslingerd tussen verwondering en verontwaardiging. Je probeert dan ook de wereld te begrijpen maar botst daarbij op een paradox tussen complexiteit en eenvoudigheid, zoals verwoord door Steve Jobbs: “When you start looking at a problem and it seems really simple, you don't really understand the complexity of the problem”. Dit doctoraatswerk was voor mij dan ook een enorme verrijking om zaken te (trachten) doorgronden en ik ben enorm dankbaar dat ik de kans heb gehad om hieraan te werken. Hierbij wil ik enkele personen in het bijzonder bedanken die dit onderzoek mogelijk gemaakt hebben.

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inzichten kunnen opborrelen tijdens het discussiëren en ik heb het gevoel dat we dit geregeld gedaan hebben. Vanzelfsprekend stond de boog niet altijd gespannen en heb ik ook erg genoten van de aangename sfeer in het algemeen en van de vele gesprekken, zowel tijdens de koffiepauze als ergens bij een Duveltje.

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Steven De Meester, 2013

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Abbreviation index

List of symbols

α	Process boundary
$\alpha_{i,j}$	The weighting factor of substance i for impact category j
β	Process boundary including supporting operations
γ	Cradle to grave boundary
ζ	Ratio of specific heats, adiabatic coefficient
η	Efficiency
$\varphi_{i,}$	The environmental impact of substance i in impact category j
λ	Latent heat
μ	Viscosity
ρ	Density
ψ	Rational Exergetic Efficiency
A	Annuity factor
C_t	Estimated cost at time t
D_a	Diameter impeller
DR_i	Extraction Rate

EF_i	Site specific equivalence factor
En	Energy
En_t	Traditional energy efficiency
En_r	Rational energy efficiency
Ex	Exergy
Ex_t	Traditional exergy efficiency
Ex_r	Rational exergy efficiency
F_{eff}	Efficiency gain for multiple effect evaporators
fn	Functional lifetime
H	Enthalpy
K_L	Pump number in the laminar region
m	Mass
MM	Molar mass
N	Rotational velocity
NA_i	The sodium concentration
N_p	Pump number
P	Power
p_c	Pressure after compression

P_d	Number of persons at distance d
q	Heat demand
r	Discount rate
p_i	Initial pressure
R	Universal gas constant
R_i	Natural Reserves
T_b	Boiling temperature
T_c	Temperature after compression
T_f	Feed temperature
T_i	Initial temperature
T_{proc}	Duration of noisy process (h)
V_i	The total volume of irrigation water
w	Weighting factor
W	Specific compression work

List of acronyms

ADP	Abiotic Depletion Potential
AE	Average Emission impact
AF	Accuracy Factor

AHP	Analytic Hierarchy Process
AJQ	Average Job Quality
AL	Average Labor quantity
AoP	Areas of Protection
AP	Acidification Potential
AR	Average resource impact
AYC	Average Yearly Cost
BCR	Benefit-Cost Ratio
BEES	Building for Environmental and Economic Sustainability
BFE	Biomass Fraction available for Energy
BFM	Biomass required as material resource
BRF	Biomass available for fossil resource replacement
BUO	Basic Unit Operation
CAPEX	Capital Expenses
CEA	Cost Effectiveness Analysis
CED	Cumulative Energy Demand
CEENE	Cumulative Exergy Extracted from the Natural Environment
CERA	Cumulative Energy Requirement Analysis

CExC	Cumulative Exergy Consumption
CFC	Chlorofluorocarbon
CHEF	Current Human Ecological Footprint
CHP	Combined Heat and Power
CI	Composite Indicator
CWRT	Center for Waste Reduction Technologies
DALY	Disability Adjusted Life Years
DATABUO	Database with process specific information
DATAPHYSCHEM	Database with information on substances
DATAROT	Database with Rules of Thumb
DDGS	Dried Distillers Grains with Solubles
DDT	Dichlorodiphenyltrichloroethane
DISPEX	Disposal Expenses
DM	Dry Matter
E	Emission impact
EATOS	Environmental Assessment Tool for Organic Synthesis
EC	Ecological Capital
EC	Electrical Conductivity

EC_{50}	Effective Concentration for 50% of species
EEA	Extended Exergy Accounting
ECF	Economic Feasibility Factor
ELCA	Exergetic Life Cycle Assessment
ELCD	European Reference Life Cycle Database
EMEP	The Cooperative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe
ENVEX	Environmental Expenses
EP	Eutrophication Potential
EPS	Environmental Priority Strategy
ETP	Ecological Toxicity Potential
ExFA	Exergy Flow Analysis
FC	Food and indirect feed consumption per capita
FP	Framework Programme
GD	Green Degree
GDP	Gross Domestic Product
GHG	Greenhouse Gas
GNP	Gross National Product
GRI	Global Reporting Initiative

GWP	Global Warming Potential
HB	Harvested Biomass
HC	Hazardous Concentrations
HDI	Human Development Index
HNU	Heat Not Used
HP	Human Population number
HTP	Human Toxicity Potential
HU	Heat Used
IEA	International Energy Agency
IES	Institute for Environment and Sustainability
ILCD	International Reference Life Cycle Data System
IO	Input output
IRP	Ionizing Radiation Potential
IRR	Internal Rate of Return
ISD	Indicator of Sustainable Development
ISO	International Organization for Standardization
JQ	Job Quality
JRC	Joint Research Centre

L	Labor quantity
LAC	Life Acquisition Cost
LC_{50}	Lethal Concentration for 50% of species
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCSA	Life Cycle Sustainability Assessment
LHV	Lower Heating Value
LINX	Life cycle INdeX
LLC	Life Loss Cost
LOC	Life Ownership Cost
LWD	Lost Work Days
MCDA	Multi-Criteria Decision Analysis
MIPS	Material Input Per Service Unit
ML	Material Losses
MP	All non recycled molecules delivered to society
NMVOC	Non-Methane Volatile Organic Compounds
NN	Noise Nuissance
NOEC	No Observed Effect Concentration

NPV	Net Present Value
ODP	Ozone Depletion Potential
OPEX	Operational Expenses
OTV	Odour threshold value
PAF	Potentially Affected Fraction
PDF	Potentially Disappeared Fraction
PEC	Predicted Environmental Concentration
PMFP	Particulate Matter Formation Potential
PNEC	Predicted No Effect Concentration
POCP	Photochemical ozone creation potential
PROSA	PROduct Sustainability Assessment
PV	Photovoltaics
QALY	Quality Adjusted Life Years
QWERTY/EE	Quotes for environmentally WEighted RecyclabiliTY and Eco-Efficiency
QWT	Qualified Working Time
R	Resource impact
RA	Risk Assessment
RAE	Relative Approximation Error

RISKEX	Expenses caused by accidents and fatalities
RTF	Resilience Threshold Footprint of the earth
SAR	Sodium Adsorption Ratio
SD	Standard Deviation
SF	Site Factor
SII	Social Impact Indicator
SLCA	Social Life Cycle Assessment
SP	Salination Potential
SPI	Sustainable Process Index
SPM	Satisfaction based on the Pyramid of Maslow
SSC	Steady State Cost
SSD	Species Sensitivity Distribution
SUO	Supporting Unit Operations
TCA	Total Cost Assessment
TMR	Total Material Requirement
UER	Unemployment Rate
UNEP SETAC LCI	United Nations Environment Programme and the Society of Environmental Toxicology and Chemistry Life Cycle Initiative
UPR	Unit Process Raw data

VOC	Volatile Organic Compounds
WAR	Waste Reduction algorithm
WBCSD	World Business Council for Sustainable Development
WCED	World Commission on environment and development
WE	Working Environment
WLC	Whole Life Costs
WTA	Willingness To Accept
WTP	Willingness To Pay

CHAPTER I: General introduction

1. Context and goal of the work

The world as we know it is rapidly evolving. Industrial revolutions have allowed humanity to grow both in numbers and in standard of living. Basically these evolutions were built on the ability to transform nature in order to increase man's capacities (Kasa, 2009). Better human capacities then allow a faster transformation of nature. The drawback is that at a certain point this cascade evolution overgrows earth's carrying capacity which in its turn has an influence on the social system. Fossil resources play a central role in this progress as they have removed a part of the human constraints; by using coal instead of wood, more land was available for agriculture, allowing a growing food supply and thus growing population (Pomerantz, 2001). However, alongside these positive effects, the downsides such as city smog and working accidents in coal plants were already noticed in the nineteenth century (Kasa, 2009). Afterwards, industrial revolutions have faced several negative side-effects such as toxicity from the use of dichlorodiphenyltrichloroethane (DDT) as insecticide, mercury pollution, the Seveso disaster, etc. (Heaton, 1994). These effects have been treated for a long time case per case and end of pipe. It is only at the end of the twentieth century that better insight was obtained in the advantages of preventing pollution by clean technology rather than solving problems ad hoc (Clift, 1995). Furthermore, several emerging global issues such as climate change and the depletion of resources require a more systematic approach.

For this purpose, the United Nations initiated a series of conferences and stimulated the creation of the World Commission on Environment and Development (WCED). In 1987, this lead to the Brundtland definition of sustainable development, i.e. 'the development that meets the needs of the present without compromising the ability of future generations to meet their own needs (WCED, 1987). This is a valuable concept that has the merit that society started thinking of the earth's capacity and the social system on a longer term.

In this context it is clear that the current generations should try to find renewable resources instead of building welfare on depleting non-renewables. Mankind has to search for a more sustainable supply of mass and energy, or in other words, exergy. Replacing the fuel of our economy is a challenging task and will probably be achieved by a combination of technologies such as wind power, photovoltaics and biomass valorization. It is however only the latter that is a direct source of renewable carbon and it is therefore expected to take an indispensable place in our future economy. In this transition, lessons need to be learnt from the historical end of pipe strategy which can be connected to a citation of Paulo Coelho: “human beings are in a hurry to grow, then lament their lost childhood, and soon lose the money they need to keep their health". New solutions such as biomass valorization pathways should thus be analyzed more in depth if there are no potential direct or indirect effects counteracting sustainable development. A decent quantification of this concept is necessary, but for this purpose, the Brundtland definition is not very tangible. More tailored for practical implementation is the “Triple Bottom Line” introduced by Elkington (1994), stating that sustainable development should benefit the three P’s: People, Planet and Profit, changing the perception that environmental and social considerations are not compatible with economic benefits. This definition already gives a good overarching direction of something sustainable, but it still does not give a concrete answer on how to get there. It is for this purpose that a sound framework and clear guidelines are necessary, in which macro scale improvement is induced by sustainable development at the micro scale (Huppes and Ishikawa, 2009).

This is especially true for the use of biomass as a resource in the food, feed, fuel and chemical industry which has its advantages, but there are obviously also restrictions. Different valorization strategies are being developed to maximize the benefit from biofeedstock. Usually this relies on a combination of different reaction types such as fermentations, anaerobic digestion, pyrolysis, etherification, etc. and different separation techniques such centrifuges, cyclones, mills, … Also new techniques are being developed that can become competitive in the future such as microbial fuel cells and microbial electrolysis cells (Foley et al., 2010). These different pathways can be coupled in a biorefinery which is defined by the IEA Bioenergy Task 42 (2009a) as: “the sustainable processing of biomass into a spectrum of marketable products (food, feed, materials, chemicals) and energy (fuels, power, heat)”. Since the focus is on sustainable processing, a profound assessment is necessary to evaluate the sense or nonsense of specific applications of biomass as a renewable feedstock (Ponton, 2009). A meaningful assessment should however consider not only the processing, but also the other parts of the life cycle, as the major impact of biobased products is often situated in the supply chain of the biomass (Zah, 2007). In order to make a complete analysis and to have fair comparisons between different options, this supply chain should thus be included and analyzed. Biomass can indeed origin directly from different types of agricultural crops such as maize, sugar beet, etc. or it can origin from industrial or domestic organic waste streams such as lignocelluloses. The latter is becoming more and more important as it faces less competition with the food chain. The advantages and disadvantages of these different feedstock options and their valorization pathways can be analyzed by using life cycle assessment (LCA) which is a structured framework focusing on the interactions between the cradle to grave chain in the technosphere and the natural environment. The LCA methodology dates back to the 1960’s and 1970’s and has developed fast since then. Starting from energy and waste analysis, it has developed to full life cycle inventory systems that are analyzed in many impact categories. Furthermore, it became broader by dealing with issues such as spatial differentiation, input-output based modeling, temporal differentiation, etc. (Guinée and Heijungs, 2011). Yet, sustainability assessment is a holistic and complex task that still needs elaboration in many directions (Guinée et al., 2011).

In this context this work has a double goal:

- As the transition to renewable resources and a more sustainable economy is ongoing and should accelerate, the available assessment methodologies have to be used to give guidance to decision makers on current and future developments. For this purpose, this works analyses several biorefinery case studies.
- The LCA methodology still has points requiring elaboration and improvement. Therefore, in this work several aspects of the methodology are analyzed, and it is attempted to search for ways to improve the understanding of the concept of sustainable development and the life cycle assessment methodology.

2. Overview of the study

To achieve the goal this dissertation is subdivided in five chapters as visualized in Figure I.1. After an introductory **Chapter 1**, the first step is to gain insight in the process of assessing sustainability of biorefinery systems. For this purpose, **Chapter 2** elaborates the which methodologies and tools are available for the (semi-quantitative) assessment of environmental, economic and social impact caused by products and services. Based on this information, **Chapter 3** focuses on the environmental sustainability of biorefinery systems. In the first subpart, the efficiency of cultivation and cascade processing of wheat to food, feed and fuel is analyzed and compared to fossil based products based on a resource footprint. In the second subpart, the supply chain of different sources of biofeedstock is studied more in depth. A case study is conducted on anaerobic digestion of domestic organic waste, farm residues and energy crops, including an analysis of the environmental benefit and burden of recycling nutrients in agriculture.

Although the used life cycle assessment framework has illustrated its significance in Chapter 3, several methodological issues are identified and elaborated in **Chapter 4**. In the first subpart the difficulty to assess novel technologies is analyzed. As the main bottleneck for prospective assessments is gathering a life cycle inventory, basic engineering approaches are developed to gather mass and energy balances of the studied processes. Subsequently the reliability of these modules is tested in a biorefinery case study. In the second subpart of this chapter, the allocation procedure is identified as a key methodological feature in multipurpose biorefineries and a link is made with the goal and scope of the study. The final part of Chapter 4 analyses the conceptual framework of sustainability assessment. An indicator is constructed that focuses both on the inclusion of macro-scale conditions and on the integration of environmental impacts with socio-economic considerations.

In the final **Chapter 5**, a general conclusion is reached, combined with an outlook on potential further developments.

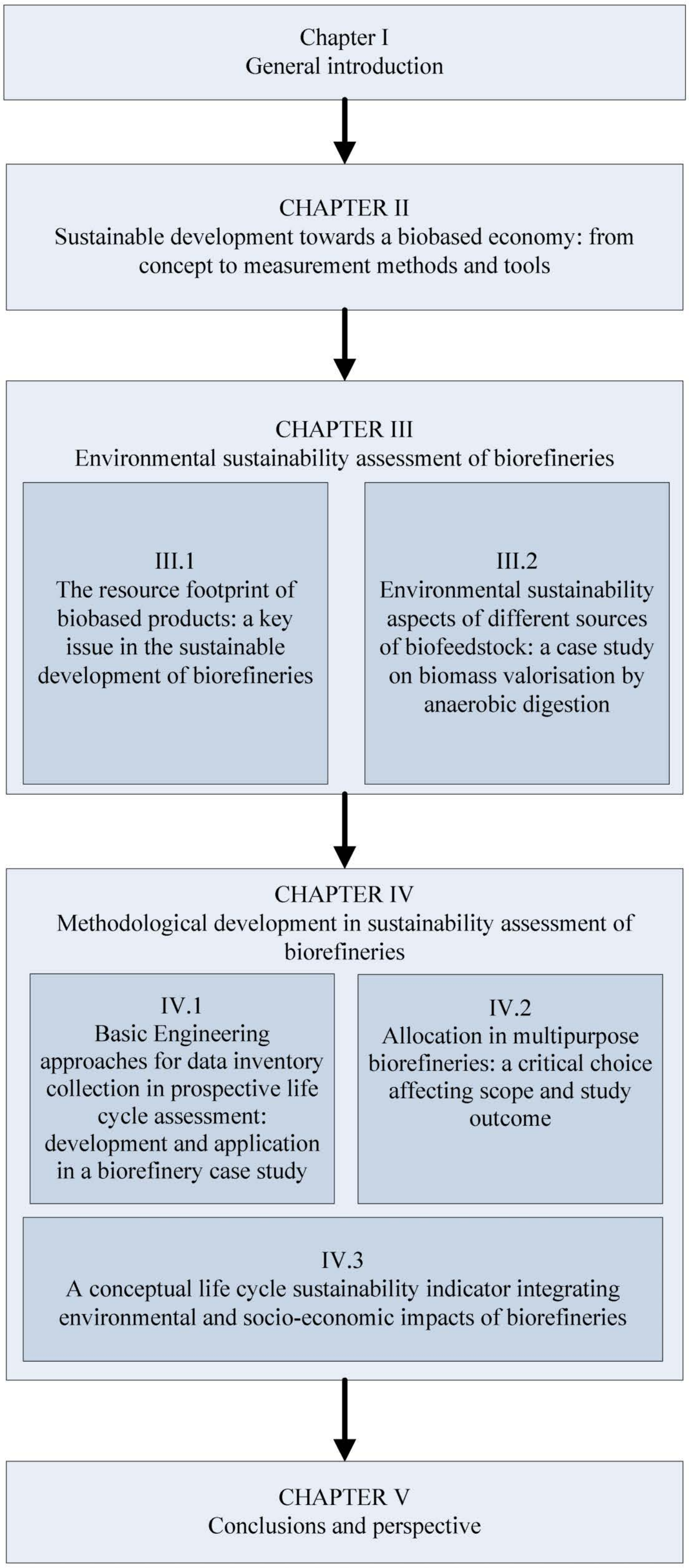

Figure I.1: A schematic overview of the different chapters in this dissertation

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CHAPTER II: Sustainable development from a fossil-based towards a bio-based economy: from concept to measurement methods and tools

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1. Introduction

The concept of sustainable development can easily be agreed upon. Conversely, the quantification of this concept and an appropriate analysis of all the complex interactions is not straightforward. Much work has already been carried out in social, environmental and economic research groups, but while this information is valuable, it is very extended and fragmented. This has resulted in the development of different combinations of principles, depending bottom-up on the available methodologies and top-down on the chosen concept (Figure II.1). In this chapter, an overview is presented of which methodologies and tools are available and for which purpose they can be used; i.e. the goal and scope of the sustainability assessment. Determining the latter, i.e. constructing an assessment framework in the light of the available means, is the first and essential phase of assessments.

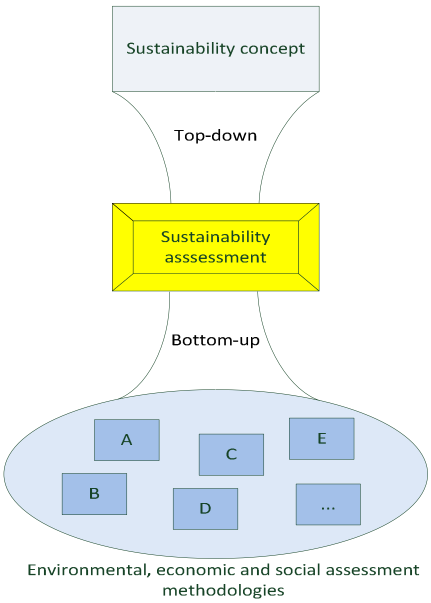

Figure II.1: A sustainability assessment starts top-down from a concept and is bottom-up dependent of the available methodologies.

2. Sustainability assessment framework and inventory

In order to perform a sound assessment, a framework should be constructed in which several conceptual and methodological choices have to be made. The ISO 14040/44 guidelines (ISO, 2006) propose an iterative four step procedure:

- Definition of goal and scope
- Construction of a data inventory
- The impact assessment
- The interpretation

Whereas this framework is originally set up specifically for life cycle assessment, it can be valid for all sustainability assessment methodologies.

2.1. Definition of goal and scope

The first aspect of the goal and scope definition is determining a starting point within the studied system; a 'function' that has to be assessed and to which the results can be linked. This functional unit can range from a process, product or service to a company, sector or a region. In this chapter, focus is on the micro scale aspects of biorefinery assessment, as macro scale improvement is the net sum of improvements at the micro scale.

As soon as the function is identified, a system boundary can be defined to decide which part of a system is included and which can be excluded or cut-off (ISO, 2006). This means that a micro scale sustainability assessment focuses on a specific part of the life cycle of a product or service which can be: a process within a company (process level); a process chain including all supporting utilities at the company level ("gate to gate" boundary); a cradle to gate system, including the production chain, or a full cradle to grave system, which encompasses the use phase and end-of-life strategy on top of the previous phases of the life cycle. The amount and nature of the unit operations that is included in the study depends mainly on the concept of the study and the available time and means. As it is impossible to give one 'absolute' advice, a simple and sound suggestion is to start thinking with involved stakeholders: "if we had no budget or time limitations, what would we include?" and then to include what is possible in the scope and with the means available for the study (UNEP SETAC LCI, 2009). To avoid confusion, each study should include a system diagram, where the system boundary is well defined with respect to the 3 different spheres and to which phases of the life cycle that are included.

2.2. Construction of a data inventory

The actual impact of the functional unit is caused by interactions crossing the system boundary and having a positive or negative effect on the ecosphere or anthroposphere. These interactions are quantified in the inventory phase and then converted to impact at the third phase of the ISO 14040/44 framework, namely the impact assessment. This is done by converting 'elementary flows' in case of the ecosphere and 'elementary interactions' or positive and negative 'pressure' in the case of the anthroposphere (Figure II.2) to actual impact. Economic assessments are more straightforward as the focus is on monetary flows thus solely requiring a decision on the costs and benefits that are of interest of the practitioner. Some economic assessments however also try to grasp environmental and social interactions by monetizing the 'external' costs. This however, could lead to double counting if a sustainability assessment is performed assessing three dimensions simultaneously.

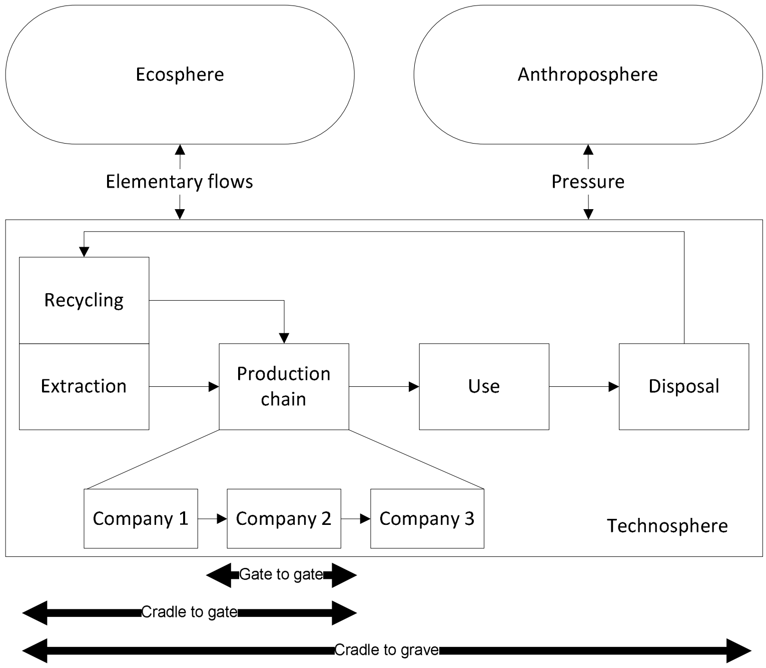

Figure II.2: The system boundary of a sustainability assessment includes unit operations within the technosphere and determines interactions with the ecosphere and anthroposhpere. Based on (European Commission, JRC, IES, 2010)

Collecting a detailed and reliable quantitative or (semi-)qualitative inventory is the most challenging, labor- and time-intensive phase (Finnveden et al., 2009), but it is the key to useful results. Data can be site specific and thus collected within a real production process chain or modeled with software. Alternatively to save time, generic/average data can be used. For this purpose, a foreground and background system can be chosen within the selected list of unit operations. The first is defined as “those processes of the system that are regarding their selection or mode of operation directly affected by decisions analyzed in the study” or as the “case specific processes”, whilst the second is defined as “those processes that are operated as part of the system but that are not under direct control or decisive influence of the producer of the good” or as the “market average processes” (European Commission, JRC, IES, 2010). Generally specific data is used for the foreground system and generic data for the background processes. For the latter, two sources exist; firstly, databases can be used that contain previous studies, such as ecoinvent (The ecoinvent Centre), the European Reference Life Cycle Database (ELCD) (European Commission, JRC, IES, 2011), etc., secondly, a hybrid assessment can be chosen, which couples micro scale assessments to meso or macro scale input output (IO) databases. This approach uses lower quality IO data to fill data gaps in a more detailed assessment (Suh et al., 2004) in which the gaps are 'purchased' from the IO database (Peters and Hertwich, 2006). In the best case, the input output tables are disaggregated to a more detailed level, such as a sector or a product group, where the best fitting and most specific IO is used or created (Suh, 2009).

Depending on the scope of the study, the assessment can be executed in a backward looking way, i.e. attributional, or in a forward looking way, i.e. consequential (or previously marginal, prospective, …) (Curran et al., 2005; Thomassen et al., 2008; Sandén and Kalström, 2007). The latter approach is very promising, as it is able to grasp the larger picture of the impact of decisions in the foreground system on the background system, the ecosphere and the social system. The research question of for example milk production changes from "what is the impact of 1kg of milk?" to "What is the impact of changing demand in the protein and fat market if 1 kg milk is introduced extra?". In this way issues such as partial equilibrium modeling can be included and several market mechanisms in the supply/demand system can be modeled (Ekvall, 2002) such as the occurrence of rebound effects (Thiesen et al., 2008). A hypothetical example in the case of the additional milk production is the fact that the profit margin of the farmer can increase, which can induce an extra investment with additional impact. Another aspect that can be included is experience curves of technologies meaning that future developments and large scale implementation can lead to efficiency gains (Zamagni et al., 2008). All these aspects can be coupled to (sectoral) input-output databases in a hybrid approach to model the impact of a change in a micro system on the meso and macro level, allowing a better understanding of the sustainability of the total system. However, this research area needs further development, as many IO databases are still based on attributional data (Finnveden et al., 2009) and furthermore, it might lead to an unachievable data collection and increased uncertainty.

As a final step, the resulting data inventory should be allocated to the 'function' of the studied system, allowing to express the final impact per unit of function. For example when it is required to allocate the impact of growing a cow to meat or milk. Whilst it is suggested by ISO (ISO, 2006) to first try to avoid allocation through system expansion or by division in subsystems, Lundie et al. (Lundie et al., 2007) conclude that this is not always possible (the cow inherently produces both milk and meat) and state that in most cases a choice is made between a physical parameter such as mass, energy and exergy or an allocation based on economical value. Weidema however, states that system expansion is a sound strategy to avoid allocation in consequential assessments (Weidema et al., 2003). To know the impact of cow meat for example, a displacement of soy milk can be modeled, whereas alternatively the cow meat can be displaced by poultry meat if the impact of the milk is required.

3. Impact indicators and assessment methodologies

The interactions included in the inventory phase should then be converted to actual impact. Assessing the impact of a product system is a very complex task, as it tries to grasp the different aspects of the broad concept of sustainability in the 3 P's; People Planet Profit. All economic interactions and the impact of elementary flows on the ecosystem and pressure on the social system have to be characterized with as a final outcome a list of indicators that give an indication on the sustainability of the studied function. It is therefore very important to understand how these indicators are constructed and applied in assessment methodologies. Furthermore, for the purpose of decision making and external communication, the different indicators are often aggregated, which simplifies decision making on the one hand, but often results in a loss of relevant information on the other hand.

Two strategies can be applied to construct indicators, as is demonstrated in Figure II.3 (Jolliet et al., 2004):

- Assessing impact at the midpoint level. Indicators are chosen at an intermediate position of the cause-effect impact pathway. It is stated that this point should be taken where it is judged that further modeling includes too much uncertainty (European Commission, JRC, IES, 2010).
- Assessing impact at the endpoint level. This strategy includes the effect of midpoints on Areas of Protection (AoP) (Udo de Haes et al., 1999) that have an intrinsic value and give an indication on the relevance of importance to society, making it better understandable for a broader audience. On the other hand, they are more uncertain and also result in a loss of information, hiding the complexity behind the calculations. Therefore, it can be useful to present both midpoints and endpoints (Bare et al, 2000).

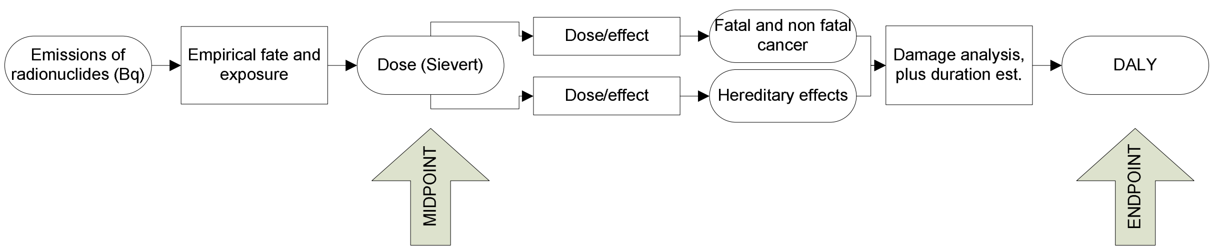

Figure II.3: Midpoint and endpoint indicators in the cause effect chain (DALY = Disability Adjusted Life Years)

In case of endpoint modeling further aggregation is often not necessary as the number of endpoints is limited. In case of aggregation of midpoint indicators, a choice can be made between the concept of strong and weak sustainability, where weak sustainability has a viewpoint that one impact category can be compensated by another, whereas strong sustainability does not accept this substitutability (Cabeza Gutés, 1996). Following the definition of strong sustainability, each indicator has a value which cannot be compensated and therefore results are left as they are, without aggregation. In the case of weak sustainability, a Composite Indicator (CI) (Gasparatos et al., 2008) can be constructed through normalization and weighting.

Normalization, i.e. putting the result in perspective to reference information, can be internal or external. Internal normalization is especially useful for comparison of different options and takes case specific data by using for example a division by the maximum or average value (Xu et al., 2006; Krajnc and Glavic, 2005; Diaz-Balteiro and Romero, 2004). External normalization is more often used and is aimed at understanding the relative magnitude of each indicator. The impact of the studied function can then be expressed relative against the impact of a certain region, population (e.g. per capita (European Commission, JRC, IES, 2010) or sector (ISO, 2006; van Oers and Huppes, 2001)). The following weighting step quantifies the relative significance of each indicator within the goal and scope of the assessment. Doing so is an arbitrary and controversial step and therefore often the simplest methodology is chosen, i.e. assigning equal weights to the different impact categories (Singh et al., 2009). When this approach is not suitable, three options are possible (Soares et al., 2006; Seppälä and Hämäläinen, 2001):

- Using a distance to target approach. In this approach impacts are considered being more if society's activities are further away from achieving the desired targets for the pollutants. This could also be seen as an additional normalization step, and does not give any information on the relative importance of impact categories to each other (Soares et al., 2006).

- Using a monetization approach by using for example the Willingness To Pay approach to rank the impact categories according to the cost that one is willing to pay to lower the impact (Huppes and van Oers, 2011).
- Using a panel approach with involved stakeholders. As this is often preferred, more systematic approaches to assign weights are used, mainly borrowed from the long existing Multi-Criteria Decision Analysis (MCDA) discipline where alternatives can be ranked based on expert judgment (Linkov et al., 2004). A promising approach to support this process is the Analytic Hierarchy Process (AHP) (Saaty, 1990) consisting out of four steps (Figure II.4):
  - Structuring the problem in a goal, in criteria for ranking the indicators, and finally in the different options that can be chosen
  - Comparing the criteria pair wise and give scores from 1 (equal importance) to 9 (one is extremely more important compared to the other).
  - Pair wise comparison of options within each criterion by giving scores from 1 to 9.
  - Combining scores of options and criteria

Zhou and Schoenung (2007) use this approach to assign weights to impact categories in a life cycle assessment case study of computer display technology. Twenty impact categories are selected (renewable resource use, energy use, radioactivity, photochemical smog, ...) which are the ‘options’. These impact categories are compared to each other based on criteria that indicate the perceived risk of that category (Figure II.4). This includes aspects such as distribution (spatial and geographic scales of the impact), frequency or intensity (the extent of impact in the affected environmental area), duration (duration of impact and remediation or reversibility time), etc . Afterwards, the impact categories (the options) are weighted pair wise within each criterion. In this study the impact categories energy use, nonrenewable resource use and global warming obtained the highest weight because of the high scores in the most important criteria: durability, distribution and irreversibility.

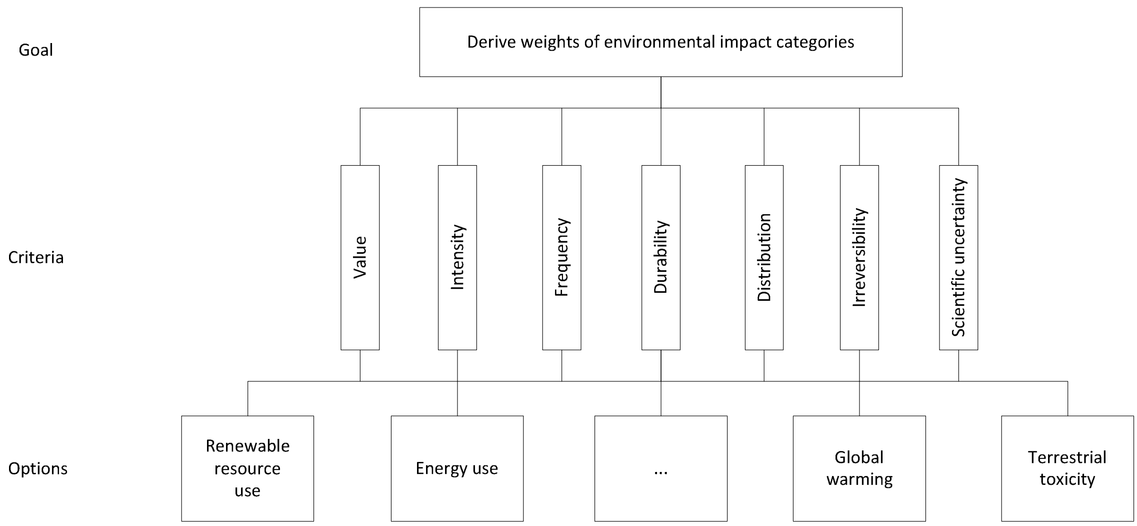

Figure II.4: The Analytic Hierarchy Process (AHP) to determine weighting factors in sustainability assessment.

In this context, several assessment methodologies have been developed, each with their specific starting assessment framework and list of midpoint and endpoint indicators. In the following, first the impact categories will be discussed and secondly, an overview will be presented of different methodologies that use a specific framework with selected impact categories. This structure will be followed for the three dimensions of sustainability; environmental, economic and social.

3.1. Environmental impact assessment

The concept of sustainable development actually grew mainly from environmental concerns. This, together with the large complexity of the environment has led to a large list of indicators with many resulting impact assessment methodologies, and therefore this is the most elaborated research area discussed in this chapter. Impact categories and methodologies related to emissions are discussed first. Resource use will be treated separately, as this is a very relevant and important parameter in modern industry and in the switch to a bio-based economy. On top of this, specific technology indicators can be constructed focusing on internal performance.

3.1.1. Emission impact indicators

3.1.1.1. Midpoint indicators

The overall approach to convert an inventory to a midpoint impact indicator is given by:

$$Category\ Indicator = \sum_{s} Characterisation\ Factor\ (s) \times Inventory\ data\ (s)$$

The inventory data of substance s is given per functional unit, whilst the characterization factor expresses the contribution of substance s to an impact category (in a unit of the equivalence factor) per unit of inventory data (Pennington et al., 2004), as such giving an estimation of the relative importance of that inventory data in a given impact category (Pennington, 2001). An overview of the most commonly used midpoint indicators assessing emissions is given in Table II.1.

Table II.1: An overview of the most common midpoint impact categories, together with the characterization and equivalence factors

Impact category	Impact specification	Most commonly used characterization factor(s) or formula to calculate the indicator	Most commonly used equivalence unit(s) for the characterization factor(s). Expressed per unit of inventory
Ozone depletion	Accounts for the depletion of the protective ozone in the earth's stratosphere due to emissions mainly of halogens (Singh et al., 2007).	Ozone Depletion Potential (ODP)	CFC-11-eq
Climate change	Refers to the change of the climate and temperature due to anthropogenic emissions disturbing the adsorption capacity of the atmosphere (Pennington et al., 2004).	Global Warming Potential (GWP)	CO_2-eq
Photochemical smog / ozone creation	Refers to excessive concentrations of ozone and its intermediate reaction products. It is influenced by different volatile chemicals such as NO_x, OH-reactive hydrocarbons and CO (Pennington et al., 2004).	Photochemical ozone creation potential (POCP)	ethylene-eq (Jolliet et al., 2003; Goedkoop and Spriensma, 2001; Itsubo and Inaba, 2003; Guinée et al., 2002) VOC-eq (Goedkoop et al., 2009; Potting and Hauschild, 2005) NO_x-eq (Singh et al., 2007) (Heijungs et al., 2002)
Acidification (can be subdivided into terrestrial and aquatic acidification	Acidification gives an indication about the increase in the hydrogen ion concentration in water and soil systems due to deposition of inorganic substances (Goedkoop et al., 2009).	Acidification Potential (AP)	SO_2-eq (Goedkoop et al., 2009) H^+ moles-eq (Singh et al., 2007) m² unprotected ecosystem (Potting and Hauschild, 2005)
Eutrophication In many cases subdivided into terrestrial and aquatic eutrophication	Aquatic eutrophication is the result of anthropogenic nutrients (specially N and P) enriching and disturbing the natural nutrient balance in aquatic environments (Pennington et al., 2004) through giving rise to biomass (algae, etc) growth (Singh et al., 2007). Terrestrial eutrophication occurs when a soil is enriched with the otherwise restricting nutrient nitrogen and nitrogen-adapted species thus get a competitive advantage (Pennington et al., 2004). Phosphorus is of less importance in the terrestrial environment, because it is seldom a restrictive nutrient (Potting and Hauschild, 2005).	Eutrophication Potential (EP)	N-eq (Singh et al., 2007) NO_3-eq P-eq / PO_4^{3-}-eq (Jolliet et al., 2003) Or combination of previous SO_2-eq (Jolliet et al., 2003) N-eq (Toffoletto et al., 2007) m² unprotected ecosystem (Potting and Hauschild, 2005)

Species and organism dispersal + gene dispersal	The dispersal of invasive species and organisms due to anthropogenic actions or processes can result in substantial change of the natural animal and plant populations of an invaded region. Also the dispersal of invasive genes from genetically modified organisms can cause harm to a region's natural composition (Jolliet et al., 2004). This indicator is still under development.		
Noise	A noise indicator is often not calculated in LCA studies, because it is stated that the existing noise of processes is taken for granted (Potting and Hauschild, 2005) or is very local and difficult to interpret in relation to other impact categories.	$NN_d = P_d * T_{proc} * NNF_{LP}$ NN_d = noise nuisance at distance d from point source P_d = number of persons at distance d T_{proc} = duration of noisy process (h) NNF_{LP} = noise nuisance factor	person hour (Potting and Hauschild, 2005)
Odour	Odour is a subjective nuisance, but above a certain level, some odours from emissions are 'experienced' as stench by everyone (Guinée et al., 2002). Despite the fact that odour is mentioned several times as a possible impact category (Toffoletto et al., 2007), it is not often calculated.	It is calculated as the reciprocal of the odour threshold value (1/OTV). (Guinée et al., 2002)	m^3 (Guinée et al., 2002)
Ionizing radiation	This impact category is related to the release of radioactive material to the environment (Goedkoop et al., 2009).	Ionizing Radiation Potential (IRP)	kBq (Becquerel) U-235 air-eq (Goedkoop et al., 2009) Bq-eq carbon 14 in air (Jolliet et al., 2003)
Soil salination	Soil salination refers to the increasing salt concentrations in the soil. It can be calculated for irrigation practices based on the Sodium Adsorption Ratio (SAR) and Electrical Conductivity (EC) (Feitz and Lundie, 2002).	Salination Potential (SP) $SP = EF_i * [Na_i] * V_i$ With EF_i the site specific equivalence factor based on EC and SAR, NA_i the sodium concentration and V_i the total volume of irrigation water	Na^+ -eq (Feitz and Lundie, 2002)

Human toxicity	Human toxicity is an adverse effect on humans as a result of exposure to a chemical (Pennington et al., 2004). Further distinction can be made between carcinogenic and not carcinogenic or even respiratory impacts for indoor air pollution (Singh et al., 2007). Midpoint indicators for this category are mainly based on reference substances, but can alternatively be more qualitative by the numbers of persons exposed.	Human Toxicity Potential (HTP)	1,4-dichlorobenzene-eq. (Goedkoop et al., 2009) Chloroethylene-eq (Jolliet et al., 2003) person.µg.m^{-3} (Potting and Hauschild, 2005) *Carcinogenic:* Benzene eq (Singh et al., 2007) *Non carcinogenic:* Toluene-eq (Singh et al., 2007) *Respiratory:* PM 2.5-eq (Singh et al., 2007)
		Particulate Matter Formation Potential (PMFP)	PM 10-eq (Goedkoop et al., 2009)
Ecotoxicity	Ecotoxicity is an adverse effect on organisms and/or the functioning of the ecosystem as a result of exposure to a chemical released in the environment (Pennington et al., 2004). Apart from reference substances, the volume of water and soil that is exposed can also be seen as a midpoint indicator. In this case spatial diversity can be introduced by a site factor (SF) (Potting and Hauschild, 2005).	Ecological Toxicity Potential (ETP)	2,4-dichloro-phenoxyacetic acid-eq (Singh et al., 2007) 1,4-DCB-eq (Guinée et al., 2002) triethylene glycol-eq (Jolliet et al., 2003) (Toffoletto et al., 2007) m^3 (Potting and Hauschild, 2005)

3.1.1.2. Endpoint indicators

Endpoint or damage categories are at the level of ultimate societal concern and thus easier to link with the sustainability concept. The best known endpoint model is presented in the Eco-indicator 99 impact assessment methodology (Goedkoop and Spriensma, 2001) and uses two damage categories for emissions, following the so-called Areas of Protection (AoP) proposed by Udo de Haes et al. (Udo de Haes et al., 1999):

- Damage to human health
- Damage to ecosystem quality or diversity

Calculating the impact of a certain flow on one of these endpoints is not straightforward as it requires complicated cause-effect models. Current environmental endpoint modeling has learnt much from the longer existing risk assessment (RA) approach, which starts from hazard identification and is followed by a release and exposure assessment and hazard characterization phase (dose/response) to obtain a final risk characterization and interpretation. Similarly, endpoint modeling typically uses four steps (Goedkoop and Spriensma, 2001):

- Fate analysis linking an emission to a temporary concentration. This requires extensive data and good models. A harmonized approach to do so is presented in "The Tool" (Wegmann et al., 2009). Three parameters are calculated in this model, which can also be used as midpoint indicators: overall persistence, characteristic travel distance and transfer efficiency.
- Exposure analysis, linking this temporary concentration to a dose (used for human health, not for ecosystem quality)
- Effect analysis, linking the concentration or dose to the effects. Typically dose-response curves are constructed, allowing comparisons between the Predicted

Environmental Concentration (PEC) and the Predicted No Effect Concentration (PNEC) based on acute (EC_{50} / LC_{50}) or preferably chronic (No Observed Effect Concentration NOEC) data (Van Leeuwen and Hermens, 1995). Whilst this should actually be determined for all species, often a more generic Species Sensitivity Distribution (SSD) approach is used, focusing on a full community or ecosystem, based on Hazardous Concentrations (HC) (Larsen and Hauschild, 2007).

- Damage analysis, linking the effects to a damage indicator. Most used endpoint indicators are:
    - Disability Adjusted Life years (DALY) for human health, representing years of "healthy" life lost (WHO, 2011).
    - Potentially Affected Fraction (PAF) or Potentially Disappeared Fraction (PDF) of the species, for ecosystem quality. The first giving an indication on the fraction of species affected above their NOEC and the second adding what happens beyond this NOEC (Pennington, 2001).

Figure II.5 is an example of the determination of the endpoint indicator from a SSD curve, plotting the NOEC of a set of species. A benchmark can then be put on the concentration where the NOEC value is exceeded for 5% or 50% of the species; respectively $HC5_{NOEC}$ and $HC50_{NOEC}$ (Smit, 2007).

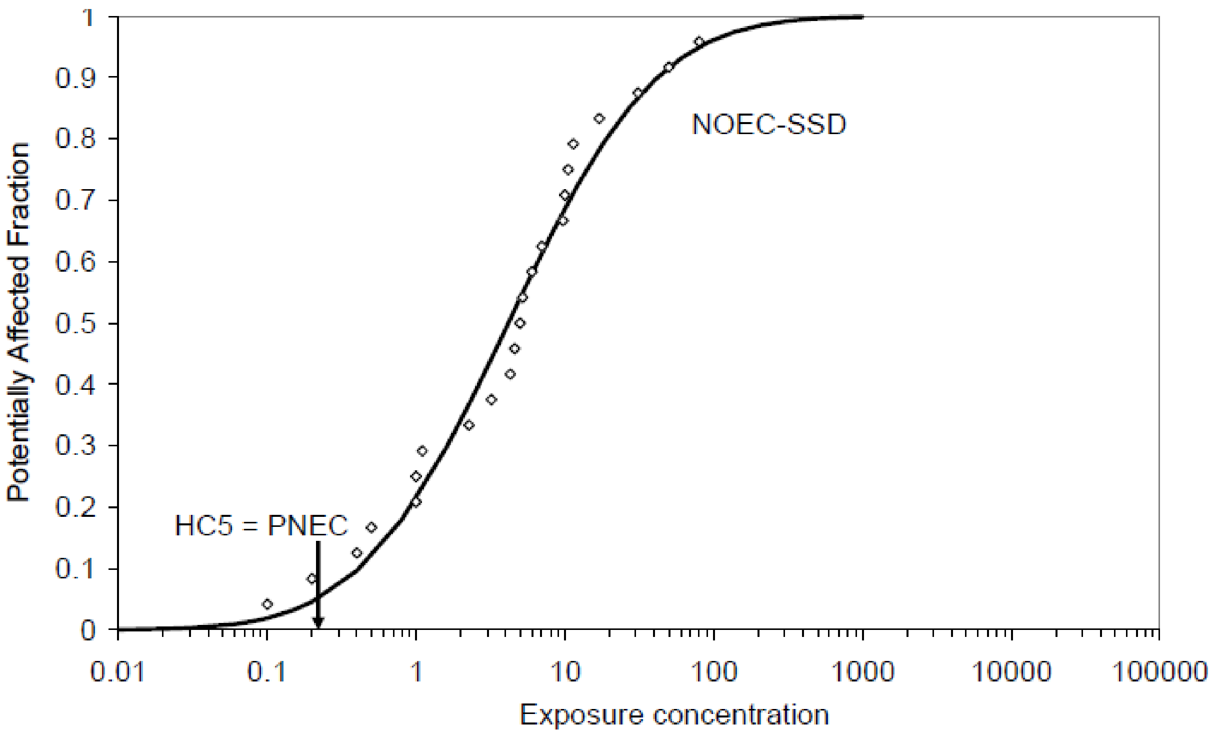

Figure II.5: A species sensitivity distribution based on NOEC values, where the exposure concentration is plotted versus the Potentially Affected Fraction (PAF) of the species. HC5 is the point where 5% of the species is potentially affected (Smit, 2007).

These curves are typically sigmoid, implying that there is a non-linear relationship between the dose/concentration and the impact. Due to the limitations of the current LCA methodology, accounting for this is not possible. However, linearity can be assumed when using marginal models, as the changes of the emission levels are often relatively small compared to the total level (Heijungs et al., 2002). On top of this, some impact curves are assumed to be of the non-threshold linear type, which means that marginal and average approaches are equal (Heijungs et al., 2002), implying that linearity can also be assumed at concentrations less than the PNEC or HC5 (Huijbregts et al., 2000). The assumption of linearity by using an average or marginal approach has led to sound LCIA endpoint methodologies such as RECIPE 2008 (Goedkoop et al., 2009), or the consensus model for toxicity USEtox (Rosenbaum et al., 2008), the latter based on previous work in the OMNIITOX project (Molander et al., 2004). Nevertheless, this assumption of linearity could be flawed if larger systems are studied, for example if LCA is combined with input-output tables and the impact of market penetration of technologies is studied. In this case, more research might be necessary to improve the characterization factors of different scales.

3.1.2. Resource impact indicators

The assessment of environmental impacts has been dominated for a long time by the characterization of emissions, but now, in the post Brundtland era, there are numerous indications that assessments should account for the emerging depletion of resources as well in order to allow future generations to fulfill their needs. The environment (ecosphere) can indeed be considered as a reservoir for energy, material and land needs (for the technosphere). From this point of view, industry and other economic activities can only exist as long as they exploit these (Dewulf et al., 2008). On top of this, mass and energy resources cost money and are thus directly coupled to economic profit. Because of this relevance, several methodologies were developed to account for the resource use of processes and products. Elaborating on the work of Steen (2006), resources can be subdivided into 5 midpoint types:

- Mass and energy
- Land use
- Exergy consumption
- Emergy consumption
- Relation to use of deposits

On top of this one endpoint indicator is constructed, focusing on future consequences of resource extractions.

3.1.2.1. Midpoint indicators

Mass and energy

Mass and energy are very tangible concepts, which are easily applicable due to their omnipresent use in industrial applications. For material use, the Material Input Per Service Unit (MIPS) indicator quantifies (in kg) how much resources are needed to manufacture a product or service (Ritthoff et al., 2002). All materials taken away from the ecosphere and technosphere, depending on the system boundary of the study, are counted and subdivided into five different input categories:

- Abiotic or non renewable resources
- Biotic or renewable resources
- Earth movements in agriculture and silviculture (consumption/erosion and alteration through farming and forestry)
- Water
- Air

When applying a similar approach at the level of national economies this is called the Total Material Requirement (TMR) (Ritthoff et al., 2002). In recent years, water use is becoming a more and more relevant indicator, especially in regions with low water availability. Recent developments focus not only on surface and ground water use, but also on the available levels (Milà i Canals et al., 2009) . Furthermore, the water quality which is discharged back to the environment can also be included (Goedkoop et al., 2009).

For energy use, the concept of Cumulative Energy Demand (CED) or Cumulative Energy Requirement Analysis (CERA) is used as a measure for the primary energy demand of a product or service, meaning that the energy content (in Joules upper heating value) of energy carriers that have not yet been subjected to any conversions is quantified (Wrisberg and Udo de Haes, 2002), whilst taking losses due to transformation and transport fully into account (Klöpffer, 1997). Generally eight categories are used:

- Non-renewable resources:
  - Fossil
  - Nuclear
  - Primary forest
- Renewable resources
  - Biomass
  - Wind
  - Solar
  - Geothermal
  - Water (Hydro-energy)

Land use

In a world where biomass is gaining importance as an alternative for fossils, the inclusion of land use in assessments is essential. Two starting points can be taken:

- From an inventory point of view i.e. occupation in m², that is occupied area multiplied with time, in m²a (Krajnc and Glavic, 2005), not considering the differentiation in occupation intensities.
- From an impact point of view: i.e. including transformation and resulting effects such as impact on biodiversity, soil organic carbon, erosion, biotic production or ecological soil quality, etc. (Milà i Canals et al., 2007; Mattila et al., 2012). Despite the difficulty to find a starting point for transformation impacts, since in modern times used land is usually already transformed (Schmidt, 2008) assessing these types of impact is indispensable. This can also be seen in the amount of work done on the assessment of biodiversity, where Delbaere (2002) has identified over

600 impact indicators. Examples focus on threatened vascular plant species (Schmidt, 2008), red listed species (Kyläkorpi et al., 2005), threatened and endangered species (Singh et al., 2007), global species diversity (Jeanneret et al., 2006), etc.

Exergy consumption and entropy production

Whilst energy is based on the first law, exergy is based on the second law of thermodynamics, which states that all processes and activities generate entropy. Exergy thus quantifies (in J_{ex}) the quality of all types of mass and energy (Dewulf et al., 2000) and the amount of useful work that can be obtained from a system or resource when it is brought to equilibrium with the chosen surroundings, or "dead state" through reversible processes (Dewulf et al., 2008). As such materials are delivered by the ecosphere and their exergy content is degraded in the technosphere.

Similarly to CED, the Cumulative Exergy Consumption (CExC) can be defined as the sum of the exergy contained in all resources entering the supply chain of the selected product system. This resource indicator can be subdivided into 10 categories (fossil, nuclear, wind, solar, water, primary forest, biomass, water resources, metals and minerals), including both flows and stocks (Boesch et al., 2007).

This approach can be applied in LCA, as an Exergetic Life Cycle Assessment (ELCA) (Dewulf et al., 2008), which is elaborated by Dewulf et al. (2007) in the CEENE (Cumulative Exergy Extracted from the Natural Environment) methodology, where wind, solar, primary forest and biomass equivalents are elaborated as 'renewable resources' and 'Land occupation and Transformation'.

As the concept of exergy is a measure of 'usefulness', it has often been coupled to economics in two directions. Extended Exergy Accounting (EEA), gives an exergetic equivalent to a monetary cost. By doing so other production costs such as labour, capital and environmental remediation activities can be added to the exergy of the resources (fuel) needed. The conversion can be made by using a case-and time-dependent equivalence coefficient equal to the total influx of exergy in a given society in a certain year divided by corresponding monetary circulation (Sciubba and Ulgiati, 2005). Thermo economics does the opposite by giving monetary values to exergy streams by writing monetary balances on components or subsystems of a system (Dewulf et al., 2008).

Emergy

The starting principle of emergy is solar (equivalent) energy/exergy which creates, helps developing and maintains all biophysical processes on earth. The emergy concept draws up a balance of all solar energy/exergy flows which were necessary and are thus 'embodied' in the final product (in solar emJoules sej) (Bastianoni et al., 2007). Apart from the constant input of solar energy on earth, geothermal and tidal energy are the two other constant forms of energy, which can be rescaled to solar equivalent (Odum, 1988; Hau and Bakshi, 2004). Emergy is calculated based on the transformity concept, which is defined as "the Solar Emergy required to make 1 J of a service or product" (Odum, 1996). This approach is interesting for ecologists, as it includes the contribution of ecological processes to human welfare (Hau and Bakshi, 2004), and is furthermore comprehensive in communication. However, putting the system boundary to the sun, might be of less interest in industrial applications.

Relation to use of deposits

Methods based on deposits use an R factor, which is a function of natural reserves (R_i in kg) of the resources i combined with their rate of extraction (DR_i in kg per year). An example is the Abiotic Depletion Potential (ADP), which is used in the CML 2002 (Guinée et al., 2002) method, where the ADP_i is derived for each extraction of element i and is seen relative to the depletion of antimony as a reference (DR_{ref} and R_{ref} in Sb-eq).

$$ADP_i = \frac{\frac{DR_i}{(R_i)^2}}{\frac{DR_{ref}}{(R_{ref})^2}}$$

The Biotic Depletion Potential can be constructed in the same way, with another reference, e.g. the reserve of African elephants (Guinée et al., 2002).

3.1.2.2. Endpoint indicators

Future consequences of resource extractions

As it is often difficult to estimate the total reserves of a certain resource, an alternative approach can be chosen, by accounting for the consequences of future extractions. This can be elaborated in an environmental context by quantifying the energy needed to extract the resource as MJ per kg (Singh et al., 2007; Goedkoop and Spriensma, 2001) or economically as money per kg extracted (Goedkoop et al., 2009).

3.1.3. Technology indicators

Technological indicators are frequently used in industry and give specific information of the performance of the studied system within a specific chosen system boundary; often at the level of the gate to gate boundary. Examples are:

- Yield, dividing the mass of product by the mass of raw material needed
- Waste indicators, dividing the amount of waste by the amount of product
- Recyclability, being the quotient of the amount of recycled material and the sum of all materials used
- Renewability, quantifying the share of renewable materials in the total amount of raw materials
- Energy efficiency, giving an indication how much energy is used for the product, and how much is directed to waste

3.2. Assessment methodologies

The impact indicators explained in the previous section are used in many different assessment methodologies with different names. These methodologies can be distinguished mainly by choices in goal and scope (in the functional unit and the system boundary) and by choices in impact indicators.

3.2.1. Life Cycle Assessment

Life Cycle Assessment (LCA) is basically a framework focusing on a product or service within a cradle to gate or full cradle to grave production chain boundary and following the principles of the ISO 14040/44 (ISO, 2006) and ILCD (International Reference Life Cycle Data System (European Commission, JRC, IES, 2010)) guidelines. Whereas the framework is similar in most cases, a choice can be made between many impact assessment methodologies such as the Eco-indicator 99 (Goedkoop and Spriensma, 2001), Recipe 2008 (Goedkoop et al., 2009), USES-LCA (Huijbregts et al., 2000), LIME (Itsubo and Inaba, 2003), IMPACT 2002+ (Jolliet et al., 2003), EDIP2003 (Potting and Hauschild, 2005), LUCAS (Toffoletto et al., 2007), CML 2002 (Guinée et al., 2002), Carbon Footprint (European Commission, JRC, IES, 2007), etc. A strong communicative alternative is the Ecological Footprint (EF). It is originally developed by Wackernagel and Rees (1996) and defined as “the biologically productive land and water a population requires to produce the resources it consumes and to absorb part of the waste generated by fossil and nuclear fuel consumption”. The basic principle to convert these impacts to biologically productive land however, can be applied in any system boundary (JRC, 2011). For this purpose, the equivalence and yield factors used in the original Ecological Footprint method can be converted to characterization factors for application in the LCA framework (Huijbregts et al., 2008). This is also suggested by the Global Footprint Network (2009) who make a distinction between a process-based Life Cycle

Assessment (P-LCA) and Extended Input-Output LCA (EEIO-LCA). It is stated that a combination of the Ecological Footprint with another LCIA method can complement each other, since both approaches have specific attributes such as the characteristic to introduce the earth's capacity in the EF and the possibility of including end-of-life scenario's in LCA for example to account for land regeneration after use (Castellani and Sala, 2011). This methodology has been extended in the Sustainable Process Index (SPI) (Narodoslawsky and Krotscheck, 1995 and 2000; Dewulf and Van Langenhove, 2006). Similarly, a Water Footprint can be constructed for nations (Chapagain et al., 2006), or for use in LCA, accounting for blue water, i.e. ground and surface water, green water, i.e. rainwater stored as soil moisture, and grey water, i.e. water polluted during production (The Water Footprint Network, 2011). Unlike these more 'default' LCA methodologies, the ECEC/ECOLCA approach uses a hybrid approach with exergy or emergy as impact indicator (Ukidwe and Bakshi, 2007; Zhang et al., 2008b).

3.2.2. Gate to gate methodologies

If the assessment focuses on the gate to gate boundary of a production chain, the Green Degree (Zhang et al., 2008a) methodology, based on and thus very similar to, the WAR (WAste Reduction) algorithm (Young et al., 2000) can be used. A flow sheet of this methodology is presented in Figure II.6. The green degree of substances (GD_i^{su} in gd per kg substance) is calculated by:

$$GD_i^{su} = -\sum_j^9 (100\alpha_{i,j}\varphi_{ij}^N)$$

In which:

$$\varphi_{ij}^{N} = \frac{\varphi_{i,j}}{\varphi_{j}^{max}},\ \varphi_{j}^{max} = \max(\varphi_{i,j})$$

$\alpha_{i,j}$ is the weighting factor of substance i for impact category j

$\varphi_{i,j}$ is the environmental impact potential of substance i for the nine midpoint impact categories j

$\varphi_{i,j}^{N}$ is the relative impact potential obtained by normalizing $\varphi_{i,j}$ by φ_{j}^{max} which is the maximum value for category j among all the substances reported. The consequence is that for each impact category the indicator is normalized from 0 to 1. For mixtures, the Green Degree value of the substances is linearly added to each other.

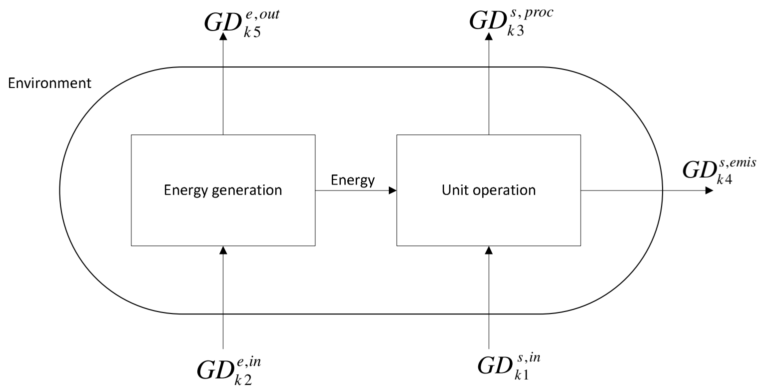

Figure II.6: The process flow sheet of the Green Degree methodology consisting of a unit operation and an energy generation process

The Green Degree value of the production of a unit (ΔGDu in gd/h) expresses the change that is caused by the material and energy conversions taking place in the unit. It therefore required that the green degree of a substance GDisu is multiplied with the respective quantity of substances entering and leaving the system per time (Figure II.6). The overall Green Degree of the unit is calculated by following equation:

$$\Delta GD^u = \sum_{k3} GD_{k3}^{s,proc} + \sum_{k4} GD_{k4}^{s,emis} + \sum_{k5} GD_{k5}^{e,out} - \sum_{k1} GD_{k1}^{s,in} - \sum_{k2} GD_{k2}^{e,in}$$

With $GD_{k1}^{s,in}$ the green degree value of the input streams of the unit operation. k1 Indicates the different input streams, such as raw materials, solvents, or catalysts. $GD_{k2}^{e,in}$ indicates the green degree value of an energy source fed into the energy generation system, such as natural gas, coal or oil. $GD_{k3}^{s,proc}$ represents the green degree value of the process streams exiting the unit, possibly to another unit, and $GD_{k4}^{s,emis}$ is the green degree value of the emissions or discharge streams from that unit directly to the environment. $GD_{k5}^{e,out}$ is the green degree value of emissions or discharge streams from the energy-generation system into the environment. It is stated that when assessing the production of a unit, a $\Delta GD^u > 0$ indicates that the unit operation is benign to the environment and $\Delta GD^u < 0$ indicates that the unit operation adds pollution to the environment.

A semi-quantitative methodology for process assessment in the early phase of development is presented by Biwer and Heinzle (Biwer and Heinzle, 2004), where substances get A/B/C scores in 14 impact categories, which can further be aggregated to two environmental factors.

3.2.3. Methodologies using technology indicators

Several methodologies focus on performance of a system by using technological indicators:

- Fijal (2007) proposes a methodology including a raw material unit index, an energy unit index, a waste generation unit index a production unit index and a packaging unit index.
- The Green Chemistry metrics (Anastas and Warner, 1998) have been extensively discussed by Lapkin and Constable (Lapkin and Constable, 2008) and have been elaborated in the EATOS (Environmental Assessment Tool for Organic Synthesis)

methodology (Eissen and Metzger, 2002). These indicators focus on mass and energy efficiency, emissions, the amount of redox reactions quantified as an hypsicity indicator and on economic cost associated with reactions.

- Dewulf and Van Langenhove (2005) combine exergy with principles of industrial ecology, to account for efficiency, re-use of materials, recoverability of waste materials, renewability and toxicity.
- Lou et al. (2004) use emergy to assess efficiency and emissions of a production plant.

3.2.3.1. Shortcut toolkits

If the means for the assessment are limited, several shortcut toolkits can be used to have a first indication of the sustainability of the functional unit, which is in this case often a single process or product, not considering for supporting processes or supply chains:

- The Green Alternatives Wizard uses a database to replace hazardous chemicals based on properties (Massachusetts Institute of Technology, 2006).
- A Solvent selection guide (Curzons et al., 1999) accounting for Environmental Health and Safety aspects of different solvents.
- The EcoScale (Van Aken et al., 2006) and the iSustain (Sopheon Corporation, 2011), semi-quantitative methodologies based on the twelve principles of green chemistry, using a system of scores or penalties for process parameters and technological properties of organic synthesis routes.
- The PBT profiler, assessing persistence, bioaccumulation and aquatic toxicity based on chemical structure (USEPA, 2011).

3.3. Economic impact assessment

Economic performance is the main driver of the industrial system. It will probably even be *the* decisive factor for the inclusion of biomass alternatives in the production chain. Nevertheless, the assessment of economics is rather straightforward in comparison to environmental and social assessment, as only one type of flow, namely the monetary one, has to be assessed. As such, the discussion of midpoint and endpoint indicators and aggregation is not necessary.

A very determining factor for the result of the assessment however, is selecting a relevant cost breakdown structure to decide which direct and indirect costs and benefits should be included. Here, two main approaches are distinguished:

- Using a company/user perspective. Kawauchi and Rausand (Kawauchi and Rausand, 1999) define three cost categories for the oil and chemical process industry:

  $$LCC = LAC + LOC + LLC$$

  With LAC the life acquisition cost (for example: equipment purchase, installation cost, commissioning cost, insurance spares, reinvestment cost, design and administration cost), LOC the life ownership cost (for example: man-hour cost, spare parts consumption cost, logistics support cost, energy consumption cost, insurance cost), and LLC the life loss cost (for example: cost of deferred production, hazard cost, warranty cost, loss of image and prestige cost). Utne (2009) goes further and defines costs as:

  $$LCC = CAPEX + OPEX + RISKEX + ENVEX + DISPEX$$

Where CAPEX + OPEX are the capital (production) and operational cost respectively. RISKEX are the costs caused by accidents and fatalities, ENVEX are the environmental expenditures, mainly based on eco-taxes for climate change and acidification, whilst DISPEX are the costs for disposal.

- Using a societal perspective. This approach focuses on top of the previous cost categories on the indirect or 'external' costs. These externalities, arise when the social or economic activities of one group of persons have an impact on another group and when that impact is not fully accounted, or compensated for, by the first group (ExternE, 2011). Efforts to quantify these costs, mainly by using the Willingness To Pay (WTP) and Willingness to Accept (WTA) principles, are made by the Environmental Priority Strategy (EPS) (Steen, 1999), the ExternE projects (ExternE, 2011) and the NEEDS project (NEEDS, 2011), the latter two available in the software tool EcoSense (Stuttgart University, 2011). Including these external costs however, might not be an appropriate approach in sustainability assessments, since double counting issues with the environmental and social assessment might occur. Furthermore, within economic assessment, several eco-taxes already include some external costs (Pearce and Turner, 1990; Hanley, 1997).

Determining the 'value' of money is another point influencing economic assessments. First, the value of the benefits should be considered, as indirect, revenue-enhancing effects, can be generated next to the direct profit (Wynstra and Hurkens, 2005). Second, the value of money changes in time due to market mechanisms. The time dependency of the value of money can be included by discounting, based on changes in inflation, cost of capital, investment opportunities and personal consumption preferences (Gluch and Baumann, 2004). This is mostly captured with the Net Present Value principle, calculated by:

$$NPV = \sum_{t=0}^{t=n} \frac{C_t}{(1+r)^t}$$

With n the number of years of analysis, r the discount or interest rate and C_t the estimated costs in year t.

3.3.1. Economic impact indicators

The result of the cost breakdown should result in a final indicator which aggregates the different values obtained during the assessment and at the same time cover the discounting issue. In this context, Huppes et al. (Huppes et al., 2004) suggest 7 different indicators:

- The NPV
- The Average Yearly Cost (AYC), which is the sum of all yearly costs divided by the functional running time. This is called the Steady State Cost (SSC) when the functional time is infinite.
- The Annuity factor (A), which accounts for the regularly paid constant amount over the functional lifetime (fn). An eternal annuity factor has an infinite functional lifetime.

$$A = NPV \times \frac{r}{1-(1+r)^{-fn}}$$

- The Internal Rate of Return (IRR) is the discount rate (r) which makes the NPV equal to 0, and thus makes the present value of benefits equal to the present value of costs.

- Profit is the benefits minus the costs.
- Pay-back time is the measure of the time required to return the initial investment and can thus be calculated by dividing the initial investment costs with the yearly net benefits.
- Benefit-Cost Ratio (BCR) is the ratio of the present value of the future benefits to the present value of the future costs, discounted at the same rate.

3.4. Economic Assessment methodologies

Due to the relevance of money, economic assessment has a widespread use. Therefore many different names have been assigned to this type of study, mostly depending on the sector where it is applied. Originating from the building sector, Whole Life Costs (WLC) and Life Cycle Costing (LCC), are used, where WLC is seen broader than LCC, by including all indirect, tangible and intangible social, environmental and business costs, and the benefits from consumption and production (ISO, 2008). The Center for Waste Reduction Technologies (CWRT) introduced Total Cost Assessment (TCA) to include environmental and health risks and costs (AIChE, CWRT 1999). Similarly, Total, Full or True Cost Accounting or Full Cost Pricing, Total Cost of Ownership, Cost Effectiveness Analysis (CEA) or Cost Benefit Analysis can be used. However, it can be questioned what the difference between these methodologies really is. It is indeed stated that Life Cycle Costing is the theory behind all economic assessment methodologies, but depending on the perspective and application, choices are being made concerning the costs to be included (which and whose) and the time frame of the assessment (Huppes et al., 2004).

3.5. Social impact assessment

The third dimension of sustainable development differs quite significantly from environmental and economic assessments, as there are no ‘flows’ going in and out a system, complicating the boundary, inventory and impact assessment. At the same time, social issues are often hardly distinguishable from their economic context. This is why some sources such as Kruse et al. (Kruse et al., 2009) rather mention socio-economic assessment. Aspects such as fair trade have been implemented for a longer time, but methodological developments concerning a quantified social impact assessment, compatible with environmental and economic impact assessments in industry, are still in a state of infancy and research has not advanced significantly last decades (Hunkeler and Rebitzer, 2005). This is why the UNEP SETAC Life Cycle Initiative started a working group and published its report “Guidelines for Social Life Cycle Assessment of Products” in 2009 (UNEP SETAC LCI, 2009). The merit of this report is not only solving some of the obstacles, but it also boosted the debate and research.

In comparison to environmental assessment, the natural link between the physical input/output and an impact such as the change in environment is absent (Dreyer et al., 2006). Collecting social data is therefore not straightforward, and could result in a never ending data collection (Nazarkina and Le Bocq, 2006). It is stated that the causal link of social issues is situated at a company/stakeholder level, and not at process level (Dreyer et al., 2006; Nazarkina and Le Bocq, 2006; Spillemaeckers et al., 2004). Furthermore, social data is difficult to quantify, and sometimes a more qualitative or semi-quantitative approach might be preferred. In this context, Swarr (Swarr, 2009) quotes Einstein: “Not everything that can be counted counts, and not everything that counts can be counted”. However, this is not necessarily a problem as Jørgensen et al. (Jørgensen et al., 2009) questioned several large Danish companies and concluded that a full list of quantitative life cycle indicators for the social aspects is not essential. Industry just wants to take well informed decisions, so it might be sufficient to simply define a process to assess the social impact in a reliable way (Swarr, 2009), rather than to construct a complete quantitative methodology.

3.5.1. Social impact indicators

The UNEP SETAC LCI selected a list of midpoint and endpoint impact categories (Table II.2) based on the definition: “social impacts are consequences of positive or negative pressures on social endpoints (i.e. well-being of stakeholders)”. These categories should then be assessed by indicators which are appropriate and fitting in the study. However, the midpoint – endpoint modeling might become very difficult. Further work on this topic is thus required, optionally using work done by other assessment frameworks such as GRI (Global Reporting Initiative) indicators, IChemE Sustainability metrics, etc. A suggestion for a generic methodology could be to include an obligatory and a mandatory list of indicators (Dreyer et al., 2006; Kruse et al., 2009).

Table II.2: The structure of the social assessment methodology developed by the UNEP SETAC LCI (2009) with stakeholder categories and impact indicators at the midpoint and endpoint level

Stakeholder categories	Impact categories	
	midpoint	endpoint
Workers/employees	Freedom of association and collective bargaining, child labour, fair salary, working hours, forced labour, equal opportunities/discrimination, health and safety, social benefits/social security	
Consumer	Health and safety, feedback mechanism, consumer privacy, transparency, end of life responsibility	Human rights Working conditions
Society (national and global)	Public commitments to sustainability issues, contribution to economic development, prevention and mitigation of armed conflicts, technology development, corruption	Health and safety Cultural heritage Governance
Local Community	Access to material and immaterial resources, delocalization and migration, cultural heritage, safe and healthy living conditions, respect of indigenous rights, community engagement, local employment, secure living conditions	Socio-economic repercussions
Value chain actors	Fair competition, promoting social responsibility, supplier relationships, respects of IP rights	

As social impacts are site specific, Dreyer et al. (2006) consider unlimited generic data unacceptable, regardless the high data demand. Therefore it is suggested that site specific data from the most relevant processes should be gathered. For example impacts that are not under the assessment executer's influence could then be handled with generic data. A hotspot approach is thus suggested to identify unit operations located in a region where problems risks or opportunities occur, where in these hotspots site specific data is assessed (UNEP SETAC LCI, 2009; Hauschild et al., 2008). Furthermore, a hybrid approach can be used, where macro data, for example social data coupled to GNP (Gross National Product)/GDP (Gross Domestic Product), can be coupled to micro assessments (Norris, 2006; Hutchins and Sutherland, 2008; UN, 2005).

3.6. Social impact assessment methodologies

Parallel to the construction of an impact assessment structure, several authors have tried to develop quantitative methodologies. Amongst others:

- A societal LCA is developed by Hunkeler (2006), which transforms the indicator 'working hours' to the ability to acquire four regionalized societal necessities: housing, health care, education and necessities.
- A Working Environment (WE) LCA can be used to grasp the direct impact, as Lost Work Days (LWD), of health and safety in the working environment (Schmidt et al., 2004; Kim and Hur, 2009).
- The Gabi methodology suggests a Qualified Working Time (QWT) approach based on working time and qualification profile. This can be extended with a health and safety aspect and humanity of working conditions (Back et al., 2009; Makishi et al., 2006).
- Weidema (2006) focuses on one endpoint indicator: the Quality Adjusted Life Years (QALY) concept, which is the elaborated version of the DALY indicator, including health-related quality of life. Six damage categories are addressed: life and longevity, health, autonomy, safety security and tranquility, equal opportunities and participation of influence. It is furthermore stated that this indicator can be linked to an overall endpoint indicator of human wellbeing.
- Labuschange and Brent (Labuschagne and Brent, 2006) construct a Social Impact Indicator (SII) based on 18 impact indicators in 4 resource groups (internal human resources, external population, stakeholder participation and macro-social performance).

3.7. Multi-dimensional assessment

According to Elkington's three dimensions of sustainability, a win-win-win situation should be obtained. Therefore, the assessment should in the best case focus on the people, planet and profit related issues similarly. Originally most research was aimed at the concept of eco-efficiency and dematerialization or decoupling economic growth from environmental impact (WBCSD, 2005), but nowadays, the inclusion of social issues is high at the agenda.

It is generally assumed that the life cycle approach will take an important role in sustainability assessment due to its holistic viewpoint (Klöpffer, 2003 and 2005), which seems essential to grasp the broad concept of sustainable development. Indeed, a good evolution in one part of the life cycle, can still have negative overall consequences. As such, Klöpffer (2008) proposes two possibilities for Life Cycle Sustainability Assessment (LCSA):

- $LCSA = LCA + LCC + SLCA$
- $LCSA = new\ LCA$

Whereas the first option is most chosen, the second option would mean that a completely new methodology should be constructed. In this context, LCSA can also be seen as a framework of different approaches with life cycle thinking as a common basis (Guinée et al., 2011). The assessment should in this case include the three dimensions of sustainability and it should not be considered exclusively as a micro scale assessment of products or services. The scope of the assessment should be elaborated from micro to meso (product groups) to economy-wide. Future research is necessary on posing exact research questions that have to be answered by a full sustainability assessment and on the additionality and overlap between different available methodologies at different levels.

3.8. Sustainability assessment methodologies

Whereas many issues are unresolved for a full sustainability assessment, several methodologies are already available. The most known example is the SEEbalance tool (Saling, 2010) developed by BASF, building on their previously developed eco-efficiency methodology (Saling et al., 2002; Kicherer et al., 2007; BASF, 2011). The environmental impact assessment consists out of 11 midpoint categories: GWP, ODP, AP, POCP, solid wastes, water emissions, energy consumption, raw material consumption, land use, toxicity potential and a risk (of accidents) potential. This is combined with an economic LCC value and social indicators in five stakeholder groups: employees, consumer, local and national community, future generations and international community. Afterwards, an external normalization is executed based on national statistics such as the GDP or impact per GDP whilst weights are determined by so-called relevance and societal factors. Doing so allows this methodology to have a communicative visualization; the so-called SEE-cube.

Other methodologies using the same strategy are the BEES (Building for Environmental and Economic Sustainability) tool (Lippiatt, 1999) using MCDA principles (Lippiatt and Boyles, 2001) and the Green Productivity methodology (Hur et al., 2004) accounting for eco-efficiency, whilst Öko-Institut has developed a PROduct Sustainability Assessment (PROSA) framework for sustainability assessment (Öko-Institut, 2007). The latter proposes a 'usual' LCSA, such as the SEEbalance, but gives more attention to a broader analysis of the product system in the market to allow a better scoping of the study. Furthermore, it has the unique feature that it also includes a fourth dimension of sustainability, i.e. utility, based on three perspectives:

- Practical utility from the perspective of the users/consumers (durability, performance, reliability, …)

- Symbolic utility accounting for the perception of stakeholders (prestige, enjoyment, …)
- Societal utility or "public value" which focuses on the essential contribution of the product or service to societal objectives (basic needs, education, poverty reduction, …)

A simpler and user-friendly LCSA is presented in the Life cycle INdeX (LINX) (Khan et al., 2004), which accounts for 4 impact categories: environment and resources (11 indicators), cost (3 indicators), technology (4 indicators) and socio-political factors (3 indicators). Each of these parameters is assessed with the use of a specific monograph where the value of the calculated parameter is directly linked to a penalty score, which eases the aggregation and interpretation step.

Other methodologies assess sustainability or eco-efficiency on a non-life cycle basis. Examples are Sustain-Pro (Carvalho et al., 2008), which uses the WAR algorithm and indicators from the IChemE metrics list, added with safety indices and seven own developed indicators and the Quotes for environmentally WEighted RecyclabiliTY and Eco-Efficiency (QWERTY/EE) methodology (Huisman et al., 2003), which is originally designed to assess the eco-efficiency of waste treatment and recycling options for electronic products.

4. Interpretation

The interpretation phase of the results of a sustainability assessment is of essential importance. It requires knowledge of the assessment framework with the choices and assumptions that are made in the study and the used indicators and possible aggregation steps. Only in this case, well founded conclusions can be made at the end of the study. Determining the uncertainty of the final result can be a helping tool for the interpretation. According to

Huijbregts (2011) three types of uncertainty can be determined, where only the last one is often quantified in assessment studies:

- Decision rule uncertainty includes the methodological choices that are made.
- Model uncertainty is caused by limitations in knowledge or techniques to quantify the impacts (e.g. endpoint cause-effect models, characterization factors, …)
- Statistical uncertainty is mainly related to uncertainty in the data inventory and is the uncertainty which is currently most analyzed by using a semi-quantitative pedigree matrix base on scores in five criteria: reliability, completeness, temporal differences, geographical differences and further technological differences (Lundie et al., 2007).

5. Conclusions

According to the Brundtland the abilities of future generations should not be compromised. Therefore renewable resources should be sought instead of building welfare on depleting non-renewables. Yet, it is clear that renewable resources also have drawbacks and that different applications and processing routes have to be assessed to enhance sustainable development in industrial and societal progress.

As the concept of sustainable development originates mainly from environmental concern, most efforts have been made to assess environmental impacts. This also seems the most obvious dimension to make comparisons between fossil-based and bio-based products, since the aimed change of resources is mainly triggered by environmental concerns such as resource depletion and climate change. Furthermore, the life cycle perspective is identified as a useful framework to assess full supply chains and trade-offs between different processes and impacts. Nevertheless, while the relations with the ecosphere are relatively well characterized, performing an environmental sustainability assessment is still challenging and several methodological aspects such as the system boundary definition, allocation, inventory collection and impact assessment still require improvement. Whereas the economic assessment is quite well established, the social dimension is elaborated, but still in a state of infancy for quantitative sustainability assessment as it faces essential methodological challenges such as identifying the cause-effect link between a technical system and the sociosphere, which currently impedes its practical implementation.

CHAPTER III: Environmental sustainability assessment of biorefineries

1. The resource footprint of biobased products, a key issue in the sustainable development of biorefineries

Redrafted from:

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1. Introduction

The valorization of fossil resources was probably one of the main catalysts for welfare generation and human development over the last decades. No other type of resource has changed the world so fast and to that extent; it has become a vital part of industry, agriculture, transport and society as a whole (Youngquist, 1999). But as this source of hydrocarbons was formed by the long term conversion of ancient biogenic material, their stock is not endless and is depleting due to disproportional exploitation rates, with price increase as a consequence. This together with climate change forces society in the direction of renewable resources, which can offer similar functionalities as fossils. Different alternatives are available, such as using the quasi infinite energy from the sun, which can be used in a direct way, e.g. photovoltaics (PV) or concentrated solar power, or indirectly, e.g. relying on photosynthesis. A first judgment would favor the first option, since the solar light capture efficiency of photosynthesis is limited and lower than for direct capture (Bolton and Hall, 1991; FAO, 1997; Green et al., 2007). However, to date the applications of direct solar capture are limited to energy generation, whilst on the other hand, biomass obtained from photosynthesis is a carbon source that can serve as food, feed, chemical, material, textile, fuel *and* energy resource. This offers the possibility to create a broad and valuable product mix from the starting resource. Due to this multifunctionality, the valorization possibilities in a so-called biorefinery are even bigger than in fossil refineries. Whereas such a diversity of options allows a large range of configurations they also imply environmental consequences such as arable land use and impact from agriculture and processing in general. Decisions taken regarding the valorization of biomass should therefore be well-thought-out and based on sound assessments to achieve an optimal sustainable development in the post fossil era. Two points seem to be critical for the sustainability of the biorefinery sector:

- Serve market demands
- An ecologically sound production chain

1.1. Serve market demands

Society has several demands of which some rely on depleting fossils and some on biomass and hence land use. In the future, slowly but surely there will be a shift to the utilization of renewable resources for many services. However, because of limited arable land availability and the limitation in photosynthesis efficiency, it is uncertain and even quite unlikely that biomass will be able to cover all these demands fully (IEA Bioenergy, 2007; Fischer et al., 2007; Ponton, 2009). Therefore a maximal valorization of each quantity of biomass should be pursued. Lessons can be learned from fossils: crude oil consists of different types of hydrocarbons, which are fractionated and valorized in oil refineries. Similarly, biomass consists out of different types of molecules, ranging from the plant reserves, mainly starches and lipids, to plant structure, mainly lignocelluloses, to proteins and microcomponents such as vitamins and pigments. Valorizing these types of molecules for specific purposes is called 'biomass cascade utilization', and is aimed at maximizing the socio-economic benefits per quantity of biomass (Haberl and Geissler, 2000).

Figure III.1.1 shows the cascade scheme of biomass valorization. After cultivation, biomass fresh matter is obtained. The different types of molecules in the dry matter can be separated if necessary and used for their specific purpose. This figure shows clearly that all molecules can be used for three different levels: food and feed, biobased products and bioenergy. This means that no biomass molecules can be considered as waste. From an economic perspective producing according to this cascading system is a major opportunity for biorefineries. For example a company specialized in processing wheat gluten to thermosetting biomaterial can valorize the other parts of the plants by making ethanol from the sugars for the fuel sector and animal feed from the DDGS (Dried Distillers Grains with Solubles) to maximize the economic profit (Raquez et al., 2010).

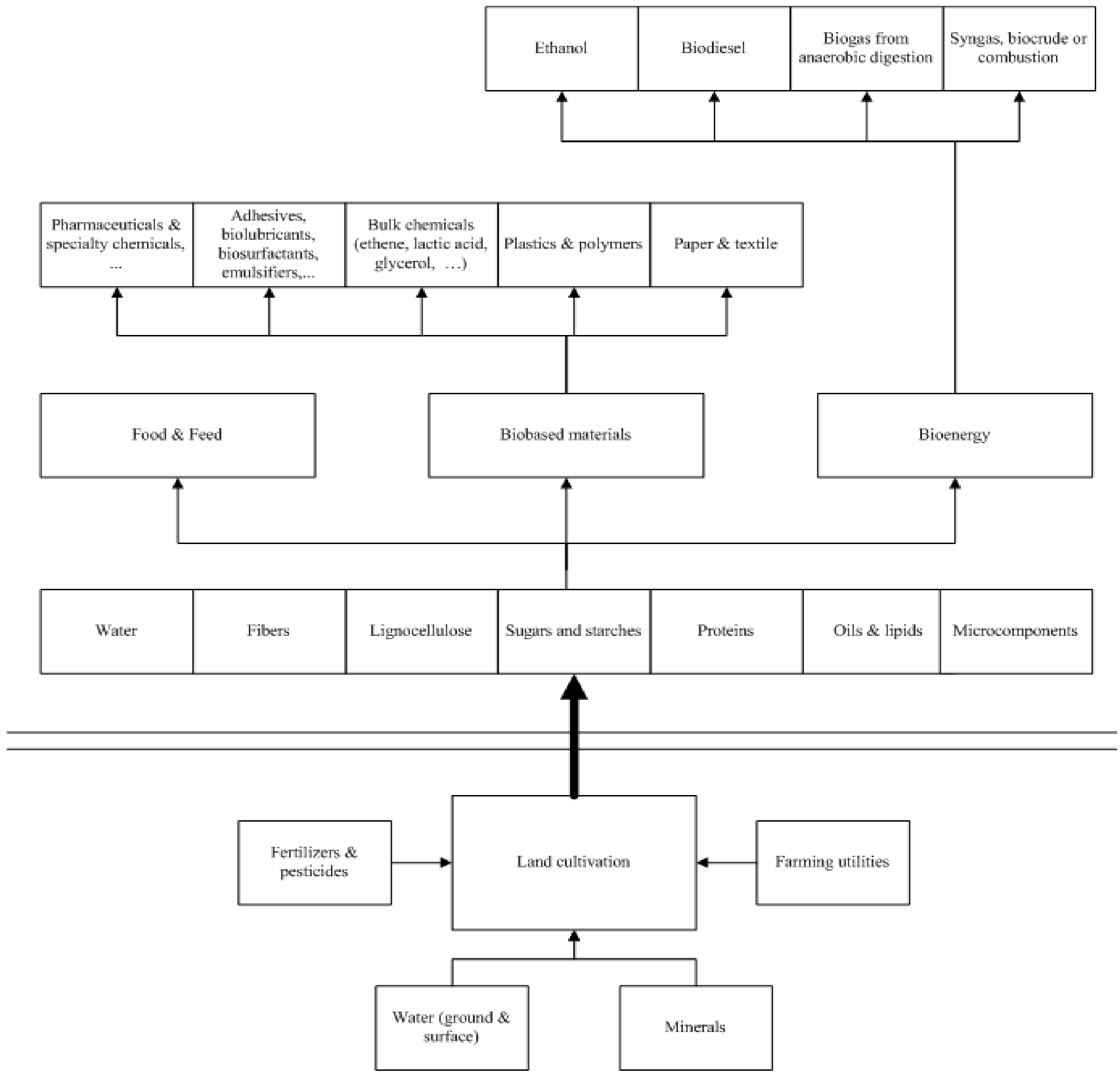

Figure III.1.1: The biomass cascading scheme. Three levels of products can be identified: food and feed, biobased materials and bioenergy. All molecules from the feedstock can be valorized for different applications inducing economic opportunities on the one hand, but creating an extra demand on the other hand. Obtaining biomass depends thus on the fragile basis of this scheme, i.e. the resource input from nature and technosphere during cultivation.

1.2. An ecologically sound production chain

At the other side of the coin however, Figure III.1.1 already illustrates the bottleneck of the bio-based economy, namely that these economic opportunities all rest on the shoulders of the cultivation of biomass. Whilst fossils originate from ancient and converted biogenic material, current biomass production requires the cultivation of a certain amount of surface area and needs inputs for growth and harvest. So whilst the limiting factor for fossils is the historically built up stock of hydrocarbons and the price it costs to obtain the next quantity of resources, the limiting factor for a large scale implementation of biomass in our economy is the physical chemical "fuel and feedstock" taken away from the natural environment for production and consumption. Such a resource footprint concerns not only consumption of fossils and arable land use and transformation, but also other natural resource stocks and flows that come from the natural environment into the technosphere such as minerals, metals, water, nuclear, renewable and atmospheric resources (Dewulf et al., 2007). This includes also the effort of the natural environment for the use of utilities such as fertilizer and pesticide, diesel for machines, water and minerals from the soil, etc. (Cherubini, 2010). Even agricultural residues or lignocelluloses, which are often seen as waste, require a certain input of natural resources, since they originally depend on agricultural processes where the agricultural system has 'invested' resources in creating the molecules. This means that the production chain of biomass is more extensive than their fossil equivalent.

Several studies pinpoint that the agricultural phase is often the main contributor to the environmental impact of the production chain of biobased products (Zah et al., 2007; Farrell, 2006). Therefore it is essential that this step is executed in a sustainable way. However, since the demand for biofeedstock will rise due to the depletion of fossils and since the arable land is limited, this implies that higher agricultural yields will be pursued. A significant yield increase per hectare is indeed expected, however, these innovations are often not focused on the simultaneous acceleration of yield and environmental protection of the natural resources (Cassman and Liska, 2007). Whilst on the one hand the extra demand can be beneficial for agricultural development, on the other hand the risk exists that a blind striving for higher yields will cause severe damage to the natural environment which would have a reverse effect on the longer term (Matson et al., 1997). For example the use of field crop residues is an extra source of useful biomass, but it is also an important precursor for soil erosion and nutrient depletion, which could induce the use of additional inputs during cultivation. Using this part of biomass, which is often seen as 'a sustainable resource' might thus actually turn out to be worse on the longer term (Reijnders, 2006).

Summarizing the previous discussion, the transition to a 'renewable' bio-based economy, offers several opportunities, for example replacing services that were previously fulfilled by fossils, but faces the main bottleneck that inputs, including land, are required during cultivation. So whilst the current industrial system exists mainly of dedicated food, dedicated bioenergy and petrochemical industry, these three sectors should think how obtained feedstock can be valorized to the fullest to obtain the lowest resource footprint per output product. In this chapter we aim to show that the cascade use of biomass in an 'integrated biorefinery' is a sound strategy to achieve a high valorization efficiency of the biobased molecules and that the integration of these sectors can indeed serve as a solution to replace fossil services. Furthermore a resource footprint can be obtained which quantifies how much additional basic inputs during cultivation and processing are necessary to replace a certain amount of fossils. This allows to offer a sound comparison between different options in the biosector and to calculate the 'environmental cost' of for example striving for higher yields. As a demonstration, a case study is executed to assess the decision of a food and feed company to integrate fuel bioethanol in its production. It focuses on a Belgian processing facility where wheat, sugar and flour are used as starting material and which initially produced starches, sugars, gluten and animal feed. To cope with the growing demand for renewable energy, a part of the wet sugar-starch streams that were previously dried to produce animal feed, is now fermented to fuel bioethanol.

2. Method

The assessed production plant consists of dry and wet milling, different separation and drying steps, and the processing of the obtained streams to salable products (868 kton in 2009). Also included is the on-site energy supply of a CHP working on natural gas, a wastewater treatment plant with biogas generation in the anaerobic treatment and all internal transport. The study is carried out before, and after the switchover to bioethanol production, where the main difference is a new ethanol fermentation and purifying section, and a decrease in animal feed production requirements.

Thermodynamics are used as a basis for the assessment in order to quantify the resource related issues in this sector in a scientifically sound manner. The first thermodynamic law states that energy is conserved, which would mean that there is no resource problem, whilst the second law states that every process generates entropy, and thus the 'quality' of the energy decreases in every step. The latter is quantified by the concept of exergy, which represents the maximum amount of useful work that can be obtained from a resource when it is brought to equilibrium with the reference environment (Dewulf et al., 2008). This is very relevant as parameter in the biorefinery sector as it can be used to quantify both:

- the efficiency of the cascade use of the raw material in the biorefinery, and
- the amount and origin of inputs necessary from nature to obtain a certain product mix from biofeedstock, i.e. the resource footprint

The first point is analyzed by an Exergy Flow Analysis (ExFA) in the gate-to-gate boundary of the processing plant. The quality decrease of the main feedstock and the relative amount of energy and utility resources used per useful output product can be quantified by calculating the rational thermodynamic efficiency of each process, with the Rational Exergetic Efficiency (Ψ):

$$\Psi = \frac{\sum \text{Exergy content of the useful outputs}}{\sum \text{Exergy content of the inputs}}$$

The exergy is quantified based on chemical and physical properties collected at the production plant by means of data available in literature, the group contribution method, the macro nutrient method, and data from Gibbs energy of formation.

Concerning the second point, life cycle assessment (LCA) is used to grasp the impact of the production chain on the natural environment. The different steps of the LCA are executed according to the recommendations of the ISO 14040/44 standards. The functional unit is processing 1 ton of incoming biofeedstock (wheat, sugar and flour) with the Belgian processing facility as foreground system, whilst the system boundary is the full cradle to gate out production. A physical allocation procedure is chosen, based on the Exergy Flow Analysis. This means that the incoming and outgoing flows per process are quantified and that the related impacts are allocated proportionally to their exergy content. The data inventory of the system is collected at the facility of Syral Aalst, Belgium. A year average of 2009 is made, based on analytical measurements, company reports and completed with information received from process engineers of the production plant. As such, an accurate data inventory is constructed, which reduces the uncertainty of the final results as much as possible. Whilst efforts are made to obtain a reliable data set, uncertainty of the results is not quantified. However this would be an interesting added value, current calculation techniques still face several limitations (Finnveden et al., 2009).

Background data for the supply chain of the facility, including transport per ‘tkm’, are taken from the ecoinvent database. Table III.1.1 lists the most dominant ecoinvent processes used to model the life cycle inventory of the incoming resources. On top of this, 5 types of transport and 56 types of chemicals and utilities are used. The natural gas used in the CHP is allocated to the produced electricity, the used steam and the used heat of the flue gas, based on their exergy content.

Table III.1.1: List of the most dominant resources processed in the studied biorefinery and the ecoinvent processes which are used to model the data inventory

Material or energy carrier (+origin)	Ecoinvent process
Wheat (France)	Wheat grains conventional, Barrois, at farm (FR)
Flour (France)	Maize starch, at plant (DE)
Potato starch (France)	Potato starch, at plant (DE)
Sugars (France)	Sugar, from sugar beet, at sugar refinery (CH)
Natural gas burned in CHP (Belgium)	Natural gas, burned in cogen 1MWe lean burn (CH)

To quantify the resources necessary in the life cycle of the biofeedstock and the final products, the Cumulative Exergy Extraction from the Natural Environment (CEENE) methodology has been chosen (Dewulf et al., 2007). This methodology is a resource footprint methodology which traces back the origin of the inputs necessary to obtain the final product(s) and the related amount of exergy deprived from the environment. Eight subcategories are used: renewable resources (excl. biomass), fossils, nuclear energy, metal ores, minerals, water resources, land resources (incl. biomass), and atmospheric resources. This is different from many case studies which are executed in the sector of biorefineries and bioenergy which focus only on the carbon footprint, or the net energy balance, whilst also the other categories, and especially the inputs during cultivation such as land occupation and transformation and water use should not be forgotten. Another option often chosen is the fossil resources saved per hectare, an indicator which is relatively sound in the sector of bioenergy, but which is less suitable for other sectors such as the food industry.

Finally a scenario assessment is executed to analyze the decision to change the services delivered by the wet sugar-starch streams and the related consequences of the decision in the foreground system on the background system. Producing ethanol from the streams saves a certain amount of fossil fuel, but also might displace the animal feed production to another facility. A comparison between the two scenarios is made for the eight resource impact categories of the CEENE methodology, with data 'after transition' taken from the current production facility (company A) and data 'before transition' taken from data files from the same company (company A') supplemented with ecoinvent data for fossil fuel production (company B).

3. Results and discussion

3.1. Cascade valorization efficiency

A thorough analysis has been made of the different steps in the production facility before and after the integration of fuel ethanol production. Figure III.1.2 shows the exergy flows through the plant in the two situations. In both cases three major biomass streams; wheat, flour and sugars are processed to specialty sugars, starches, gluten and animal feed, whilst in the newer situation an additional fermentation section is added. The different parts of the wheat plant are 'refined', allowing cascade processing to serve different markets: firstly the wheat brans and germs are separated to serve as animal feed and the gluten proteins are separated in a wet milling process to serve as an additive in the food industry. Afterwards the starches and sugars fractions are valorized for the food industry. In the new situation the wet sugar-starch streams that were previously dried and used as animal feed are now first fermented to ethanol, whilst the DDGS is processed further to animal feed. Table III.1.2 shows the exergy content of the categorized inputs and the sold outputs. Furthermore it summarizes the exergy flows going in and out the studied system after transition relative to 1 ton incoming biomass. The complete plant was and is very efficient: in the situation after transition, the Rational Exergetic Efficiency of the complete facility is 81.1%, whilst it reached 81.5% in the situation before transition. The most prominent, but inevitable losses are located at the energy generation processes: the CHP (Ψ = 58%) and the steam boiler working on biogas from the anaerobic wastewater treatment (Ψ = 23%). On a mass basis almost no incoming biogenic material is wasted; only in the ethanol fermentation step, 17% of carbon of fermented biomass is wasted through CO_2 production, however the related exergy loss is small (1%), due to the fact that the exergy content of ethanol is higher per mass unit and the fact that the exergy content of carbon dioxide is low. An additional factor causing the small change in efficiency between the situations is the fact that a unit ethanol requires relatively more utilities in comparison to a unit of animal feed. The efficiency in both situations is thus very similar, since the biomass was previously used as animal feed, however, the newer configuration offers the possibility to be flexible and to deliver a range of services to different markets, including previously fossil based services without losing efficiency. For example, gluten and cellulosic materials can be used as food or feed but can also be used as a resource in the plastic industry. Similarly, the bioethanol can serve as fuel or as a basic building block in the petrochemical industry. In all these cases it is essential that the biobased product is used as efficient as possible after its production as well. For example the combustion of bioethanol as a transport fuel can induce an efficiency loss that cancels the higher upstream efficiency and therefore makes alternatives such as bio-electricity more attractive (Campbell et al., 2009).

Table III.1.2: The categorized inputs and outputs of the factory after transition relative to 1 ton incoming biomass (wheat, sugars and flour), with exergy contents of the incoming and outgoing products, their relative share of the total and their total quantity. The CEENE values of the inputs are indicated and allocated to the outputs, first as absolute value and secondly relative per kg product. Mass units are on a wet basis, i.e. salable products.

INPUT	Exergy content (MJ/kg input)	MJ CEENE/ kg input	INPUT	INPUT UNIT	Total exergy at gate in (GJ)	% of total exergy input at plant	Total CEENE input (GJ)
Wheat	16.3	107.2	568.7	kg	9.3	48.4%	61.0
External flour	16.7	131.9	33.4	kg	0.6	2.9%	4.4
Sugars	13.4	71.7	397.9	kg	5.3	27.9%	28.5
Chemicals	6.8	32.1	39.3	kg	0.3	1.4%	1.3
Nat. gas	41.3- 49.5	65.0	80.5	kg	3.7	19.4%	5.2
Transport	n.a.	n.a.	322.6	ton.km	n.a.	n.a.	0.5
				Total	19.1	100%	100.9

OUTPUT	Exergy content (MJ/kg output)	MJ CEENE/ kg output	OUTPUT	OUTPUT UNIT	Total exergy at gate out (GJ)	% of total useful exergy output	Total CEENE output (GJ)
Dried starch	16.4	134.0	98.0	kg	1.6	10.4%	13.1
Gluten	23.4	170.1	38.0	kg	0.9	5.7%	6.5
Animal Feed	17.3	126.3	180.0	kg	3.1	20.2%	22.7
Sugar	12.7	78.1	622.3	kg	7.9	51.1%	48.6
Ethanol	29.5	216.5	37.6	kg	1.1	7.1%	8.1
Electricity to net	n.a.	n.a.	0.2	MWh	0.8	5.5%	1.9
				Total	15.5	100%	100.9

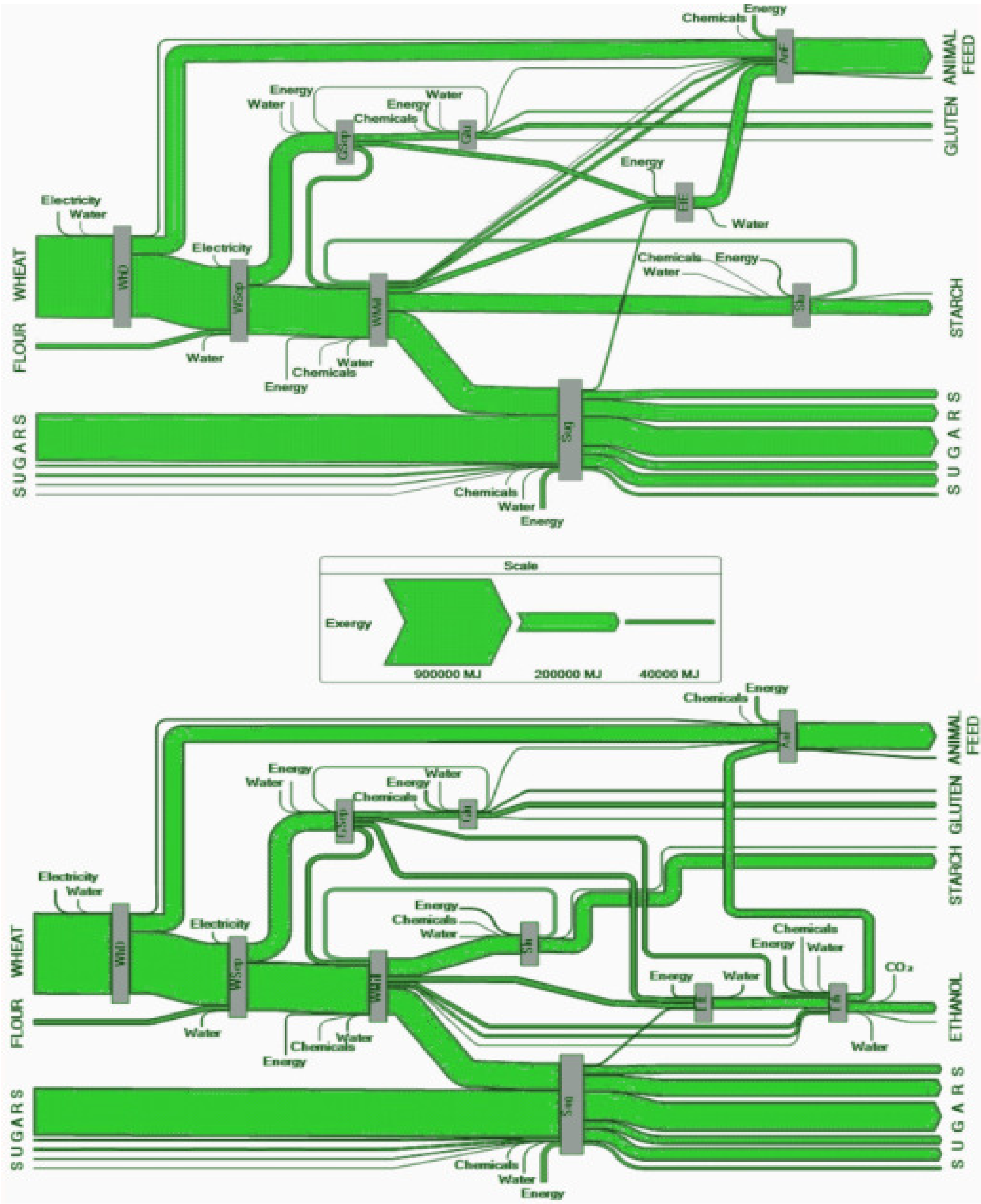

Figure III.1.2: Exergy flow diagrams (Sankey) on an hour basis of the main processing steps in the biorefinery before and after fuel bioethanol integration. The thickness of the flows indicates the relative amount of exergy. The different process steps: WhD: Dry wheat processing, WSep: Wet separation, GSep: Gluten separation, WMill: Wet milling, Slu: Slurry processing, Glu: Gluten processing, AnF: Animal feed production, EfE: Effluent evaporation, Eth: Ethanol production, Sug: Sugar refining. Energy originates

from the CHP and biogas steam boiler; wastewater is treated in a WWTP. The latter ones are not visualized for the sake of simplicity.

3.2. Life Cycle resource use

Whilst the processing plant itself is rather efficient, the steps necessary to produce the inputs of the factory from elementary flows from nature contribute to additional resource quality losses in both the agricultural phase of biobased resources and in the industrial system of the utilities. Table III.1.2 summarizes the origin of the environmental impact according to the CEENE methodology and how the life cycle resource consumption is captured in the end products. From an environmental life cycle perspective, the Rational Exergetic Efficiency is calculated by dividing the total exergy of the useful outputs by the CEENE value. In the situation before transition this efficiency reached 15.6% in comparison to 15.3% in the situation after transition. This means that currently only 15.3% of the exergy of the elementary resources deprived from the environment (CEENE) is captured in the final products. It should be noted that in the calculation of the CEENE impact category land use, 2% of the solar irradiation is included to account for biomass production, since this is approximately the maximum energy that is captured by photosynthesis per land area and which is therefore not available for a natural ecosystem.

Table III.1.2 clearly demonstrates that the biofeedstock used in biorefineries is responsible for a large share (93%) of the life cycle resource requirements and the related impacts of the output products. Utilities to process it further in the biorefinery account only for 7.0% of the total exergy extracted from nature (1.3% for chemicals, 5.2% for natural gas used in the CHP and 0.5% for transport). A more detailed picture of the resource footprint of the different end products can be obtained by considering the different categories in the CEENE methodology, which represent the relative amount of exergy deprived from nature per category for a kg of end material. Figure III.1.3 depicts this footprint for the situation after transition. The main difference between the two situations is the footprint of the animal feed which is slightly lower before transition (A') because of the larger production rate on a mass basis. The highest resource extraction from nature is the land use, mainly originating from agricultural production of the incoming biomass. Indeed, in contrast to fossil resources, biobased materials require a land intensive cultivation step depriving the natural ecosystem from this potential territory. The second highest resource extraction is the use of fossils, which originates mainly from natural gas used in the CHP of the production plant (49.7%), whilst the life cycle of the biobased resources accounts for 39.9%, the life cycle of the chemicals for 6.5% and the transport for 3.9%,

Due to the fact that the allocation procedure was based on exergy flows per process, insights on the origin and size of the environmental impact per product can be obtained. As such, the amount of fossils used indicates the energy intensity to obtain the direct processing and production chain of the different products. For example the gluten are separated with energy intensive centrifuges and the ethanol needs a significant amount of steam for the purification section, both requiring fossil natural gas from the CHP. Furthermore, more impact from the agricultural phase is allocated to the gluten and ethanol because they both have a higher exergy content than the sugar/starch streams. The sugar stream has the lowest resource footprint. However, it should be considered that the incoming sugar stream is accounted for as 'sugar, from sugar beet', since the ecoinvent database does not contain sugar syrup from wheat. In comparison to wheat, sugar beet has a dry matter yield which is approximately three times higher per hectare than wheat and a relatively larger sugar concentration. However, on the other hand it is more difficult to store and furthermore it offers fewer opportunities for refining.

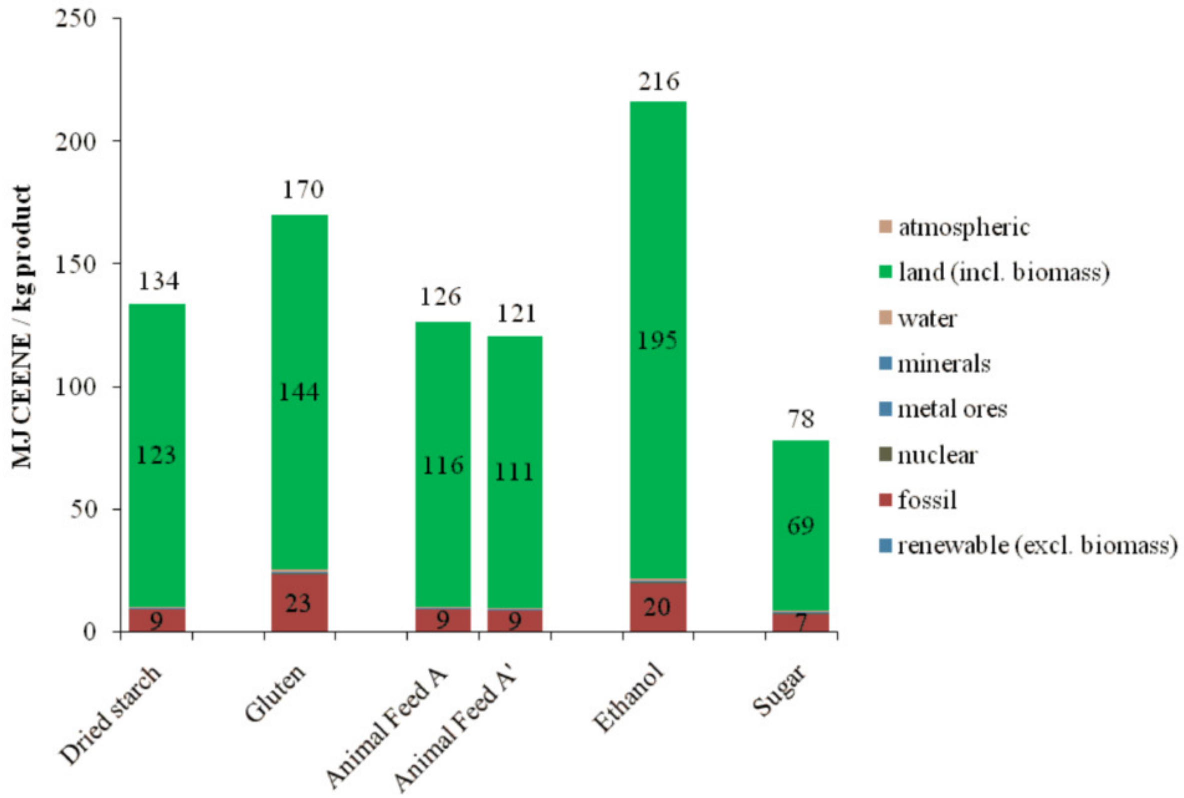

Figure III.1.3: The resource footprint of the different output products expressed in MJ CEENE per kg end product, which expresses the relative amount of exergy deprived per resource category. The difference between the situation before (A') and after (A) transition is situated in the footprint of the animal feed.

3.3. Scenario assessment

A scenario assessment is used to analyze the dynamic character of decisions in the bioresource sector and the implications of taking the opportunity to replace fossil services with biomass. In the case study ±30% of the previously produced animal feed is now converted to fuel bioethanol. Per ton animal feed replaced, 13.6 GJ fuel bioethanol is obtained, thus replacing 13.6 GJ fossil fuel. It is supposed that the market demand for animal feed remains constant and that the production of the replaced tons animal feed is displaced to another facility. Table III.1.3 summarizes the consequences on the resource impact of this decision. The transition to the valorization of the biomass stream as a biofuel results in an overall saving of 7GJ fossil resources per ton animal feed displaced, resulting in an automotive fuel based on 43% less fossils than regular petrol. It should be noted that this number could be higher, because the studied production facility uses mainly energy from a CHP working 100% on natural gas, thus saving nuclear energy which is related with grid power. However, when considering the other categories, the pressure on nature increases. In this case, the production of biofuel requires overall more electricity (nuclear and renewable), uses more water and furthermore, the amount of minerals, metals and land use and transformation nearly doubles (193%), mainly due to the fact that fossils do not need current land cultivation. This means that replacing fossils by biomass decreases the pressure on the atmosphere by mitigating GHG emissions but on the other hand it increases the pressure on the inputs from the earth's crust. Assuming that electricity will become renewable in the future through solar energy and that metals can be recycled, the water, land and minerals demand remains problematic. In other words, there is a tradeoff in the biosector between the Carbon Footprint of products and the Land Footprint, Water Footprint and Minerals Footprint. Figure III.1.4 visualizes this by using internal normalization by using the average of the two scenario's. Biomass is thus a renewable resource, but definitely not a 'gratuite' or an 'endless' resource.

Table III.1.3: The consequences of a strategic decision regarding the valorization of a biomass stream according to the eight resource impact categories of the CEENE methodology (in GJ). The animal feed production is displaced to another company (A'), whilst a certain amount of petrol, previously produced at company B, can be substituted by bioethanol. Company A represents the company after transition and A' before transition.

					Reference situation				
	Amount	**Renewable**	**Fossil**	**Nuclear**	**Metal ores**	**Minerals**	**Water**	**Land**	**Atmospheric**
Animal feed company A'	1 ton	0.14	9.03	0.39	0.01	0.02	0.28	111.02	0,00
Petrol company B	13.6 GJ	0.05	17.53	0.18	0.00	0.00	0.18	0.07	0,00
Total CEENE GJ		0.19	26.56	0.57	0.01	0.02	0.45	111.09	0.00

					Situation after transition				
	Amount	**Renewable**	**Fossil**	**Nuclear**	**Metal ores**	**Minerals**	**Water**	**Land**	**Atmospheric**
Animal feed company A	1 ton	0.15	9.38	0.42	0.01	0.02	0.32	116.04	0,00
Bioethanol company A	13.6GJ	0.19	9.96	0.56	0.01	0.02	0.41	98.99	0,00
Total CEENE (GJ)		0.34	19.33	0.98	0.02	0.04	0.73	215.03	0.00

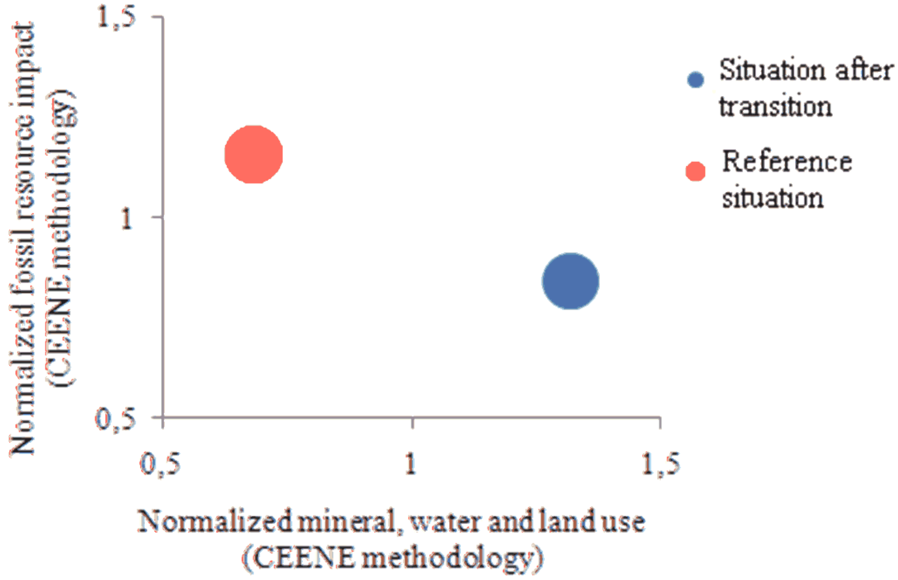

Figure III.1.4: Normalized (internal normalization by using the average of the two scenarios, higher is worse) fossil resource savings versus the mineral, water and land use according to a scenario assessment with the CEENE methodology. The savings of 27% fossil resources in the scenario assessment 'costs' 93% additional inputs of land, minerals and water, mainly due to higher cultivation requirements.

4. Conclusions

Refining biomass to different end products is a major opportunity to offer different market services. As such, fossil resources can be replaced without losing thermodynamic efficiency in biomass processing. However life cycle assessments show that the production chain of biomass requires a demanding cultivation step nuancing the renewability of bio-based products. Furthermore, every decision to change a product mix results in a displacement of production due to a constant demand, implying that a certain amount of biomass and the related inputs are necessary for every quantity of food, feed, bioproducts and bioenergy needed by society. Because of the fact that the availability of these factors is limited, even if the inputs are minimized, it is highly uncertain if biomass will be able to deliver all required services to replace fossils. Therefore, the decisions concerning biomass taken in the political and industrial system should be well-thought-out and based on sound assessments. Apart from economic concerns, these decisions are currently mainly driven by greenhouse gas emission targets or in other words, lower Carbon Footprints. However, the main limiting factors for the development of biorefineries, are the use of the inputs during cultivation such as land, water and minerals. This chapter has stressed the importance of quantifying these inputs and of weighting the 'cost' of lowering GHG emissions through the use of biomass. Introducing such calculations, e.g. as a basis for subsidies, allows objective comparisons and might encourage sustainable agriculture and efficient production. Furthermore, it might also deliver a more balanced market regulation, by including the limiting factors for feedstock production for food, feed and bioproducts in the energy sector. The large range of opportunities for biorefining should thus be taken, but it should be considered that replacing the carefully built-up stock of valuable fossils will always require other types of natural resources.

2. Environmental sustainability aspects of different sources of biofeedstock: a case study on biomass valorization by anaerobic digestion

Redrafted from:

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1. Introduction

Mankind currently depends heavily on depleting fossil resources and although it is clear that they will keep on taking an important place in our resource supply for the next decades, it is also clear that a transition to more sustainable sources of material and energy is necessary. Biomass is such an alternative resource, which has a large potential in application range and in the mitigation of climate change. On the other hand it is not an endless renewable feedstock as it depends on its resource footprint caused by agriculture and limited photosynthetic efficiency, resulting in competition with the food and feed chain. For this purpose, a detailed environmental sustainability assessment of different sources of biomass can give more insight in future possibilities of the bio-based economy. Biomass can origin from arable field crops such as maize, sugar beet, wheat, etc. whereas also lignocellulosic crops can be produced on marginal lands. Alternatively domestic and industrial waste streams can be used or in the longer term, aquatic biomass (algae) could make a significant contribution (McPhail et al., 2012). In this chapter, the currently most implemented resource choices, i.e. energy crops, field residues and organic waste are assessed with a focus on anaerobic digestion as a biomass valorization strategy.

Anaerobic digestion, basically defined as “a process that converts biomass to biogas under oxygen free conditions”, exists in many configurations depending on temperature (psychrophilic, mesophilic and thermophilic), moisture content (less than 15% dry matter is considered as wet, a higher dry matter is considered to be dry), reactor type, (plug flow, completely mixed, film, …), horizontal and vertical, single- or multistep reaction, and continuous or batch (NorthEast Biogas, 2010). In general however, anaerobic digestion is able to convert almost all sources of biomass, including different types of organic wastes, slurry and manure to a highly energetic biogas (Holm-Nielsen et al., 2009) as long as conditions such as C/N ratio are within an acceptable range. Only strongly lignified organic substances such as wood are not suitable for digestion (Weiland, 2010). When using digestable biomass, the different molecules such as carbohydrates, proteins and lipids can be hydrolyzed to soluble sugars, amino acids and long chain fatty acids in order to start the further microbial conversions. Afterwards, during acidogenesis these components are degraded to acetate, hydrogen, carbon dioxide and a number of organic acids, the latter converted further by acetogenesis. Methanogens then convert this mixture to biogas (Gujer and Zehnder, 1983) consisting of approximately 50-70% methane, 30-50 carbon dioxide and smaller amounts of N_2, H_2O, NH_3 and H_2S (IEA Bioenergy, 2009b). The remaining fraction in the digester, the digestate, can be further treated and processed, or can be used directly as a fertilizer. These complex microbiological reaction pathways allow conversion of all types of biomass which is a major advantage in comparison to other forms of bioenergy such as bioethanol and biodiesel. In these options respectively the *Saccharomyces cerevisiae* convert only the glucose fraction to ethanol and only the oil and fat fractions undergo transesterification to biodiesel. This results in better conversion efficiencies of biomass to biogas compared to other biofuel production alternatives (Börjesson and Tufvesson, 2011) which is an essential parameter in the environmental sustainability of bioenergy because the cultivation of biomass is generally responsible for the largest impact over the life cycle of bioenergy (Zah et al., 2007). As a result, a better overall energy balance of biogas compared to for example ethanol can be achieved, where extra pre- and post treatment steps might enhance higher yields but do not have a beneficial effect on the energy balance (Schumacher et al., 2010).

Although it is a promising technology, up to now biomass contributes by only 3 to 13% of the total energy supply of industrialized countries in which incineration for heat or electricity, in many cases by fuelwood, covers most of this supply. Liquid biofuels represent a smaller contribution, mainly as biodiesel and bioethanol. Energy from biogas from anaerobic digestion is producing only a small but steadily growing share (IEA Bioenergy, 2010a). However, the role of biogas can become more substantial. The broad applicability and relatively simple setup of anaerobic digestion, is a major opportunity for the worldwide implementation of this technology as a way to treat waste, i.e. a stabilization of the waste can be achieved and to produce energy simultaneously (Weiland, 2006). It is also implemented more frequently for the digestion of energy crops, by using a large diversity of possible plant materials (IEA Bioenergy, 2010a), whilst furthermore, digestion is a potential option for (organic) farmers to become energy self-sufficient where digestate application can maintain soil fertility (Oleskowicz-Popiel et al., 2012).

These opportunities have resulted in a growing interest in anaerobic digestion; for example in Germany, a leading country in biogas production, it is considered as a key technology to meet the renewable energy and GHG mitigation targets (Pöschl et al., 2010). On a more international scale, it is stated that up to 18% of primary energy demand can be fulfilled by cultivating energy crops on 30 % of the arable land (IEA Bioenergy, 2010a), excluding the potential of organic waste streams and possible new bioresources such as biodegradable polymers (Guo et al., 2011). To highlight the potential, in 2010 already 197 plants were already operational in Europe converting the organic fraction of municipal organic waste with an average capacity of 29170 tons per year (Mattheeuws, 2012).

In this context, this chapter makes a detailed analysis of the environmental sustainability of using different types of biofeedstock in dry anaerobic digestion for the production of electricity and heat to contribute to renewable energy targets in Northwestern Europe. As input materials the currently most common biomass sources are studied, namely domestic organic waste, farm residues and energy crops. These feedstock alternatives are analyzed by using energy and exergy efficiency assessment and by performing a resource and emission fingerprint based on ISO 14040/44 LCA with an additional focus on the benefits of the valorization of the produced heat and digestate, the latter as a fertilizer. The limitation that many studies base themselves on small-scale test data or literature was avoided by studying full scale and operational dry digesters. The conclusions of this study are thus based on a high quality dataset with realistic data of for example the input composition, internal material and energy use, industrial conversion efficiencies, transport distances, digestate application in agriculture, etc.

The assessment is thus performed at two levels:

- First, the conversion efficiency of the different types of biomass to energy is assessed by using an energy and exergy balance, as an efficient use of the feedstock is a critical factor in the sustainability of biomass valorization chains. Exergy assessment was used to identify process inefficiencies based on the second law of thermodynamics (Dewulf et al., 2008).
- Second, Life Cycle Assessment was used to obtain a more holistic view on the environmental profile of the different types of biomass feedstock. For this

purpose, a combination of a resource based and emissions based LCA approach was chosen.

2. Method

In the following, the two studied full scale case studies are elaborated with a process diagram, followed by a system description and a clarification of the data sources (year average of 2010) used to construct the inventory. Afterwards, the assessment techniques are explained more in detail. The inventory of the studied cases is confidential, but can be obtained upon request.

2.1. System description

2.1.1. Case study 1

The first case study focuses on a typical setup of dry digestion in an agricultural context situated in Germany and having a capacity of approximately 20,000 tonnes biomass inputs per year (Figure III.2.1). The vertical digester is currently mainly fed by silage maize, supplemented with smaller amounts of rye silage and poultry manure. After storage, biomass is fermented with a residence time of approximately 21 days. The produced biogas is collected in a gas bag, where water is condensed. Afterwards, the biogas is converted into electricity and heat in generators of 250kW. The digestate is stored and used as a fertilizer on the surrounding fields. Because of the importance of agriculture in environmental LCA studies, the farming of silage maize was studied more in depth, with a specific focus on the impact of using digestate instead of traditional (organic and mineral) fertilizers. Data of these processes were collected together with the involved farmers and experts. Methane emissions from the digestate storage tank are taken from Liebetrau et al. (2010). Emissions from agriculture are calculated by applying the models used by Nemecec and Kägi (2007), with more detailed data of metal emissions and of nitrogen leakage taken from Freiermuth (2006) and Svoboda et al. (2011) respectively. Data of diesel consumption was obtained from the involved farmers and the resulting air emissions are taken from EMEP/CORINAIR (2000). Two alternative digester feeds were elaborated for this system in collaboration with involved experts, where all parameters of the inventory can remain constant, except for the agricultural inputs and the energy and digestate output; in the first alternative sugar beet, grass silage and poultry manure, whilst in the second alternative corn stover, cow manure and poultry manure are digested.

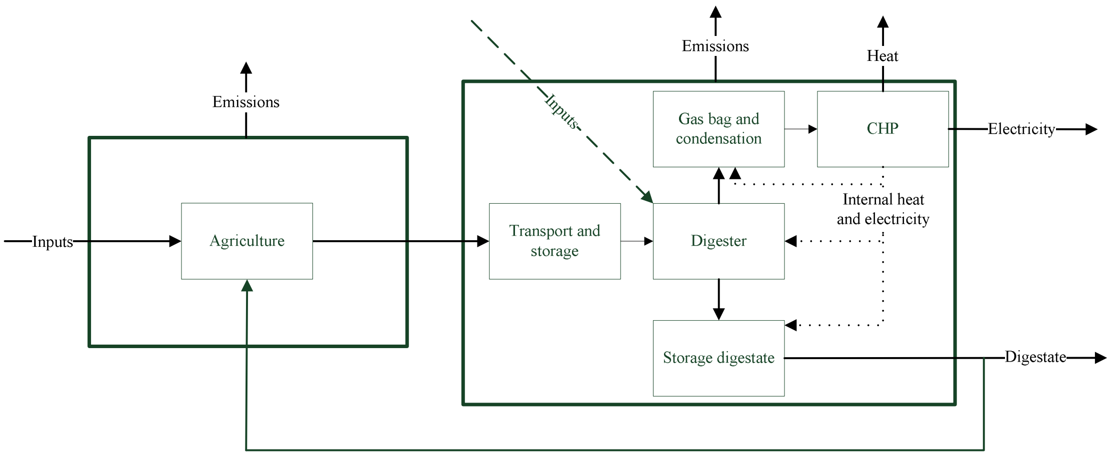

Figure III.2.1: Process flow sheet of the agriculture based anaerobic digestion setup

2.1.2. Case study 2

In the second case study a Belgian production plant was studied where domestic organic waste (±45,000 tonnes per year) is converted into electricity, heat and compost by dry digestion (Figure III.2.2). Biomass is collected by selective municipal organic waste collection. The collection in one part of the region is organized by using a temporary waste terminal, whilst the municipal waste collectors in the second part of the region supply the organic waste directly to the facility. The transport distances were collected in collaboration with the involved stakeholders. Because of the diversity of organic waste and contamination due to sometimes careless waste sorting, a specific pretreatment is necessary by means of drum sieves and magnets. Afterwards a piston pump feeds the digester, where the organic fraction is converted to biogas with a residence time of approximately 20 to 25 days. After a water condensation step, the biogas is burned in engines of 625kW to produce electricity and heat. The resulting digestate is post treated by means of a press, centrifuge and sieve, where the separated heavy fractions are landfilled and the wastewater is treated in a treatment plant. The lighter fraction is further composted in an aerobic composting hall where air is extracted and filtered in a biofilter. All data of resource use and emissions of this plant, including the composting process and the wastewater treatment is collected based on measurements and judgement of involved stakeholders and experts.

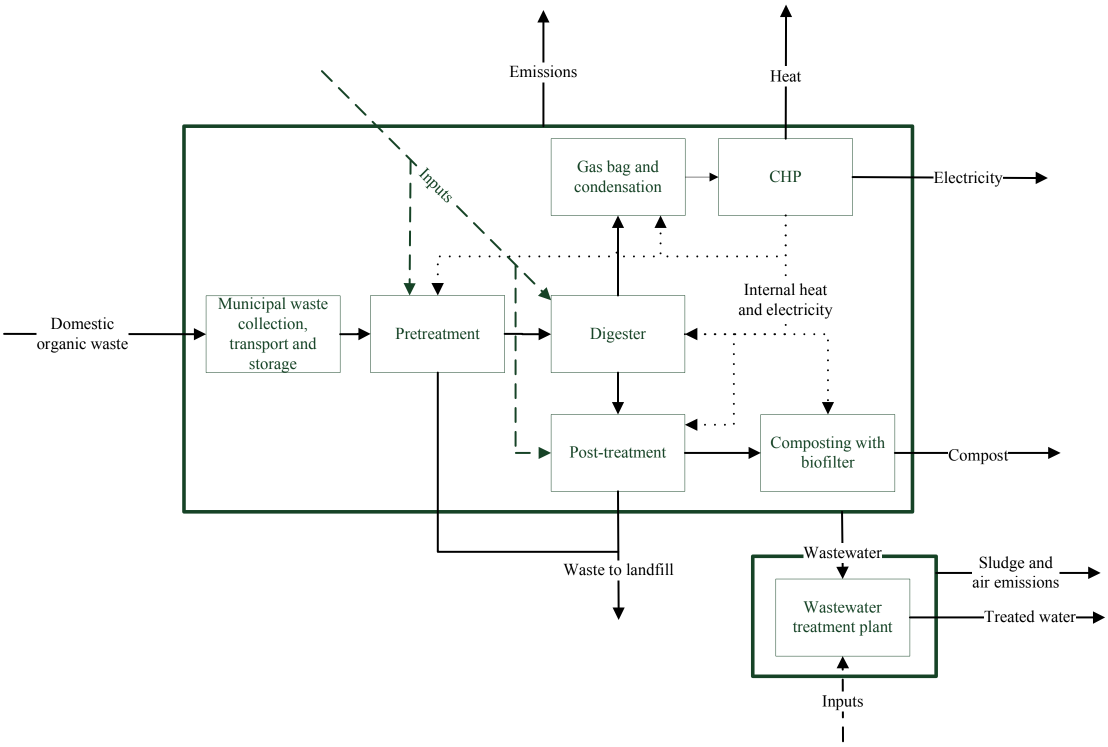

Figure III.2.2: Process flow sheet of the organic waste based anaerobic digestion setup

2.2. Technological Assessment based on energy and exergy efficiency

The efficiency of electricity production per digested biomass is calculated based on energy (Lower Heating Value) and exergy. This is a sound strategy, as the efficiency of the conversion of biomass to energy is a bottleneck in the environmental sustainability of this technology. Including heat would not contribute to the results since a fixed amount of heat is produced per kWh electricity generated and since this would be less comparable with literature. Other aspects such as agriculture and required material and energy inputs are considered in the LCA part of this chapter. Two types of efficiencies are calculated:

- First, a 'traditional' electricity efficiency is calculated by dividing the exergy (Ex_t) or energy (En_t) content of the produced electricity by the ex(n)ergy content of the input biomass.

$$Ex_t \ or \ En_t = \frac{Ex(n)ergy \ of \ electricity}{Ex(n)ergy \ content \ of \ input \ biomass}$$

- Second, a 'rational' electricity efficiency based on exergy (Ex_r) or energy (En_r) is calculated by subtracting the ex(n)ergy content of the not digested matter from the ex(n)ergy content of the total biomass input, as this exergy/energy is still available for other purposes such as fertilizing, incineration, etc.:

$$Ex_r \ or \ En_r = \frac{Ex(n)ergy \ of \ electricity}{Ex(n)ergy \ content \ of \ input \ biomass - Ex(n)ergy \ content \ of \ not \ digested \ matter}$$

  In the case of organic waste digestion, the total 'not digested' incoming biomass is considered. This means not only the final compost fraction, but also the fractions that are separated in the pre -and post-treatment steps.

The energy and exergy calculations are based on experimental and literature data, where heating values are calculated according to Sheng and Azevedo (2005) and Fowler et al. (2009). Exergy is calculated by using Gibbs calculations, the group contribution method and by using the β LHV methodology (de Vries, 1999).

2.3. Life Cycle Assessment assumptions and value choices

Life Cycle Assessment was executed according to the ISO 14040/44 guidelines (International Organization for Standardization, 2006) and the ILCD handbook (European Commission - JRC, IES, 2010). The study includes the cradle to gate production of electricity, heat and digestate/compost by anaerobic digestion in full scale plants in Belgium and Germany. Infrastructure was excluded from this study, except for the land use of the facilities and for the agricultural phase. The ecoinvent database 2.0 is used to model datasets in the background system. The life cycle assessment is structured in three comparisons which are elaborated in Table III.2.1. The detailed allocation factors based on energy and exergy are presented in Table III.2.2.

Table II.2.1: A clarification on the life cycle assessment based comparisons elaborated in this chapter

	C1: Electricity production from waste and energy crops	C2: Agricultural fertilization	C3: Options in agricultural digestion
Goal	a) Compare electricity production of domestic organic waste, energy crops and reference electricity from the grid. b) Study the influence of using heat	Studying the effect of using digestate as a fertilizer compared to 'traditional' mineral and organic fertilization	Comparing different feedstocks available in an agricultural context in North West Europe
Functional unit	1MJ electricity	1kg silage maize	1MJ electricity
Allocation	Based on exergy. In the case of energy crops: a part of the digestate remains within the system boundaries (no allocation on internal stream) Domestic organic waste: compost fully out of system (allocation applied)	n.a.	Based on exergy. Digestate leaves system boundary: allocation applied in all cases.
Heat	Heat used and heat not used compared	n.a.	Heat used
Feedstock data	Real data from case study	Real data for digestate agriculture, ecoinvent studies for alternatives	Real data for maize digestion, data from ecoinvent for the others
Impact assessment	Resource and emission based	Resource and emission based	Resource based

Table III.2.2: Exergetic (and energetic) allocation factors (in %). HU = heat used, HNU = heat not used

		Electricity	Heat	Digestate/ compost
C1	Domestic organic waste digestion, compost used outside system boundary, HU	36.7 (28.4)	22.1 (44.8)	41.2 (26.8)
	Domestic organic waste digestion, compost used outside system boundary, HNU	47.2 (51.5)	0 (0)	52.8 (48.5)
	Silage maize digestion, digestate used within system boundary, HU	51.0 (47.3)	26.1 (49.3)	22.9 (3.4)
	Silage maize digestion, digestate used within system boundary, HNU	69.1 (93.4)	0 (0)	30.9 (6.6)
C3	Silage maize digestion, digestate used outside system boundary, HU	33.7 (44.0)	17.2 (45.8)	49.1 (10.2)
	Corn stover and manure digestion, digestate used outside system boundary, HU	19.5 (26.1)	8.2 (28.8)	72.3 (45.1)
	Sugar beet and grass silage digestion, digestate used outside system boundary, HU	31.7 (42.4)	13.0 (45.7)	55.3 (11.9)

As a life cycle impact methodology, the Cumulative Exergy Extracted from the Natural Environment (CEENE) (Dewulf et al., 2007) methodology is chosen to construct a resource fingerprint consisting out of seven resource categories: renewable resources (excl. biomass), fossil fuels, nuclear energy, metal ores, minerals, water resources and land occupation (incl. biomass). To account for emissions, six categories are taken from the RECIPE methodology with midpoint indicators and the hierarchist perspective: climate change, ozone depletion, photochemical oxidant formation, terrestrial acidification, freshwater and marine eutrophication (the latter also influenced by emissions from the field). Other categories such as toxicity have not been taken into account due to the requirement of a very detailed and specific inventory. Especially in studies involving agriculture, the emissions of metals and pesticides are determining for life cycle toxicity results. These flows are difficult and very case specific to quantify, and therefore, the authors consider the used models of Nemecek and Kägi (2007) not sufficient for further impact modeling of toxicity. The uncertainty of the results is analyzed by using the most commonly used approach relying on the pedigree matrix followed by a Monte Carlo simulation. In this type of uncertainty quantification it should be considered that only data uncertainty is taken into account, without analyzing the impact of model uncertainty, allocation choices, etc. (Huijbregts, 2011).

3. Results and discussion

3.1. Technological assessment: energy and exergy efficiency

Table III.2.3 summarizes the exergy and energy efficiency of the studied biomass to energy routes. When considering the traditional efficiencies, electricity from silage maize production is the best strategy, with a En_t of almost 33%. Electricity production from sugar beet and grass is less efficient and is therefore less suitable from a technological perspective. The digestion of agricultural residues and municipal organic waste has a lower efficiency compared to the digestion of energy crops as the molecules in these fractions such as lignocelluloses are less straightforward for biological decomposition. However, especially the digestion of agricultural residues produces a highly energetic and stabilized digestate resulting in the highest (36%) rational energy efficiency. Organic waste digestion performs worse compared to the agricultural options, however, the En_r reaches 22.6%, demonstrating that the digestable fraction of the organic waste is converted approximately as efficient as solid waste incineration (22% according to IEA Energy Technology Essentials, 2007), however, efficiency of incineration will lower rapidly for fractions with a higher moisture content. In this discussion the ‘traditional’ efficiency ignores the fact that not all biomass is lost or converted. After biological conversions, a digestate remains with a high energetic value (in the dry matter) and containing valuable macro- and micronutrients. This fraction can therefore be useful as a fertilizer (compost), or can be pyrolized/incinerated for additional energy production. The rest product after incineration, ash, can cause additional phosphorus leaching and is not a carbon and nitrogen source (Piirrainen et al., 2013). Therefore it obtains lower credits compared to digestate as a fertilizer which often results in a better performance on a life cycle basis of anaerobic digestion compared to incineration (Bernstad and la Cour Jansen, 2011; Hermann et al., 2011). Recently, the more effective valorization of highly concentrated metals, phosphorus and micronutrients receives more attention and evolutions in this field could have an influence on this balance (Simon and Adam, 2012).

A clear difference between the internal use of energy of domestic organic waste digestion and digestion in an agricultural facility can be observed. In the agricultural facility, 5.6% of the produced electricity is used internally, whilst 6.4% of produced heat is necessary, mainly for heating the digester. In contrary, the domestic organic waste digestion process, requires 36.1% of the produced electricity and 1.6% of the produced heat. The large share of internal electricity consumption, mainly needed for the separation of non-fermentable/compostable fractions is a drawback for domestic organic waste digestion and lowers the rational exergetic (energetic) efficiency to 9.8% (14.5%).

Table III.2.3: Exergy and energy efficiency of electricity production from different types of biomass by anaerobic digestion

	Electricity from organic waste digestion	Electricity from corn stover and manure digestion	Electricity from silage maize digestion	Electricity from sugar beet and grass silage digestion
Electricity produced (MJ)	1.0	1.0	1.0	1.0
Exergy in (MJ)	10.2	6.7	4.4	5.3
Energy in (MJ)	6.6	4.5	3.0	3.5
Ex_t	9.8%	14.8%	22.8%	18.9%
En_t	15.1%	22.2%	32.9%	28.8%
Exergy out in side streams/digestate (MJ)	3.7	3.7	1.4	1.7
Energy out in side streams/digestate (MJ)	2.2	1.7	0.2	0.3
Ex_r	15.3%	32.9%	33.3%	28.3%
En_r	22.6%	36.0%	35.4%	31.3%

3.2. Life Cycle Assessment

3.2.1. Comparison 1: electricity production

From a resource perspective, Figure III.2.3 shows that anaerobic digestion of both energy crops and domestic organic waste scores ‘significantly’ better than the current electricity mix in almost all categories. Only metal and mineral consumption results in relatively comparable values; however in absolute terms, they are of minor importance. A very good performance is achieved for other categories such as renewables, fossils, nuclear and water resources. Compared to the current electricity reference (of Germany), a saving of over 90% is achieved for all these categories, except for the fossil fuel use in domestic organic waste digestion. The latter is mainly caused by the transport distances necessary for a selective municipal organic waste collection, however a positive balance is still achieved with a consumption of 0.59MJ fossil exergy consumption (0.76MJ if heat is not used) per MJ electricity. Furthermore, waste collection is a service to society which is indispensable, independently to what finally happens to the waste. Regarding land use, a saving is achieved for domestic organic waste scenarios, but for energy crop digestion, a significant amount of land is needed for the agricultural processes. In this case 6.1MJ land (8.3MJ if heat is not used) or 0.09m² (0.12m²) for 1 year is necessary to produce 1.0 MJ of electricity. This means that an average German inhabitant, using approximately 6642kWh/y (Nationmaster, 2007), would need an arable area of 2144m² (2903m²) cultivated with silage maize to fulfill his yearly electricity demand, whilst Germany has approximately 1500m² arable land available per inhabitant (Worldstat, 2007). Covering 20% of electricity demand with energy crops would thus require 29% of the arable land available on a life cycle basis (39% if heat is not used). Using organic waste as a feedstock does not have this direct land necessity, and the digestion of this biomass source can thus be seen as a valorization pathway with an overall positive balance (0.67MJ primary exergy inputs from nature per MJ electricity if heat is used and 0.86 MJ primary exergy inputs from nature if heat is not used). The different studied options of anaerobic digestion in general thus score relatively good from a resource point of view. In this assessment, the utilization of the generated heat is an important factor, with an overall poorer performance of 32% in the scenarios where heat is not used. A maximum amount of energy contained in the valuable biogas should thus be used as the waste of heat would detract from the efforts and accompanying resource footprint necessary to obtain the biomass resources. This is logic from a thermodynamic point of view, but causes difficulties in reality, since both the agricultural and organic waste digesters are mainly located in rural, non-industrial areas. Nevertheless, solutions should be sought for this problem, where heat demanding processes can be executed in the proximity of digesters (e.g. drying steps, domestic and rural heating such as greenhouses, stables, etc.). An alternative is a transportation of the heat or the biogas itself. An upgrade to biomethane for example, is stated to have a positive environmental effect when being burned in a small-scale CHP unit (Pöschl et al., 2012), whereas the biomethane could be transported in the currently available gas supply.

The emissions assessment (Figure III.2.3) obtained by the Recipe midpoint methodology shows that climate change gives similar results to the fossil fuel use except for digestion relying on agriculture, where methane emissions occur at the digestate storage tank and during digestate application on the field. Controlling these emissions would give a balance which performs almost 50% better in the mitigation of climate change. Whilst the data was collected in 2010, more recently a post-digester was installed, eliminating a significant part of these emissions and increasing electricity yield, which is expected to lower the overall impact (Pöschl et al., 2012). Ozone depletion and photochemical oxidant formation are mainly caused by transport, which results in the highest impact for the organic waste digestion due to a transport intensive waste collection step. Acidification, freshwater and marine eutrophication are mainly caused by agriculture and therefore, the agriculturally cultivated feedstock digestion scores bad on these impacts except for freshwater eutrophication which is also caused by the disposal of coal in the current electricity mix.

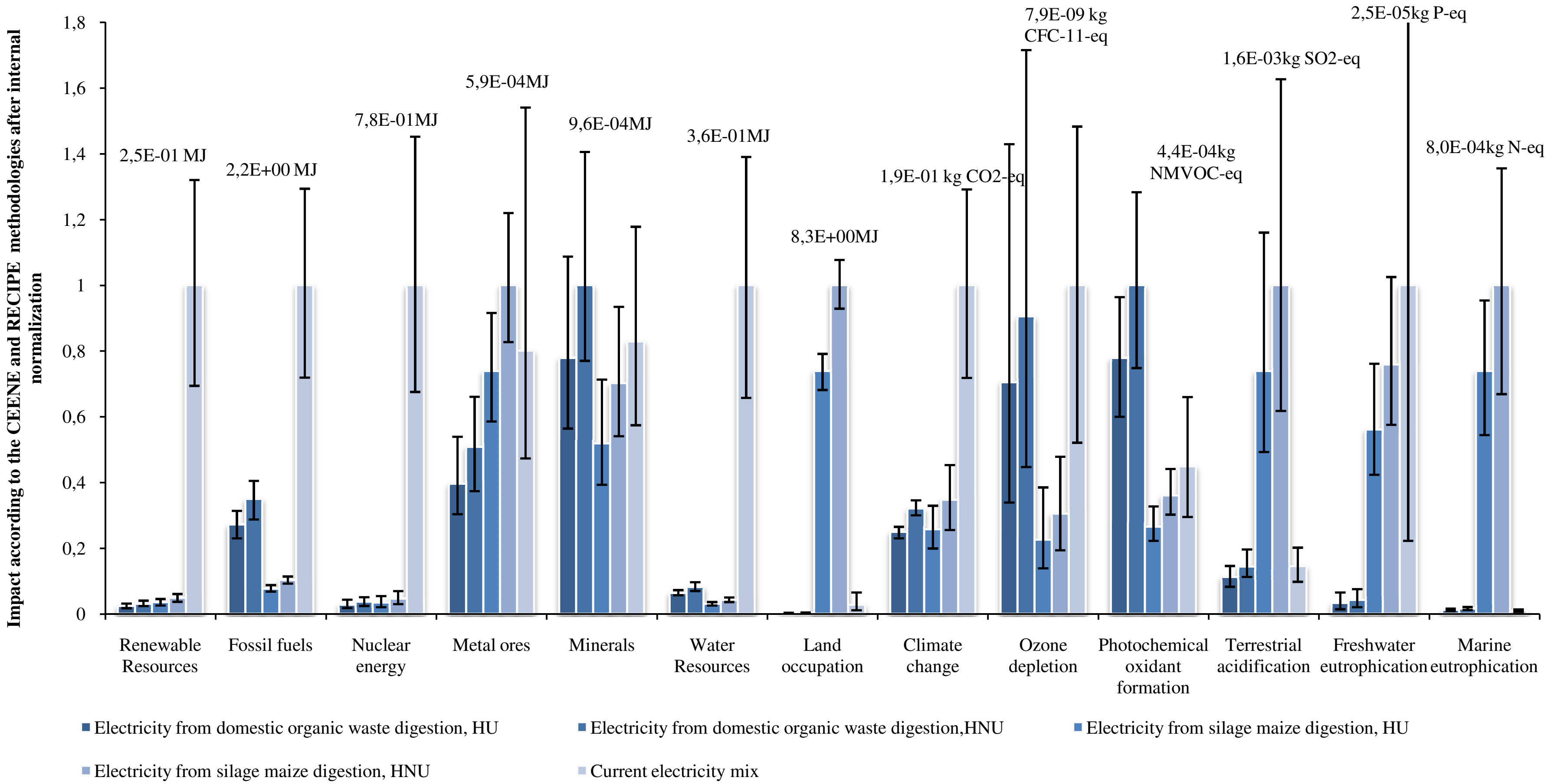

Figure III.2.3: Resource and emission footprint of electricity alternatives by using the CEENE and RECIPE methodology with uncertainty indication. Internal normalization is used, meaning that all alternatives are divided by the maximum value of the five options. Absolute values are given on top for the maximum value per MJ electricity

3.2.2. Comparison 2: agricultural fertilization

The byproduct of anaerobic digestion is a digestate containing valuable nutrients that can be used as fertilizer on the surrounding fields, as such evolving to a 'closed loop' system which is a sound strategy in the light of renewability, but which could also induce risks, that are studied more in depth by analyzing a comparison of the silage maize with digestate fertilization with the 'traditional' intensive production and organic cultivation (Figure III.2.4). Concerning yield and resulting land necessity, the studied system scores average compared to the intensive and organic production, whilst for most other resource categories it scores best. The main reason for this is the replacement of fertilizers by nutrients available in the digestate. This internal use of nutrients is a major advantage compared to the traditional intensive production which requires resource consumption for the production of mineral fertilizers. As such a saving of over 70% minerals and approximately 35% fossils is achieved. The high water use of the silage maize production can be explained by the production of diammonium phosphate, which is added as only fertilizer, but which might be omitted when digestate application practices are improved.

The good performance on a resource basis is linked to a better score in related emissions categories such as climate change, ozone depletion and photochemical oxidant formation. The difference, however, is smaller compared to fossil fuel use in the resource assessment, mainly due to direct emissions from the field such as N_2O and CH_4. The best performance for ozone depletion is achieved by organic agriculture. This can be explained mainly by the production of pesticides which are applied in both the intensive production and in the digestate fertilization scenario. In contrary to these impact categories, digestate application on the field causes more problems with acidification and eutrophication. Acidification is mainly caused by ammonia emissions during application, while marine eutrophication occurs when nitrate leaks to the groundwater. Freshwater eutrophication is mainly caused by the diammonium phosphate production and could be lowered by omitting this additional mineral fertilizer from the cultivation if digestate application would be sufficient as a nitrogen and phosphorus source.

The environmental impact assessment of digestate application thus shows that digestate is a rich source of nutrients with often a high dry matter content, making it useful as a fertilizer, but also inducing risks of pollution. Whilst the total nitrogen content remains constant before and after the digestion (IEA Bioenergy, 2010b), the pH of this biological matter is higher, causing high NH_4^+-N concentrations and thus more ammonia emissions during field application (Amon et al., 2006). This was also confirmed by experiments comparing digested with not-digested slurries (Immovilli et al., 2008). Nitrogen leaching could also become a problem, but the quantities are stated to be comparable to cattle slurries (Svoboda et al., 2011). Heavy metal components such as copper (42mg/kg DM) and zinc (217mg/kg DM) measured in the digestate of this study do not exceed concentrations in different types of manure (IEA Bioenergy, 2010b) and would therefore not require additional precautions. Other risks include the contamination of digestate with pathogens, pesticides, seed residues and other toxic compounds (IEA Bioenergy, 2010b), especially in digestates obtained after solid waste digestion.

Nevertheless, using digestate as a fertilizer can be beneficial for crop growth (e.g. maintaining carbon balance) and saves resources compared to traditional agriculture.

The large scale introduction of these nutrients however, is subjected to legislation. For example the stringent phosphate regulations in the Manure Action Plan of Flanders restrict the application of digestate as a fertilizer (VLM, 2012). On the other hand, from an ecological micro-scale perspective it can be stated that the benefits exceed the risks, especially if good agricultural practice is applied (e.g. injection of fertilizer, lowering of pH by acids, timing of application, etc.) (IEA Bioenergy, 2010b; Holm-Nielsen et al., 2009; Mokry et al., 2008).

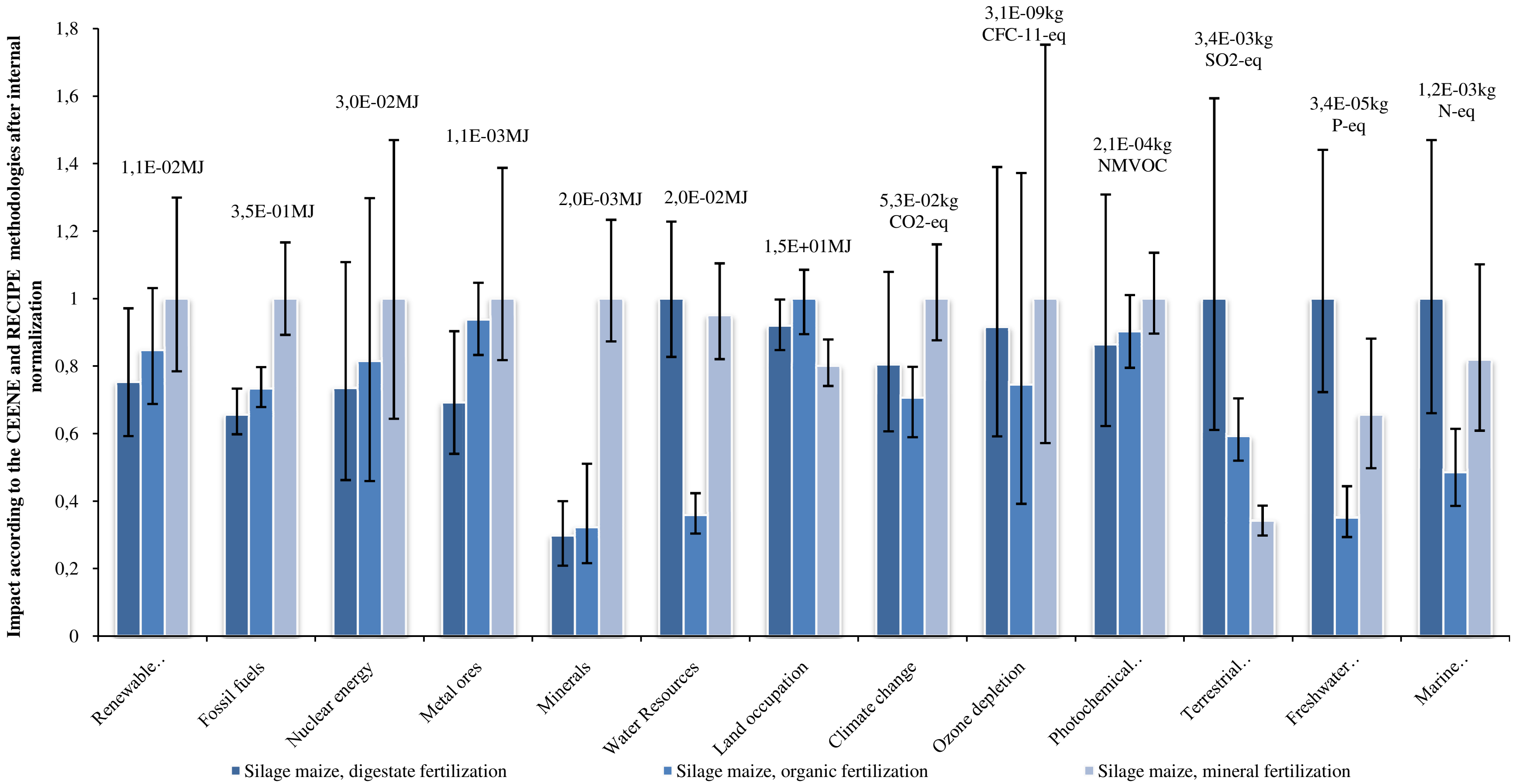

Figure III.2.4: Resource and emission footprint of fertilization alternatives in silage maize cultivation by using the CEENE and RECIPE methodology with uncertainty indication. Internal normalization is used, meaning that all alternatives are divided by the maximum value of the three options. Absolute values are given on top for the maximum value per kg silage maize

3.2.3. Comparison 3: options in agricultural digestion

In an agricultural context, several feedstocks are possible of which three scenarios are analyzed in this study; silage maize, corn stover and cow manure, and sugar beet and grass silage (Figure III.2.5). From a resource perspective, the digestion of agricultural residues such as manure and corn stover is favorable. Conversion efficiencies are relatively high compared to the limited inputs needed during the life cycle. Especially manure is seen as a 'free' resource, whilst the use of corn stover is beneficial as the impact of grain maize is allocated over the grains and stover, therefore making better use of the biomass yield obtained by cultivation. It should however be noted that this study excludes the effects of additional work processes and a possible destabilization of the soil or necessity of additional fertilizer compensating the extra harvest of biomass. This seems acceptable in most cases, as digestate is returned on the field after biogas production restoring the nutrient balance, whereas otherwise CO_2 would be emitted directly from the field during organic decomposition. When considering the digestion of energy crops, the use of silage maize performs better compared to the sugar beet and grass silage scenario. This can be explained by a better conversion efficiency of maize, as can be seen from Table III.2.2. A relatively simple but scientifically sound parameter for the environmental performance is given in IEA Bioenergy (2010a), where the yield per hectare is multiplied with the biogas potential per mass of biomass. As such, silage maize has a potential of maximally 18540m³/ha whilst grass and sugar beet have lower maxima (6538 and 6096m³/ha respectively). Biomass sources such as potatoes and fodder beet also achieve high yields, however, underground crops can result in other disadvantages such as difficult handling, higher moisture content and sand clogging in the digester (IEA Bioenergy, 2010a). As such, silage maize conversion to biogas can be seen as one of the most efficient energy crop pathways, where in this study only 0.14MJ fossil exergy is required per MJ electricity. This positive balance, which is even better for the digestion of farm residues (0.10MJ/MJ), is therefore an opportunity for (organic) farmers to become energy self-sufficient.

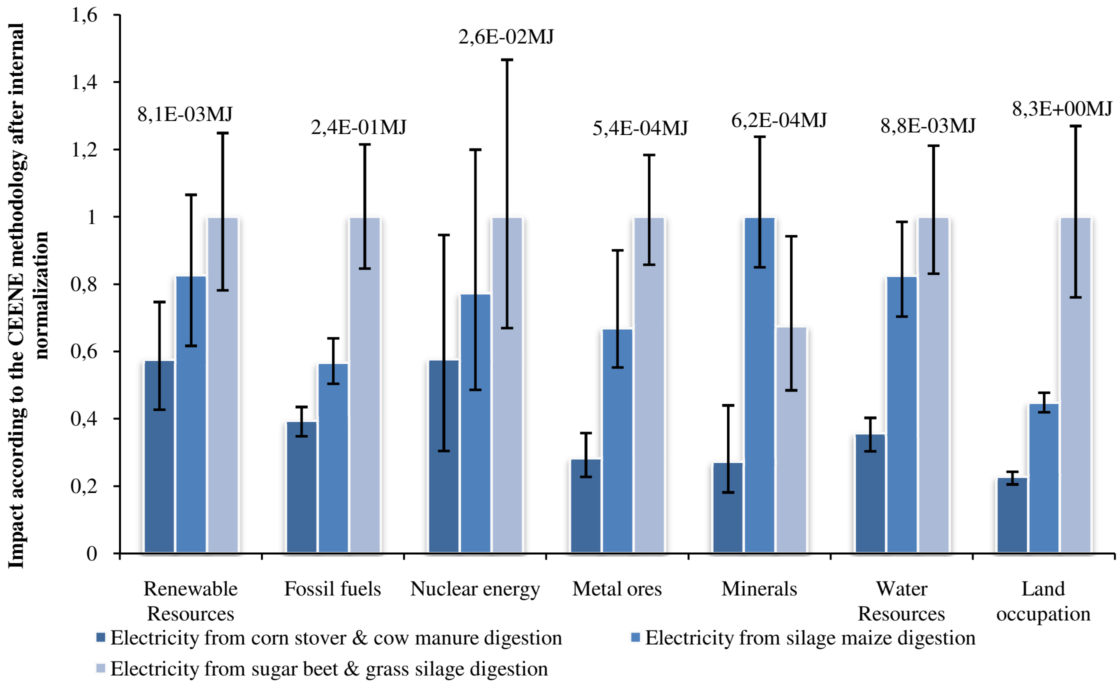

Figure III.2.5: Resource footprint of electricity alternatives in an agricultural context by using the CEENE methodology with uncertainty indication. Internal normalization is used, meaning that all alternatives are divided by the maximum value of the three options. Absolute values are given on top for the maximum value per MJ electricity

4. Conclusions

This chapter highlighted that the different types of biomass all have their advantages and disadvantages. It is shown that energy crops such as silage maize are most efficiently converted and are thus easiest to use as a feedstock in biorefineries whereas farm waste and domestic organic waste achieve lower efficiencies because they often contain contaminants and more difficult molecules to convert such as lignocelluloses. For this purpose more mass, energy and utilities are required per functional unit. In a life cycle perspective however, the ‘waste’ streams generally have a lower footprint as they do not directly rely on the intensive agriculture step or do not need arable land for cultivation. This is also has an influence on the economics of anaerobic digestion. Only a few crops such as fodder beet, wheat, sugar beet and forage maize are stated to be profitable for conversion of biogas to electricity (Jones, 2010). Apart from the ecological impact of arable land use, the economics are therefore also a limiting factor for several feedstock options. Generally waste streams have a low price or induce a gate fee, whereas competition for other sources of biomass with the food industry can have an increase in feed price as a consequence, threatening profitability of different digester feed configurations. Since electricity is still a relatively cheap commodity, new markets for biogas could however lead to a more competitive business. If the methane is purified for example, it can be injected in the natural gas grid, used as fuel in cars or even used as building block in the chemical industry.

Nevertheless, anaerobic digestion is identified as an efficient technology for the conversion of different types of biomass and also from a life cycle perspective, anaerobic digestion performs well in most categories by inducing significant resource savings compared to reference energy production. The technology is able to produce biogas from many different sources of biomass whilst co-producing a rich digestate that can be used for ‘closed loop’ nutrient recycling, as such lowering the resource footprint of biofeedstock by excluding the need for mineral fertilizers. Therefore this technology can become a sound strategy in the production of renewable energy. On the other hand, to increase environmental sustainability of this system, it is necessary to control (agricultural) emissions in the biogas production chain.

CHAPTER IV: Methodological development in sustainability assessment of biorefineries

1. Basic Engineering approaches for data inventory collection in prospective life cycle assessment: development and application in a biorefinery case study

Redrafted from:

De Meester, S., Van Langenhove, H. and Dewulf, J. Basic Engineering approaches for data inventory collection in prospective life cycle assessment: development and application in a biorefinery case study. To be submitted to the Journal of Cleaner Production.

1. Introduction

In the transition to a more sustainable society, Life Cycle Assessment (LCA) is considered as a valuable assessment framework for the quantification of the environmental impact of products and services (European Commission, 2003). For this purpose it is more and more included in the decision making process at different levels of policy and industry. The LCA supported decision should then make a choice between options by outweighing the positive and negative environmental effects of each option. Obtaining meaningful results requires that all options are thoroughly known; LCA is indeed a data intensive procedure (Mueller et al., 2004) that typically requires full material and energy balances of the system under study. However, this might not be available for the different options in development, which is a major shortcoming for the implementation of prospective environmental assessments.

Especially in biorefineries this is an important issue. The transition from fossil based to biobased refineries is seen as a big step in greening the economy mitigating climate change and giving the ability to obtain renewable and thus more sustainable products and services (IEA Bioenergy, 2009c). Nevertheless, it is already shown that this transition is challenging as renewable resources also have a production chain with significant environmental impact, e.g. through land use (De Meester et al., 2011). Strategic choices should therefore be made before final implementation in order to achieve the highest degree of sustainability with the biomass that is available.

A typical question would be if a biorefinery should change configuration and what kind of by-products can be produced. It could for example make sense to analyze the environmental consequences of including a wet milling step to separate proteins before fermentation of corn grains (Figure IV.1.1).

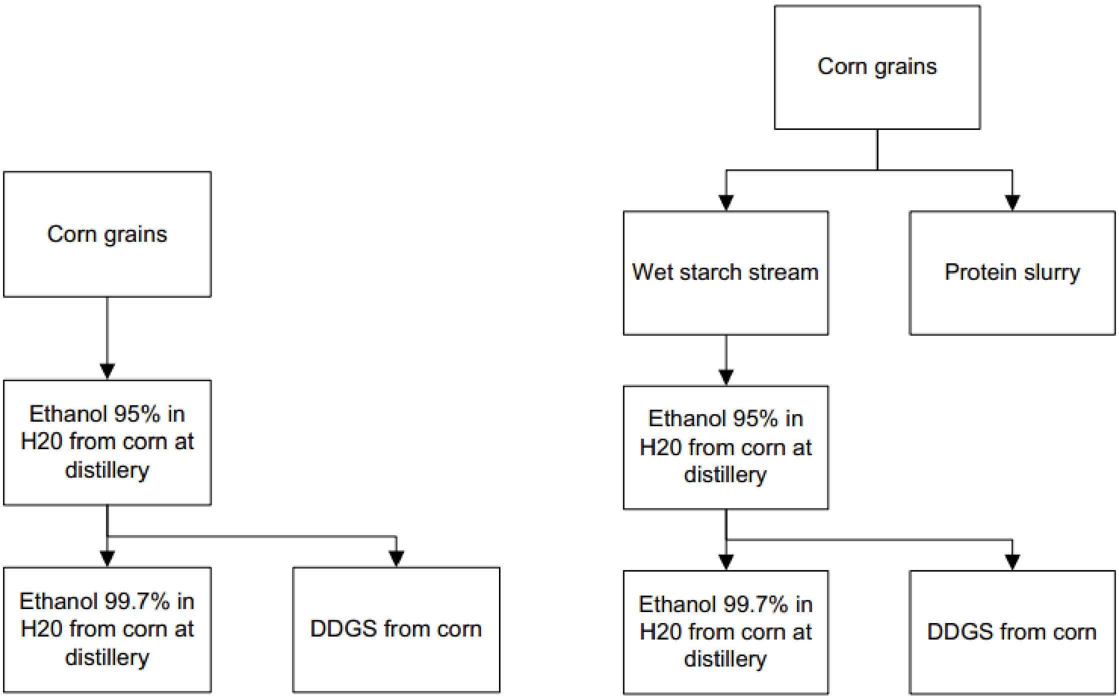

Figure IV.1.1: The product system of traditional corn ethanol (left) versus an alternative product system where the proteins are first separated (right). DDGS = Dried Distillers Grains with Solubles.

To address such a typical question with Life Cycle Assessment, a choice can be made between the 'usual' options to compile a data inventory, namely data collected in a real facility or taken from literature, life cycle databases or process simulation software. The first option is often not possible as the question is prospective and data is therefore not readily available. Alternatively looking at similar installations is a possibility, but these are not likely to be identical and furthermore this can result in confidentiality issues. The second option is only applicable in a few cases. In the example presented in Figure IV.1.1 the current product system is available in a life cycle database (Jungbluth et al., 2007), but the new option with the additional milling step is not at hand. These life cycle databases indeed use static, often aggregated and generic data, not being flexible for case specific modifications. This leaves only the last option open, where process simulation software such as ASPEN, SuperPro

Designer and GProms can be used. Following this last approach however has several disadvantages in the use of life cycle assessment; first the software tools are not open source and expensive, second, they are not compatible with common life cycle practice (types of flows, units, reports, …) and third they are not easy to use and offer moderate flexibility. It is often a time consuming process to work with these tools requiring a lot of detailed data which might not be available at the time of decision making.

As an alternative to the aforementioned three possibilities, this work, performed in the framework of the European FP7 project PROSUITE (Prospective Sustainability Assessment of Technologies), aims at developing engineering modules that can be used as parameterized unit operations where raw data and formulas are used to determine the data inventory, instead of fixed values (Cooper et al., 2012). This allows the completion of the life cycle inventory by assembling material and energy balances of basic unit operations (BUO; single process steps such as a distillation column) whilst being flexible and straightforward in use and easily accessible to life cycle scientists as the modules can be implemented in LCA software such as OpenLCA (Greendelta, 2012). Returning to the example given in Figure IV.1.1, the process flowsheet can indeed be assembled with the BUO approach, based on engineering approaches combined with rules of thumb and default values, in order to model the extra milling step in the production of bioethanol. In this chapter, the modules developed in the PROSUITE project are elaborated and tested in a biorefinery case study to demonstrate the operability and accuracy of the proposed approach.

2. Methodology

2.1. The BUO approach: structured parameterization

The starting point of the presented approach is the so-called 'basic unit operation' as these single processes are the fundament of each production chain. Every factory is indeed the combination of a specific sequence of processes. In this light, parameterized modules were elaborated for 22 common processes applied in (bio)refineries and chemical industry. The list is subdivided in four types of processes:

- Reactions: chemical reactions, incineration for heat and power, fermentation
- Separation processes: evaporation, distillation, filtration, sedimenting centrifuges, electrostatic precipitation, electrodialysis, pressure swing adsorption
- Physical mechanical processes: mechanical compression – single stage, mechanical compression – multi stage, pumping incompressible fluids, pumping incompressible fluids through packing, agitation and mixing of liquids and suspensions, comminuting, fluidization, pneumatic drying and pneumatic conveying, conveying solids, fans, blowers & vacuum pumps
- Utilities: heating, cooling, steam generation

For all these processes, a systematic approach is presented where the system is analyzed at α, β and γ system boundary level. The structure of this work is visualized in Figure IV.1.2, being a further elaboration of Van der Vorst et al. (2009).

The BUO is situated within the α boundary where the scope and exact boundary of the module is clearly defined per process to avoid confusion. The description then considers not only the processes that are included, but also the range of application. The β system includes supporting unit operations (SUO) such as pumping, mixing, etc which are excluded from the calculations within the α level, and which should therefore be modeled separately. Afterwards the information of the α and β boundary, which is typically a material and energy balance, delivers Unit Process Raw data, which can be coupled to life cycle databases such as ecoinvent or the ELCD database to obtain the life cycle inventory at the γ boundary (cradle to gate/grave). This stepwise procedure should be executed for every BUO in the production chain. The information on the material and energy balance of the process obtained can be used in modeling the subsequent process.

To facilitate the calculations, three databases are established:

- DATAPHYSCHEM: delivers data on the physical and chemical properties of material flows such as chemicals, biomass, ..
- DATABUO: delivers typical data of the BUO, such as efficiency factors
- DATAROT: delivers rules of thumb values that can be used as first estimate of order of magnitude

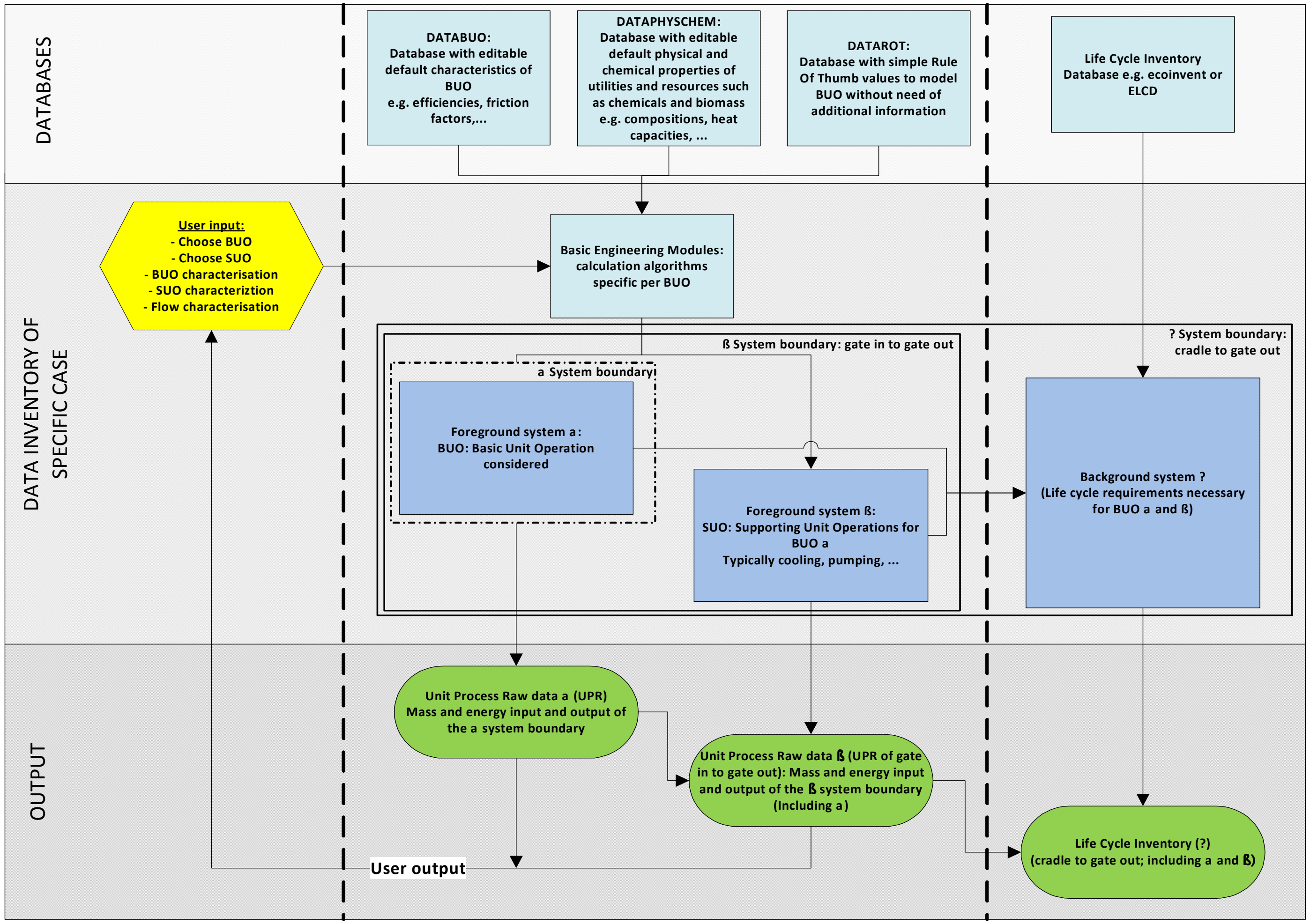

Figure IV.1.2: An overview of the structure of the basic engineering modules

In the following, two modules are presented for clarification, which will also be elaborated with an example in the results section. The other twenty calculation procedures can be found in the Appendix (A1).

2.1.1. Mechanical compression – single stage

Compression uses mechanical energy to increase the pressure of a gas. This can be used for steam to recover the latent heat, or for other gases such as air to obtain higher driving forces.

System boundary description

The BUO 'single stage mechanical compression' includes the mechanical energy consumption of compression in a reciprocating or centrifugal compressor. It assumes the adiabatic compression of ideal gases, which is a reasonable approximation for most compressors (Perry and Green, 1999). Supporting operations (SUO) such as pumping are not included in the α system boundary and should be modeled separately (Figure IV.1.3).

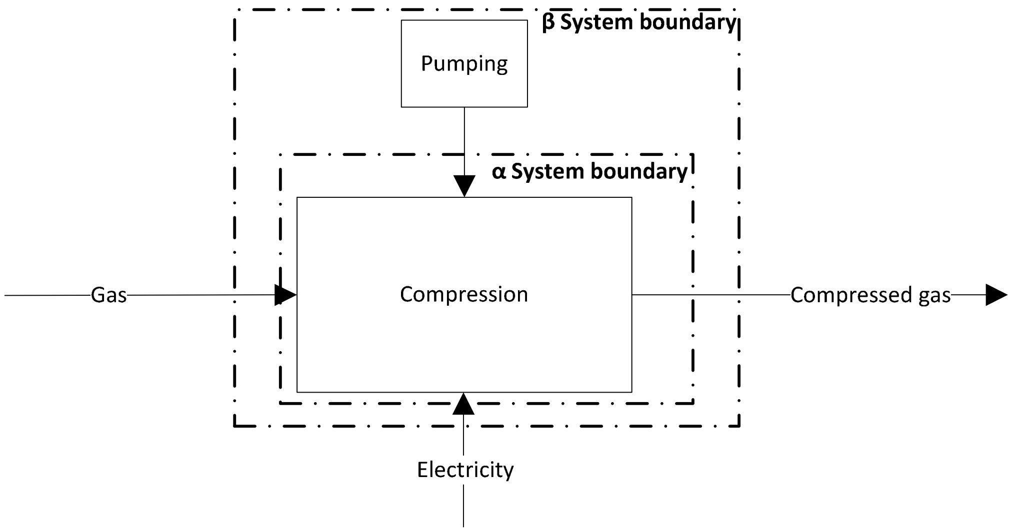

Figure IV.1.3: System boundary of the BUO compression

Calculation algorithm

The mechanical energy needed for the compression (P, in kW) can be obtained by:

$$P = \frac{m}{MM} \times W$$

With m the gas mass flow in kg/s, MM the molar mass of the gas and the specific compression work W (in kJ/kmol). In the case of ideal gases, the specific work can be obtained by (Perry and Green, 1999):

$$W = \frac{\zeta \times R \times T_i}{\eta \times (\zeta - 1)} \left[\left(\frac{p_c}{p_i} \right)^{\frac{(\zeta-1)}{\zeta}} - 1 \right]$$

With

R = universal gas constant (J/mol K)

p_c = pressure after compression (Pa)

p_i = initial pressure (Pa)

T_i = initial temperature (K)

η = efficiency factor

ζ = ratio of specific heats, adiabatic coefficient.

To facilitate this calculation procedure, DATAPHYSCHEM and DATABUO contain default values for adiabatic coefficients (Table IV.1.1) and efficiencies (Table IV.1.2) respectively. The first depends mainly on the type of flow (The Engineering Toolbox, 2012), whereas the second depends on the type of compressor and compression ratio or flow rate (Chemical and Process Engineering Resources, 2012).

Table IV.1.1: Information from DATPHYSCHEM: default adiabatic coefficients for different flow types (The Engineering Toolbox, 2012)

Range	Typical ratio of heat capacities
Steam 0.068 atm 50 – 316 °C	1.32
Steam 1 atm 107 –316 °C	1.31
Steam 10.2 atm 182 – 316 °C	1.28
Air	1.41

Table IV.1.2: Information from DATABUO: default evaporator efficiencies for different types of evaporators (Chemical and Process Engineering Resources, 2012).

Compression ratio (p_c/p_i)	Efficiency (%)
Reciprocating compressors	
1.5	65
2	75
3-6	80-85

Gas flow rate (m3/s)	Efficiency (%)
Centrifugal compressors	
2.8 to 47	76-78

In order to facilitate further calculations with the output flow, the following equation can be used to link temperature and pressure before and after compression (Perry and Green, 1999):

$$T_c = T_i \times \left(\frac{p_c}{p_i}\right)^{\frac{(\zeta-1)}{\zeta}}$$

With T_i the initial and T_c the temperature after compression.

This module is summarized in Table IV.1.3.

Table IV.1.3: Summary of the BUO Mechanical compression – single stage

Input values required	DATABUO	DATAPHYSCHEM	Output
Mass and type of feed Feed temperature Type of compressor Compression ratio	Efficiency	Adiabatic coefficients	Electricity use Physical properties of output stream

2.1.2. Evaporation

The module 'evaporation' calculates the energy required to concentrate a solution consisting of a non-volatile solute and a volatile solvent, where the latter is typically water. Unlike drying, the residue of an evaporation is a (sometimes highly viscous) liquid, whereas the main difference with distillation lies in the efforts to obtain a concentrated vapour product (McCabe et al., 2004).

System boundary description

The BUO 'evaporation' includes 1 to 3 effect evaporators. Vacuum pumps and possible recompression systems are not included in the α system boundary (Figure IV.1.4). These operations should be added as SUO if necessary. Calculations are valid over a broad temperature range, as long as the substance dependent coefficients for heat calculations remain valid.

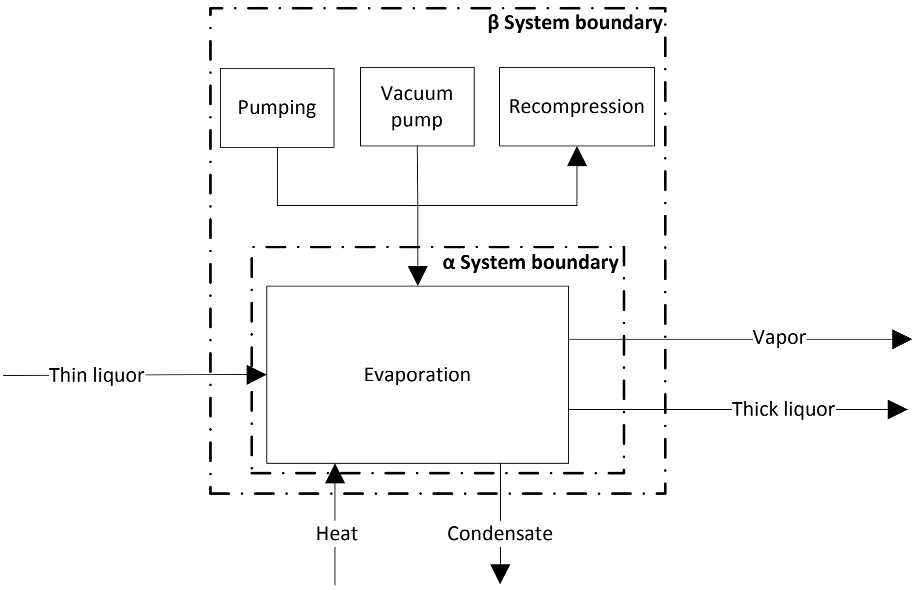

Figure IV.1.4: System boundary of the BUO evaporation

Calculation algorithm

The heat required for evaporation processes (q) can be obtained by making an enthalpy balance, with a thin liquor coming in as feed (f) and thick liquor going out (o) (McCabe et al., 2004):

$$q = \left(\left(m_f - m_o\right) \times H_v - m_f \times H_f + m_o \times H_o\right) / \eta$$

With m the respective masses of feed and thick liquor, H_v the specific enthalpy of the generated vapour, H_f the enthalpy of the incoming feed, H_o the enthalpy of the thick liquor and η an efficiency factor accounting for heat losses.

This equation can be converted to:

$$q = \left(\left(m_f - m_o\right) \times \lambda + m_f \times c_p \times \left(T_b - T_f\right)\right) / \eta$$

With λ the latent heat of vaporization, c_p the mean heat capacity of the feed, T_b the boiling temperature of the mixture and T_f the temperature of the feed. This last equation assumes a negligible heat of dilution, which is a reasonable assumption for flows such as sugars, organic salts and paper mill liquors (McCabe et al., 2004).

In order to save energy, a part of the enthalpy in the vapour is recovered in sequencing vessels or 'effects', which is called multi-effect evaporation. To estimate the amount of heat savings per effect and assuming no recompression, the default values in Table IV.1.4 from DATABUO can be used for one to triple effect evaporators (Earle and Earle, 2004). The effective heat required (q_{eff}) then becomes:

$$q_{eff} = q \times F_{eff}$$

Table IV.1.4: Default steam savings in one to triple effect evaporators (Earle and Earle, 2004)

Number of effects	Calculated amount of heat required per amount evaporated (F_{eff})
1 effect	1.00
2 effects	0.52
3 effects	0.37

The module is summarized in Table IV.1.5.

Table IV.1.5: Summary of the BUO evaporation

Input values required	DATABUO	DATAPHYSCHEM	Output
Mass and type of feed Temperatures Pressure Mass flow of thick liquor Number of effects	Steam savings for 1 to 3 effect evaporators	Heat capacities Enthalpy of vaporization Boiling temperature	Required heat Output product flows with temperature

2.2. The biorefinery case study

The presented approach is tested in a case study where a biorefinery processes wheat, flour and sugars as into specialty sugars, starch, gluten, ethanol and animal feed. The conversion of the biofeedstock concerns typical processes of a biorefinery, starting with dry and wet milling steps and further separations mainly with centrifuges and sieves. Afterwards the intermediate flows are upgraded to final products, mainly by drying and evaporation. In this type of biorefinery, few ‘reactions’ occur as it is more the separation of the different molecules of the biofeedstock as such, possibly after a hydrolysis step. There are two exceptions, namely the fermentation of wet starch streams to bioethanol with a subsequent distillation section, and a combined heat & power (CHP) engine where natural gas is converted into steam, hot water and electricity.

The case study is a complex system with a large number of single processes where an extensive dataset was gathered as a year average of 2009 for many of these processes. Yet, it was not possible to collect all data of all processes. Therefore a selection has been made of ten of the twenty-two elaborated processes based on confidentiality, availability of detailed data and availability of a specific BUO that is applicable for the considered process. This is still valuable as it gives a first indication of the accuracy of the results and it can serve as guidance for further work on the quantification of life cycle inventories for prospective assessments by means of parameterized modules. In total, ten of the twenty-two BUO approaches were tested, often based on several subsamples within their own α boundary. This test is elaborated in Table IV.1.6, where also the sample size is given. In total, 41 subsamples were tested, where identical processes that are in a parallel configuration (e.g. two centrifuges), are only counted once.

Table IV.1.6: The elaborated BUO categories with case specific information and sample size

BUO	Case specific process information	Sample size
Comminuting	The wheat grains are first dry-milled by using a complex system of rolls and rotors	3
Agitation and mixing of liquids and suspensions	Both the agitation in the fermentation tanks and the dough mixer are studied	3
Sedimenting centrifuges	Centrifuges are mainly used for wet separation of dough, gluten, etc.	7
Evaporation	After wet separation, the dry matter content of flows is increased by evaporators with 1 or more effects.	3
Mechanical compression – single stage	Recompression is used to upgrade vapor of evaporators	4
Fermentation	Wet starch streams of the factory that are less suitable as food or feed are fermented to bioethanol	1
Binary distillation	The 'beer' solution obtained from fermentation is distilled to purify the ethanol	1
Heating	Several flows are preheated before evaporation, drying, etc.	5
Incineration for heat and power	A CHP working on natural gas produces hot water, steam and electricity to supply the factory with energy. Excess electricity is sold to the local grid	1
Conveying solids	Before the wet milling steps, biomass is mainly transported and ensilaged by different types of conveyors	13

The results of the modeling of mass and energy balances within the α system boundary are validated with the actual mass and energy balances of the factory. As the sample size (n) was limited for some operations, no statistical uncertainty is elaborated. Instead, per calculation of a basic unit operation within the α system boundary, an Accuracy Factor and a Relative Approximation Error (RAE) is calculated, which are defined as respectively:

$$\text{Accuracy Factor (AF)} = \frac{\text{calculated value}}{\text{actual value}}$$

$$\text{Relative Approximation Error (RAE)} = \frac{\sum_n |1 - \text{AF}|}{n}$$

2.3. The application in a Carbon Footprint calculation

In this chapter, the greenhouse gas emissions caused by products of a biorefinery are assessed in a life cycle perspective. The parameterized BUO modules are used mainly to predict energy consumption of the different processes. The accuracy of this calculation is then tested with the actual data obtained from the factory. Afterwards, the results are linked to life cycle assessment by calculating a Carbon Footprint based on the IPCC 2007 (Solomon et al., 2007) impact assessment method, relying on the ecoinvent database for the datasets to model the γ system boundary.

3. Results and discussion

Within the aforementioned limitation, it was possible to calculate 27% of heat and 42% of the electricity use of the factory. In the following, first two examples of BUO validations are presented. Second, an overall overview on the tests is discussed and third, the application in a Life Cycle Assessment is analyzed.

3.1. Validation examples

3.1.1. Mechanical compression – single stage

Most compressors in the factory are used for recompression of vapour in evaporator systems. One of the compressors upgrades the vapour of 377K to usable steam of 439K and has an actual energy use of 2599kJ/kmol. Using the calculation procedure for this BUO with the values given in yields a predicted energy use of 2829 kJ/mol (Table IV.1.7), obtaining a Relative Approximation Error of 9% for this process. By applying this BUO approach, the output temperature and pressure are obtained, allowing further calculations with the available heat of the steam, and the electricity use of the compressor is known when linked to the flow rate. Coupling this to a life cycle database allows obtaining the carbon footprint of the operation. Based on the Belgian electricity mix (medium voltage), the carbon footprint of compression of 100 kg steam according to the parameters in Table IV.1.7 results in an emission of 1.48 kg CO_2-eq according to the calculations, whereas the actual emission is 1.36 kg CO_2-eq.

Table IV.1.7: Parameters in the calculation procedure of the BUO mechanical compression – single stage

DATA source	Symbol	Value	Unit
INPUT	pi	101325	Pa
INPUT	Ti	377	K
INPUT	Tc	439	K
DATAPHYSCHEM	R	8.31	J/mol*K
DATAPHYSCHEM	γ	1.31	
DATABUO	α	77	%
OUTPUT	Pc	192769	Pa
OUTPUT	p_c/p_i	1.90	
OUTPUT	W	2829	kJ/kmol

3.1.2. Evaporation

After the different wet milling and separation steps, different starch streams require higher dry matter concentrations. One of the stream enters in an evaporator at a dry matter concentration of 2.8% and leaves at 4.9%. The actual energy delivered by the steam is 998kJ per kg incoming feed, whereas the calculated value indicates 973kJ per kg (Table IV.1.8), resulting in a RAE of 3%. Using this BUO thus allows to estimate the heat requirement of the evaporation process. Coupling this to a life cycle database gives a Carbon Footprint of 2.65 kg CO_2-eq according to the calculations, and 2.72 kg CO_2-eq based on the actual data (by using Heat, at cogen 1MWe lean burn, allocation exergy/RER).

Table IV.1.8: Parameters in the calculation procedure of the BUO evaporation

DATA source	Symbol	Value	Unit
INPUT	m_f	1.00	kg
INPUT	m_o	0.56	kg
INPUT	T_i	108.0	K
INPUT	T_b	108.6	K
DATAPHYSCHEM	c_p	4.10	kJ/kg*K
DATAPHYSCHEM	λ	2230	kJ/kg
DATABUO	η	90	%
OUTPUT	q	973	kJ

3.2. Overview of the validation

Figure IV.1.5 summarizes the Accuracy Factors obtained by the validation of the different samples, where 1 would be a perfect fit of the actual mass and energy balance of the factory. An overall average relative approximation error of 22% is obtained, whereas the majority of parameterized modules give estimates within a reasonable 10% RAE range.

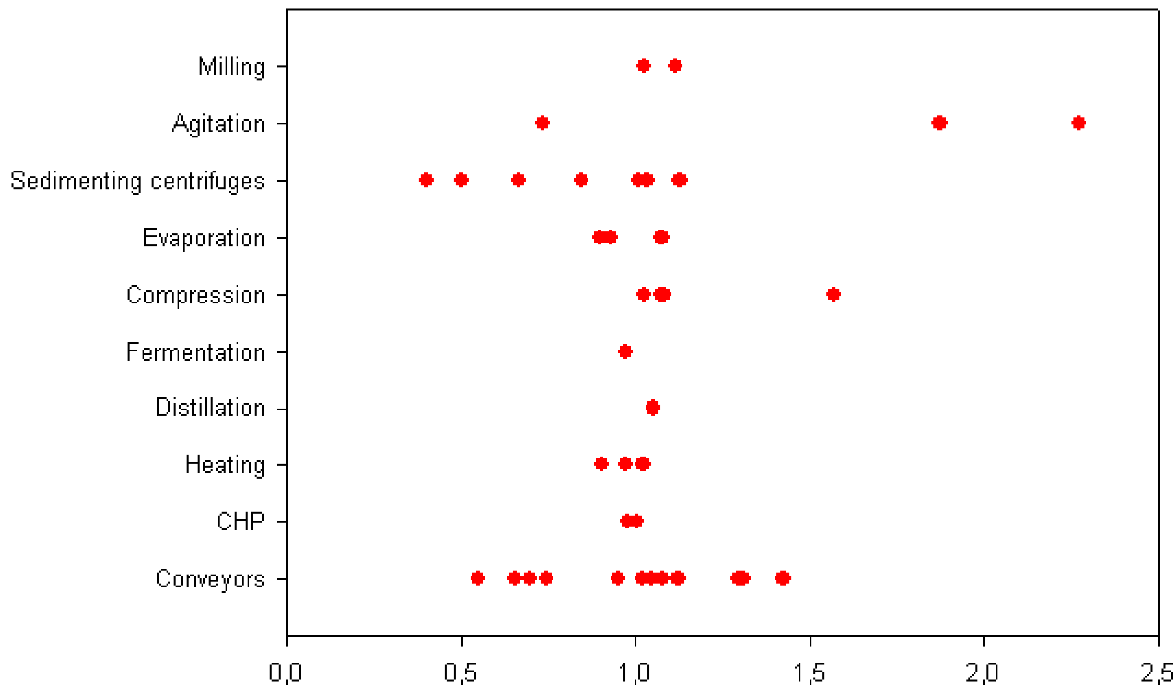

Figure IV.1.5: A summary of the Accuracy Factors of the different Basic Unit Operations that are tested in a case study. A value of 1 means a Relative Approximation Error of 0%.

The Combined Heat and Power (CHP) plant is the starting point and is accurately predicted with a RAE of 0% for electricity and 2% for heat production. The standard efficiency factors for an efficient CHP on natural gas producing electricity and heat are thus reliable in this case, which is essential in the sustainability assessment of the factory as this CHP delivers energy to all other operations and thus has a large influence on the final result. It should however be noted that the heat availability is predicted accurately, but not necessarily all heat is required in the processes. The allocation factors in LCA studies should thus be based on the real heat use instead of the potential heat use.

The calculations for milling (comminuting) result in a RAE of 7%. A good Bond Work Index (information on this can be found in the appendix (A1)) should however be found for the milled material, which might not be available in some cases. For wheat grains however, a reliable value was found in literature (Das, 2005). It should also be noted that the calculations are valid if the power of the mill is put directly on the particle. In case the particle size is reduced by rotational forces causing friction between the particles, other calculation procedures should be sought.

The deviation in the agitation model is larger; the validation highlights RAE values of up to 107% for the fermentation and 27% for the dough mixer. As a clarification the used equations in the parameterized module of agitation power (P) should be considered (McCabe et al., 2004):

$$P = N_P \times \rho \times N^3 \times D_a^5$$

for the turbulent region and

$$P = K_L \times \mu \times N^2 \times D_a^3$$

for the laminar region. With μ the viscosity, ρ the density and N_p and K_L flow regime dependent pump numbers. The prediction of equipment power thus depends heavily on the impeller velocity (N) and diameter (D_a). As these parameters are in most cases approximated, small deviations from the real value result in a large sensitivity of the final result. Furthermore, this calculation requires fluid properties, which are approximated by the Power Law for 'slurry' type of flows, resulting in an additional potential source of deviation. The same is true for pumping incompressible fluids in a biorefinery. It is very difficult to obtain all exact parameters for the calculation (e.g. amount of turns, length of pipes, etc.). This is more straightforward for conveyors where the module basically requires only the type of conveyor, the flow rate and an approximation of the length. The calculations based on 13 samples yield RAE of 23%, which is reasonable as a first estimate, knowing that this operation is of a smaller relevance relative to the total power use in the factory.

The average RAE for sedimenting centrifuges is 25% if each type is counted once. This factor is lower for the total absolute centrifuge power (10%) as the most accurately predicted centrifuges have the largest contribution to total power use. In 4 of 7 samples the power was predicted accurately (average RAE = 8%), but in the other samples a larger RAE was obtained (33 to 60%). This is the disadvantage of the fact that this module is not based on a continuous equation, but on integer ranges depending on typical combinations of liquid and solid throughput. The largest deviation occurs when it is not obvious to which exact range the centrifuge should be assigned.

The fermentation section was predicted with a RAE of 3% for the fermentation yield and 4% for the energy use of the distillation column. This module is however highly sensitive to the reflux ratio applied in the column, as this is multiplied with the latent heat, causing the largest part of the energy requirement. The (pre)heating steps are predicted with a relative approximation error of 4% and also the heat use per evaporator is predicted fairly accurate (RAE = 8%) based on the thermodynamic balance. The configuration of the different evaporators can however be complex, with different effects and with intermediate compressors to upgrade vapor streams. As a result, the total heat required is not the sum of each heat requirement separately. Instead the BUO modules for heat consumption also require heat integration and consideration of valorization of 'waste' heat from other processes and of the use of recompressors to upgrade vapor. The compressors themselves are relatively accurately predicted (RAE = 6%). It should however be noted that two adjustments had to be made; first one of the compressors is known to have a lower efficiency than 'traditional' current equipment where a default value of 77% is assumed for centrifugal compressors. Second, it is possible that in industry equipment is reused from a previous application and therefore not optimally sized for their current task, which might lead to additional energy consumption, but which is sound from an economic perspective.

3.3. Applying the BUO approach in a Carbon Footprint case study

The carbon footprint (γ system) of the calculated modules of the factory is 96% of the carbon footprint based on actual data when excluding the 'milling' steps based on rotational forces causing friction and including only the optimally designed compressors (87% including these excluded processes). This good score can be explained by the fact that the results of the parameterized modules with the highest accuracy factor have a large share in the absolute carbon footprint of the factory (Figure IV.1.6). Additionally, the obtained impact is the sum of energy use in the α system boundary of the ten applied BUO approaches and has a better score than each BUO separately, which can be explained by considering Figure IV.1.5, from which no generic trend of over- or underestimation can be observed resulting in a compensation of higher and lower approximations. Furthermore, when assembling the results of each BUO separately, we performed a similar heat integration over the different modules compared to the real factory. This aspect requires care, as the sum of heat calculated per module is much higher than real total heat use. The degree of heat integration however, cannot be generalized as it depends on the specific process chain, availability of 'waste heat' and company policy. Another difficulty is integration of the β system boundary in the assessment. In the studied biorefinery these SUO operations are not negligible: approximately 22% of total electricity use is used for pumping liquid fluids and as the biorefinery is situated in a densely populated area, an elaborated system of controlling air streams by ventilation and aspiration is used. This SUO system accounts for approximately 16% of the plant's electricity use and was also not validated because of its complexity. This system of SUO is difficult to generalize or to model separately; information such as length and amount of turns in piping systems or the pressure drop in ventilators is essential but needs detailed designing which is not straightforward. Another shortcoming is the unavailability of the BUO drying, which accounts for almost all heat use that was not incorporated in this validation. It is indeed a challenging task to find a suited generic engineering module for this process, as there is a large range of dryer types each with their specific configuration. The energy demand of this process depends on this configuration and is a combination of interlinked factors such as air humidity, temperature, velocity, surface area, equilibrium moisture content, etc. A large range of company specific choices is possible impeding generic calculations, such as the balance between more electricity to achieve a higher air flow rate over the material or using hotter air to increase efficiency per volume of air used. On top of the parameterization of energy consumption, also the mass flows in a studied system should be studied, as the impact of the agriculture of the biofeedstock should also be allocated to the output products. In this work, the fermentation yield was approximated with an relative approximation error of 3%. Apart from the various hydrolysis steps (chemical reaction), the other mass flows are separations of different molecules of the plant (e.g. gluten, starch, …). The latter are user specific choices that are rather straightforward and are therefore not included in this work. The use of utilities such as foam inhibitors, silica, cleaning agents, buffers and enzymes is case specific and requires expert judgment rather than generic parameterization. While the contribution to the Carbon Footprint of the latter is relatively small (approximately 6%), the combination of the different drawbacks might cause a significant increase in the deviation of the total carbon footprint of a prospective LCA with the BUO approach might increase significantly.

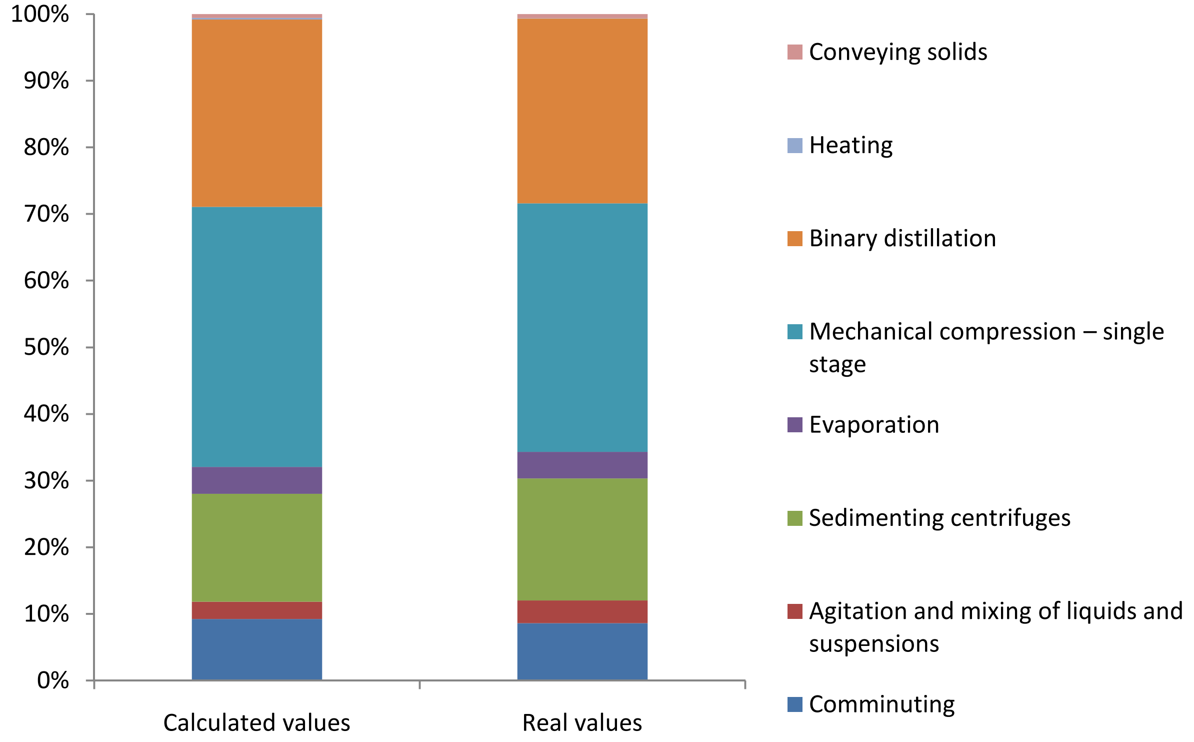

Figure IV.1.6: A comparison of the real and calculated value based on the relative contribution of the different processes to the final carbon footprint

4. Conclusions

The proposed approach of using engineering calculations, rules of thumbs and default values to obtain the mass en energy balance of a system by applying a modular BUO approach is identified as a useful and reliable way to support prospective life cycle assessments. Of the twenty-two parameterized modules, ten were tested in the case study. Apart from agitation, most of these modules yield relatively good results with an overall average relative approximation error of 22%. The carbon footprint of the tested sample was approximated with an accuracy of 96%, partly corrected by over- and underestimation. Three major shortcomings were identified however. Firstly, whereas the inventory of the α boundary was obtained with an acceptable error, the supporting unit operations such as pumping are very specific and difficult to obtain whilst not being negligible. Secondly, a factory is complex and processes are not independent from each other; a successful application of the BUO approach therefore requires a careful integration of heat use instead of a linear summation of heat use of different processes. Thirdly the list of selected BUO is still limited to twenty-two, whereas other operations also occur in industry. For example in biorefineries, operations such as cyclones and dryers are frequently used. More parameterized modules should thus be developed in the future.

Nevertheless, while more case studies are necessary for confirmation of the results in this study, the currently available modules produce relatively reliable results. The possibility of integration of these modules as parameterized unit operations in LCA software can be of major value to obtain a detailed data inventory necessary for prospective assessments. The modules should however be used with care and with a realistic design of a production chain in mind.

2. Allocation in multipurpose biorefineries: a critical choice affecting scope and study outcome

Redrafted from:

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1. Introduction

Life Cycle Assessment (LCA) is a valuable approach to assess the environmental burden of products and services by identifying and quantifying flows between the technosphere and the natural environment. Applying LCA is therefore sound from a scientific perspective, but it is also an ambitious task, which has led to several methodological issues that often do not have a simple solution. One of the most discussed methodological issues is the allocation procedure used in LCA (Finnveden et al., 2009). The ISO 14040/14044 series define allocation as "the partitioning of the input or output flows of a process or a product system between the product system under study and one or more other product systems". The guideline furthermore suggests a three step procedure for dealing with the allocation problem; first, allocation should be avoided by subdivision of the process or by system expansion. The second and third point of the ISO guidelines are the partitioning allocation procedures and propose the use of physical causations, or the use of another measure as the last preference. In practice however, subdivision only solves multi-functionality by gathering more detailed data of separable processes, but it is not sufficient if the studied process is inherently multifunctional such as in the case of a centrifuge (Azapagic and Clift 1999; Ekvall and Finnveden 2001). Allocation methodologies most often applied are therefore using system expansion and applying allocation on a mass, energy or economic base (Lundie et al. 2007).

While the ISO guideline still leaves a relatively arbitrary choice between these options, it is necessary to understand that the base of the allocation problem is actually inherent to the nature of the (initial) LCA methodology which starts from a functional unit approach, often a product or service, to which the life cycle inventory and thus impact should be assigned to. On the other hand it is obvious that all these products and services are part of a complex multifunctional economic system. This actually raises the question if it is required to separate the functional unit from reality, or if reality should be assessed as an integral system. This question is obviously linked to the goal and scope of an assessment. In the CALCAS project (Zamagni et al., 2009) three study objects are identified:

- Product oriented technosystems
- Meso-level technosystems
- Economy-wide technosystems

The first is the area of ISO LCA studies and focuses on single products with an equal function. Doing so inherently faces the challenge to distill one functional unit out of the complex reality, which is stated to be an artifact requiring an artificial solution (Guinée et al., 2004). The second and third study objects focus on groups of products and on geographical or political entities respectively. While the time frame can be retrospective or prospective in all three study objects, it is clear that the main difference is the inclusion of additional processes and interactions in the technosphere, also known as the distinction between attributional and consequential assessment. The latter indeed includes those processes that are affected by the consequences of the decision at hand (Zamagni et al., 2012).

In this context, this study focuses on the role of allocation in the assessment of different study objects and the challenges accompanying its practical implementation. For the purpose of demonstration, the Carbon Footprint of a multipurpose biorefinery product system is calculated. As an exponent of the increasing popularity of life cycle assessment, the Carbon Footprint is more and more introduced by governments and industry in legislation and marketing, especially regarding to biorefineries and the biobased economy. This has resulted in several methodological documents with different allocation procedures, but often without a clear rationale why that specific allocation procedure was chosen. It is therefore the goal of this study to compare the impact of the allocation procedure between the different methodologies, similar to other studies such as the work of Curran (2007a), Mendoza et al. (2008), Luo et al.

(2009), Kaufman et al. (2010) and Sayagh et al. (2010) next to analyzing why these results vary and which consequences of the specific allocation choice can be expected in biorefineries. This work is therefore subdivided in three parts:

- First, the link between the study object and the allocation procedure is made for biorefineries. A distinction can be made between partitioning methods and system expansion (Frischknecht, 2000; Ekvall and Finnveden, 2001), of which Weidema (2003) argues to use partitioning, preferably economic allocation, in attributional studies and system expansion in consequential assessments.
- Second, the inherent properties to characterize flows of each partitioning allocation option are discussed. This study deals with allocation based on monetary value, dry matter fractions, energy (LHV; Lower Heating Value) and exergy content.
- Third, allocation is considered as a source of variation following the conclusions by Curran (2007b) who states that one should not question the variation in calculation results, but determine the amplitude of variation. From this perspective, variation can be quantified and incorporated in the final result. This phenomenon can eventually be called decision rule uncertainty (Huijbregts 2011). If the term 'uncertainty' however is defined as "the fact that measured values frequently do not match the true values, but differ from them in a probabilistic manner" (Ciroth et al. 2004), using it in the context of model uncertainty would be slightly misplaced. The authors therefore prefer to use the terminology decision rule variation, defined as "the coefficient of variation caused by the subjective choice of allocation methodology". This variation can then be quantified and combined with the more commonly calculated data uncertainty which is likely to be determined by the pedigree approach and a subsequent Monte Carlo simulation.

2. Methodology

2.1. Case study specification

A case study has been executed, focusing on a Belgian biorefinery processing wheat, flour and sugars to starches, specialty sugars (amongst others fructose-glucose syrup, maltodextrin, high maltose and dextrose), gluten, animal feed and bioethanol. The complexity of the factory can be demonstrated in the process diagram of the gate to gate production facility as shown in Figure IV.2.1. The assessed production steps include dry and wet milling, several separation and drying steps and a fermentation section for ethanol production. Furthermore, a wastewater treatment facility with biogas generation and a CHP (Combined Heat and Power) fed by natural gas are included, of which part of the produced electricity is consumed within the factory gates and part is redistributed to the local electricity grid. In this type of biorefinery, the difference between main products and byproducts or waste is not relevant, since all molecules of the incoming biomass are used for certain end applications and are therefore considered to be 'useful'. This factory is thus a typical example where a certain type of allocation is necessary and where a Carbon Footprint is required because of regulations on biofuels (European Commission, 2009).

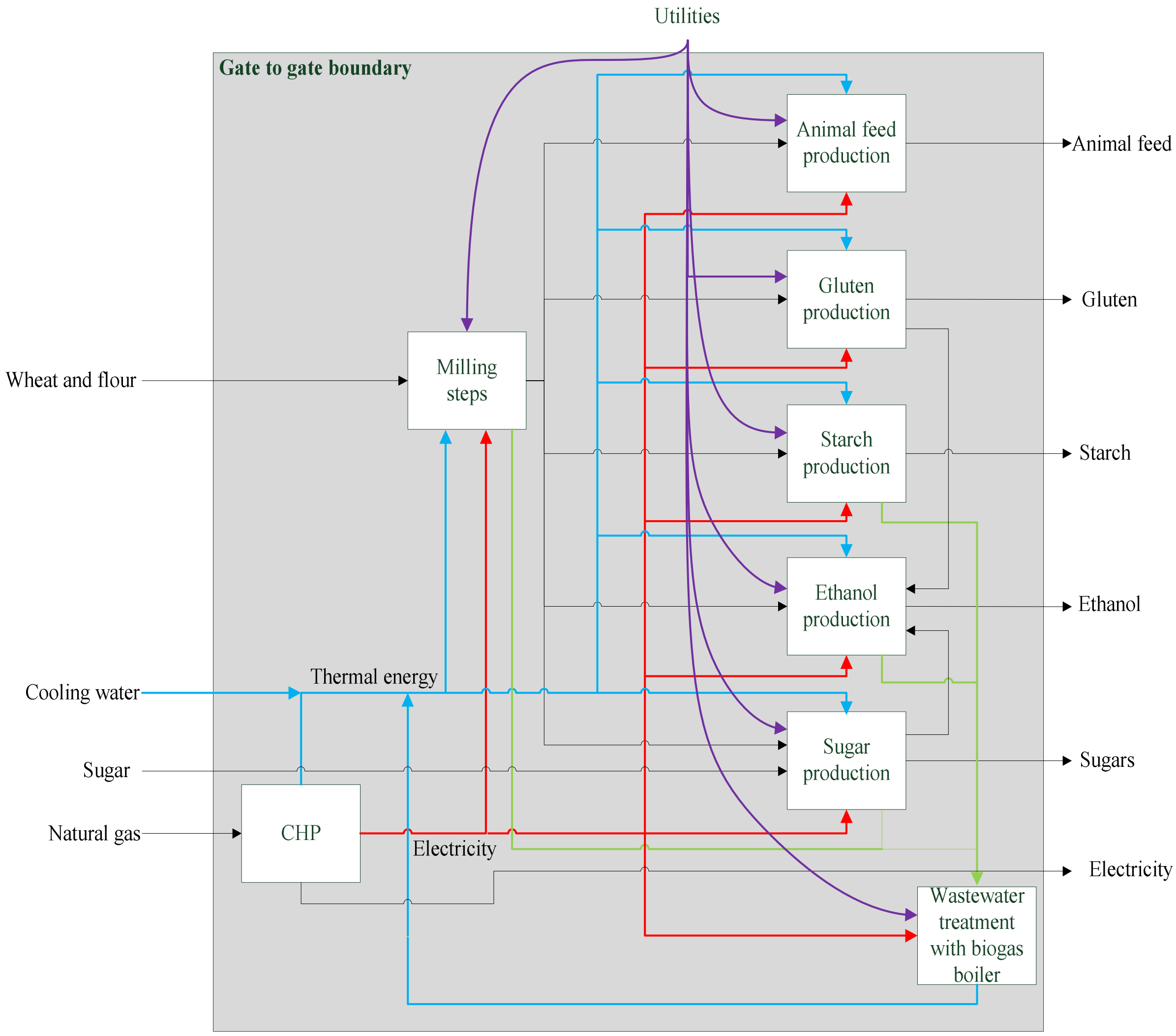

Figure IV.2.1: Process diagram of the gate to gate boundary of the studied biorefinery

2.2. Life Cycle Assessment specification

The LCA was performed according to the ISO 14040/14044 guidelines in which the impact of the studied system is allocated to the different functions delivered by the system. The results are scaled to 1 kg animal feed, 1 kg gluten, 1 kg starch, 1 kg bioethanol and 1 kg sugars. The system boundary includes the full cradle to gate production chain, for which data of the foreground system, within the gate to gate boundary, was collected at the Belgian processing facility as a yearly average of 2009 and data of the background system was retrieved from ecoinvent v2.1 datasets. Key datasets used are: 'wheat grains conventional, Barrois, at farm

(FR)' for the incoming wheat, 'maize starch, at plant (DE)' for flour, 'potato starch, at plant (DE)' for potato starch, 'sugar, from sugar beet, at sugar refinery (CH)' for the incoming sugars and 'natural gas, high pressure, at consumer (BE)' for the natural gas delivered to the CHP. This was combined with the necessary background processes for 56 different chemicals and transportation by means of truck, train or boat. The direct emissions at the CHP were taken from analytical measurements in the factory and checked by constructing mass balances.

First, system expansion was applied by using the 'substitution or avoided burden method' by subtracting the impact of equivalent market products from the total impact of the product system (Guinée et al., 2002). In the theoretical framework of system expansion a detailed market assessment is required to approximate consequences on production volumes and changes in demand (Weidema, 2001). This is a challenging aspect, as for example ethanol can be used as base chemical or as fuel. Similarly, gluten can be used as protein source for vegetarians replacing meat or other protein sources or as additive in bakeries where it can be replaced by xanthan gum or guar gum. On top of this complex market mechanisms, it is also difficult to find reliable datasets to model the inventory of the displaced products. Therefore in this study the substitution method was applied in two possible, but theoretically imperfect scenarios in which wheat starch is replaced by starch from other sources of biomass, gluten is considered as a protein source, ethanol is used in the fuel market, the specialty sugars such as maltodextrin are replaced by generic sugars and animal feed is substituted by soybean meal. The used ecoinvent processes are 'potato starch (DE)', 'protein concentrate, from whey, at fermentation (CH)', 'soybean meal, at oil mill (US)' and sugar, from sugar beet, at sugar refinery (CH)' in scenario 1. Alternatively, 'maize starch, at plant (DE)', 'proteins, from grass, at fermentation (CH)' and 'soybean meal, at oil mill (BR)' are used in scenario 2. In both scenarios bioethanol is considered as fuel and substituted by the petrol reference as defined by the European Directive 2009/28/EC (European Commission 2009).

For the partitioning methods, allocation was applied at two levels; first, the factory was considered as a ‘black box’, where dry matter, energy (LHV), exergy and economic allocation were used, and second, a ‘subprocess level’ allocation, was executed for the dry matter, energy (LHV) and exergy factors. At the subprocess level an economic allocation was not possible due to unavailability of data on prices and costs of the intermediate flows. The black box economic allocation was based on annual average selling prices of 2009. Dry matter allocation was based on data of proximate analysis of process streams. This approach was combined with energy (LHV) allocation at the CHP, because of the limitations of mass as a physical parameter in energy systems.

Lower Heating Values were obtained by combining experimental data on compositions with literature data on heating values. To calculate the exergy content of substances chemical and physical properties were required. These were collected at the production plant by means of different analytical measurement methodologies and data available in literature. Based on these compositions, the exergy contents were calculated by using the values presented by Szargut (1988) or by using the group contribution method, the macro nutrient method or data from Gibbs free energy of formation (Szargut, 2005). Generally, the group contribution method can be used to estimate the exergy content of organic substances. An example for glucose is given in Table IV.2.1, where the chemical exergy of this substance is calculated to be 2976.09 kJ/mol or 16.53 MJ/kg.

Table IV.2.1: The chemical exergy calculation of glucose by using the group contribution method

Group	Specific Chemical Exergy (kJ)	Number of groups	Total chemical exergy from this group (kJ)
CH (ring)	543.05	5	2715.25
CH2	651.46	1	651.46
-O- (ring)	-106.64	1	-106.64
OH (to CH ring)	-58.16	4	-232.64
OH (to CH2)	-51.34	1	-51.34
Total			2976. 09 kJ/mol

The macro nutrient method can be based on the group contribution method by analyzing carbohydrate, protein, fat, ash and water content of the biomass, eventually generating the total exergy content of the biomass as the weighted sum of its components. For inorganic substances the exergy content can be calculated based on the Gibbs free energy of formation by using the following formula:

$$ex_{ch} = \Delta G_f^0 + \sum_k v_k \times ex_{ch,k}$$

With ΔG_f° the standard Gibbs free energy of formation of the compound and v_k and $ex_{ch,k}$ respectively the amount of moles and specific chemical exergy of products and reactants k.

Due to confidentiality, only a limited data inventory can be shown (Table IV.2.2), in which also the dry matter, energy and exergy contents of the biomass streams are represented. This table also highlights that, apart from some small mass losses in the fermentation section and some loss in the wastewater, the incoming biomass is converted with a rather high efficiency (De Meester et al., 2011).

Table IV.2.2: The mass, energy and exergy balance of the factory per 1000 kg incoming biomass

IN	Mass (kg)	DM content	Dry matter (kg)	Energy content (MJ/kg)	Energy (GJ)	Exergy content (MJ/kg)	Exergy (GJ)
Wheat grains	568.7	84.0%	477.7	13.9	7.9	16.3	9.3
External Flour	33.4	86.0%	28.7	14.3	0.5	16.7	0.6
Sugars	397.9	76.1%	302.8	12.3	4.9	13.4	5.3
OUT	**Mass (kg)**	**DM content**	**Dry matter (kg)**	**Energy content (MJ/kg)**	**Energy (GJ)**	**Exergy content (MJ/kg)**	**Exergy (GJ)**
Dried starch	98.0	88.1%	86.3	14.7	1.4	16.4	1.6
Gluten	38.0	92.8%	35.3	22.4	0.8	23.4	0.9
Animal feed	180.0	84.5%	152.0	16.3	2.9	17.3	3.1
Ethanol	37.6	99.9%	37.6	27.0	1.0	29.5	1.1
Sugar	622.3	74.1%	461.0	12.0	7.4	12.7	7.9

As an impact assessment methodology the GWP 100 of the IPCC 2007 report was chosen (Solomon et al., 2007). As such the total life cycle GHG emissions and the resulting Carbon Footprint of the output products of the factory is known.

3. Results and discussion

3.1. Linking the allocation procedure to the scope of the assessment

According to the ISO guidelines, the first step of an LCA is to define the goal and scope of the study. In many cases this phase seems disconnected from the choice of allocation procedure. However when comparing system expansion and the partitioning approach, it is clear that the theory of system expansion has a completely different starting point. Expanding the system inherently means that the functional unit of the system is expanded from 1 product or service to a basket of products and services (Guinée et al., 2002; Wardenaar et al., 2012). Furthermore, because the displacement of products is often only practically feasible for marketable products and not so easily for intermediates, the study automatically becomes a ‘black box’ assessment. In the studied biorefinery, the basket of services (the different products produced in the factory) has an impact of 680 kton non biogenic CO_2-eq per year whereas the production chain of equivalent products in scenario 1 and 2 emit 538 and 734 kton non biogenic CO_2-eq per year respectively. When applying system expansion consistently over the full life cycle by including all background datasets, automatically more functions become involved (e.g. all products from the oil cracker if petrol is replaced by bioethanol) elaborating the assessment to the complete economy. This choice in allocation procedure thus changes the research question from: “what is the impact of this product”, to “what is the impact of this activity on the economy”. The latter is an interesting research question to analyze for example which product mix a biorefinery should produce and to which markets the products should be delivered to save most fossil fuels. Furthermore, it allows companies to attribute energy intensification in the gate to gate boundaries to the complete product mix. On the other hand, the functional unit has been extended in such a way that the product specific information is lost. Knowing the impact of one function in the created service basket is actually not the purpose of system expansion and it requires the solution to substitute other functions in the basket with equivalent market products. The consequence is that the impact strongly depends on the configuration of the factory which makes comparisons between functions difficult. In the performed case study for example, the impact of bioethanol by applying substitution is obtained from the research question “is the produced food of the biorefinery more sustainable than food from the food industry”. Such meso-level or economy-wide technosystem assessment indeed ‘trades’ emissions between product systems and sectors, allowing impacts to become negative such as for gluten in this case study. The gluten is thus a ‘good’ product mainly because the animal feed of the factory potentially displaces soybean from Brazil (and the related land transformation). This larger scope can therefore give interesting insights for scenario modeling, but induces a loss in information that might be required in product specific research and policy questions. A biofuel for example is seen as a 'renewable resource' that should typically save fossils and meet emission targets at the level of the product and production processes. This difference in scope is commonly overlooked in Carbon Footprinting, where the goal can be to attribute a guilt or responsibility (Weidema, 2003) to one product and not necessarily to a basket of products. System expansion might therefore not be used to 'avoid allocation' in any kind of study, but rather it might be used to perform a different type of study.

Apart from this theoretical difference, there are also practical aspects. This work has elaborated two scenarios in which a comparison is made between system expansion and the average values of the different partitioning allocation approaches with lower and upper limits to be discussed in the second part of this work (Figure IV.2.2). The Carbon Footprints obtained by using these two scenarios show a larger variation compared to using different partitioning approaches confirming the high dependency on the reference scenario and the increase of uncertainty by introducing this approach in LCA studies (Lundie et al. 2007). This dependency on factory configuration and the uncertainty involved in market scenario modeling might be misleading for product policies (Wardenaar et al., 2012).

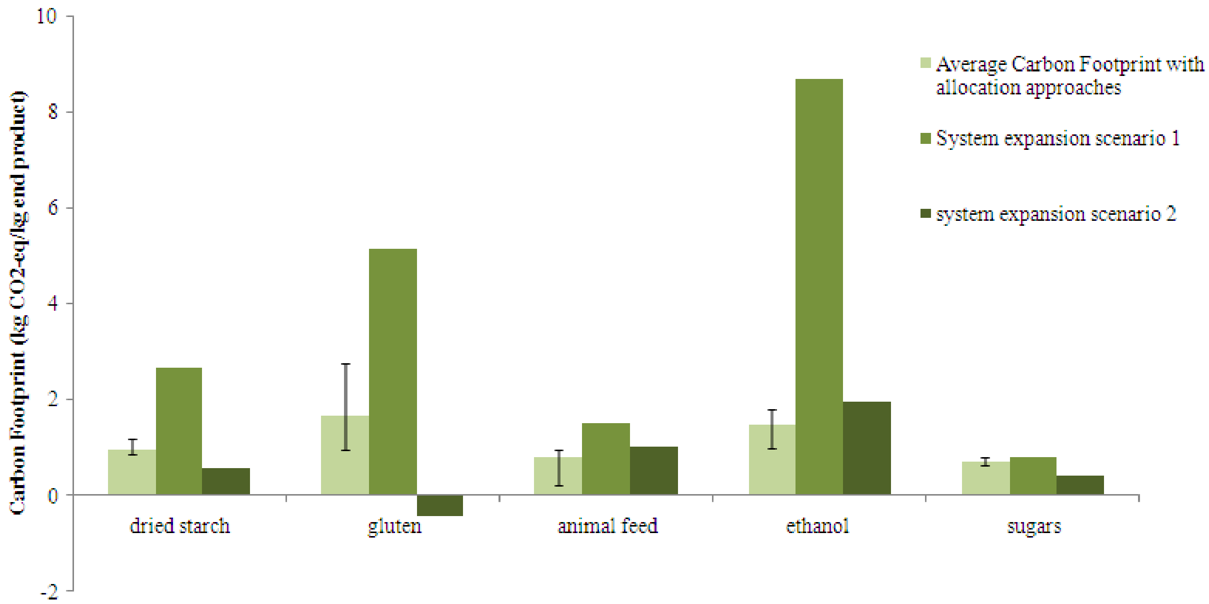

Figure IV.2.2: The comparison between system expansion and the average (with lower and upper value; n=7) of the different partitioning procedures

Nevertheless, this induced uncertainty can gradually be decreased in the future and should not inhibit the interesting theoretical perspective of meso or economy wide assessments. This will however require further research; first it is required to collect more data inventories, because all functions of the economy are required to have a complete analysis, second, functions should be recognized as equivalent to each other, and third, detailed market studies are necessary to understand and quantify how these equivalent functions react on changes within the market. Suh et al (2010) developed a generalized framework for system expansion based on matrix calculations taken from input-output literature, however the presented approach is only feasible when the process and product matrices can be inverted and thus are rectangular. This rectangularity problem, which is actually the basis of the allocation problem, is already known for a long time (Konijn, 1994; Heijungs and Frischknecht, 1998), but still causes difficulties because solving the system expansion problem is basically solving a number of equations with a number of unknowns. A possible solution is the partitioning of the product systems based on economic value (Weidema et al., 2012) allowing straightforward integration with meso or macro scale input output tables. On the other hand this procedure parts the impact from datasets similarly to economic black box allocation. Furthermore, the linking and trading between sectors should ideally be based on the actual functionality of the product (e.g. amount of proteins, effectivity of pesticides, …) and not necessarily on the economic value.

3.2. Properties of partitioning allocation approaches

System expansion thus has its merits in consequential meso or macro scale assessments and in maintaining mass balances of datasets (Weidema and Schmidt, 2010), but for some research questions that are typically required in biorefineries, a partitioning approach might still be useful. In this part of this chapter the obtained allocation factors for the specific product groups can be found in Table IV.2.3. Within the black box approach, the physical allocation factors are relatively similar to each other (limited to a difference factor of 1.58 (7.6/4.8)) whereas the economic factors are different from these physical factors (up to a factor 4.1 (21.4/5.2)). The choice between an economical or physical ground for allocation can be heavily debated, as it can be argued that economics is the actual inventive of the production facility, but on the other hand price fluctuations in time and space can devaluate the meaning of the results in the context of ecological sustainability (Pelletier and Tyedmers 2011). Two identical factories in other countries could indeed have another life cycle resource efficiency. When considering the scope of environmental life cycle assessment with a partitioning allocation approach, we argue that for product policies a physical value should be preferred whereas the use of an economic ratio has its merit in the meso and macro level modeling. Similarities can be made with the REACH regulation (Registration, Evaluation and Authorisation of CHemicals) where the impact of chemicals on human health and on the environment is also fixed, not depending on the price of the chemical. When the amount of released chemical in the same type of environment remains identical, there is no physical ground to argue that the impact should change.

Furthermore, when assessing product oriented technosystems, the assessment should include as much detail as possible requiring a focus on the different subprocesses and not considering the factory as a black box. From Figure IV.2.3, where the life cycle greenhouse gas emissions are allocated according to the allocation factors in Table IV.2.3, it can easily be deducted that the black box approach has its drawbacks. The total impact, including cradle to transport, transport to gate and gate to gate is allocated linearly, resulting in one factor of 17% contribution of gate to gate emissions to the total Carbon Footprint of the different products, systematically underestimating energy intensive production routes and overestimating less intensive processing steps. This is different to subprocess level allocation, where it can be seen that for example gluten is separated with energy intensive centrifuges (35 to 42% of the total impact origins from gate to gate emissions), and ethanol is purified in a distillation step and a molecular sieving section (21 to 37% origins from gate to gate emissions). Similarly, the causal link between the factory inputs and outputs should be respected. For this purpose, the allocation procedure should be applied at the level where the partitions actually occur.

Table IV.2.3: The final allocation factors of the different partitioning allocation approaches (%)

	Black box				Subprocess level		
	Economic	Dry matter	Energy	Exergy	Dry matter	Energy	Exergy
Dried starch	11.5	11.2	10.5	11.0	12.6	14.7	12.0
Gluten	13.2	4.6	6.2	6.1	7.4	9.5	8.2
Animal Feed	5.2	19.7	21.4	21.3	21.9	16.2	21.8
Ethanol	8.4	4.8	7.5	7.6	7.2	4.7	8.4
Sugars	61.7	59.7	54.4	54.0	50.9	54.9	49.6
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0

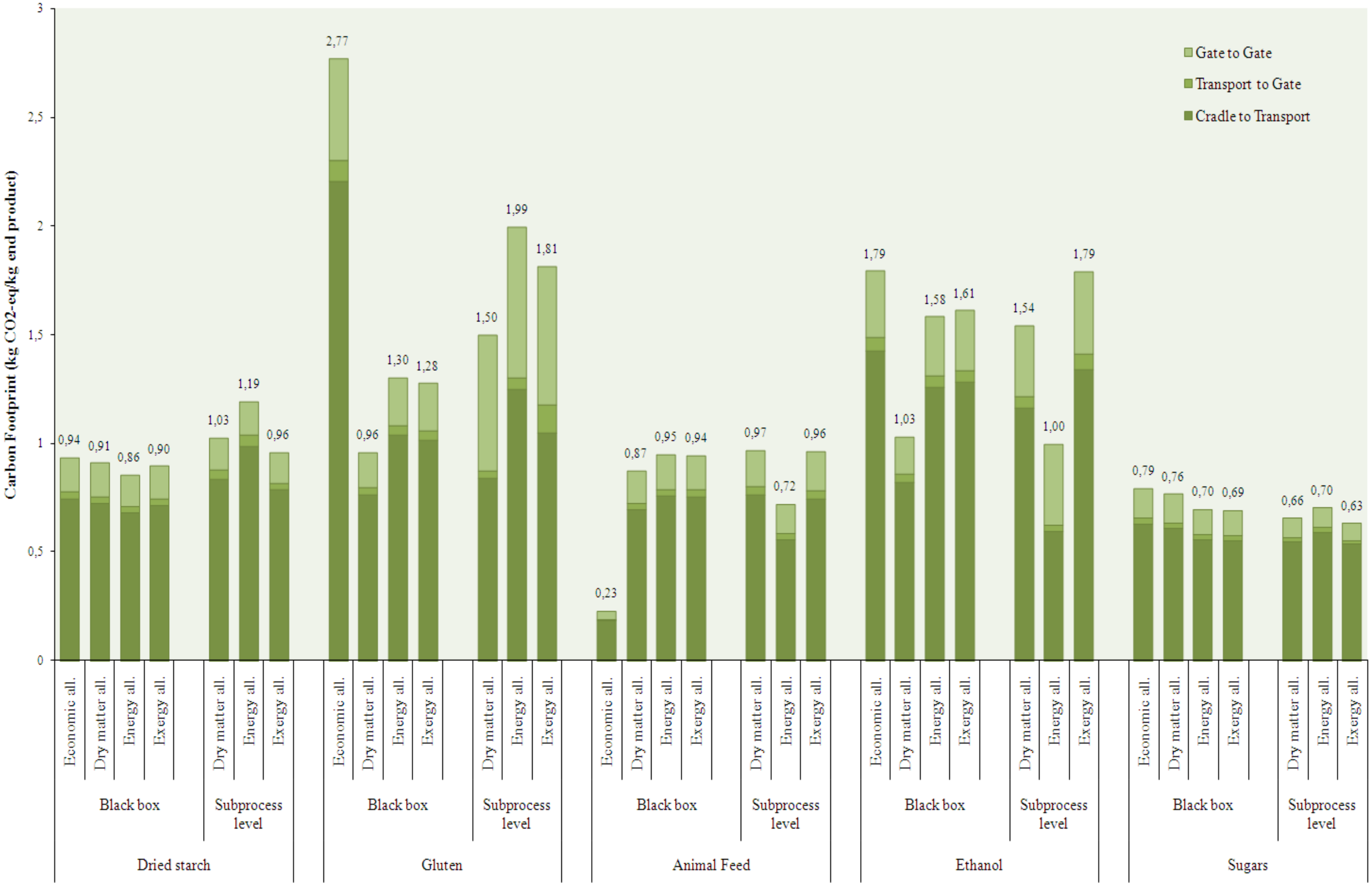

Figure IV.2.3: The Carbon Footprints per kg salable product according to the different allocation approaches

When choosing a physical allocation procedure, several options are possible. In this work, only dry matter, energy and exergy allocation are discussed as these are most commonly applied, especially in biorefineries. Dry matter allocation however, fails in addressing the ISO guidance to apply a uniform allocation procedure over the full life cycle, because masses face limitations in the characterization of energy flows. Furthermore, the mass of a substance does not give any information on the composition of a product; one kg of sand would indeed be treated exactly similar to one kg of ethanol. Using energy or exergy allocation is a solution for both of aforementioned issues as they can be used for both mass and energy flows and depend on the composition of the substance.

Remarkable is the difference between energy and exergy partitioning. When using a black box approach, the difference is small for all products (<5%), whilst for the subprocess approach, the difference between energy and exergy allocation can amount up to 44%. It is therefore essential to identify the different starting points of heating values and exergy. Whereas the former focuses only on the heat being released during combustion, the latter focuses more generically on the difference with the reference environment, usually expressed in potential, kinetic, physical and chemical exergy. For carbon, the reference is usually taken as carbon in carbon dioxide in air. The breakdown reaction of these carbon based fuels to their respective 'dead state' is thus an oxidation, explaining the analogy for some fuels between the LHV and the chemical exergy. Therefore, in some cases these values can be linked to each other by using a β factor (de Vries, 1999; Dewulf et al., 2008). Despite these similarities, this study clearly highlights that the LHV approach is limited to energy carriers as all wet intermediate flows are not valuable from a Lower Heating Value perspective. For example all wet starch streams that are directed to the ethanol fermentation can hardly be combusted due to their high moisture content, explaining the low energy subprocess allocation for bioethanol. Unlike this penalization of liquid water in the LHV approach, the exergy content of the different components of the mixture is determined by the sum of the different components and a certain amount of mixing exergy. The distance to reference environment approach is therefore applicable for all streams such as biomass, chemicals, electricity, metals, etc. and gives relevant physical information on these streams. For example the exergy content of metals and minerals depends on the abundance in and the reference reactions with the earth's crust (Szargut, 1989). Its universal applicability therefore makes exergy an attractive allocation approach within the aforementioned scope of the partitioning approach. Furthermore, the attribute of studying the relation between a substance and the natural environment seems to fit in the methodological framework of a life cycle assessment. However, exergy also faces its limitations. First, the exact composition of all substances is required to be able to calculate the exergy content, and second, the exergy content depends on the chosen reference environment. For all carbon containing molecules for example, this means that the value is determined by oxidation and that the practical utility of products (e.g. a plastic) is missed. The exergy value of a flow is also based on the current situation of the molecules without considering the efforts of the industrial production process. A possible improvement could be using cumulative exergy as an allocation basis, which would be more in line with economic allocation, as prices are also the result of cumulative efforts over the life cycle. Such an approach however, would require more research for its practical operability.

3.3. Considering allocation as decision rule variation

An alternative approach to choose one partitioning allocation approach is to avoid making a choice of allocation base and to consider allocation as a source of decision rule variation. In Figure IV.2.4, the Carbon Footprint of bioethanol is visualized with the different partitioning allocation procedures and the uncertainty of the data indicated, calculated with the combination of a pedigree matrix and a Monte Carlo simulation. All foreground data used in this study was retrieved from from real measurements in the biorefinery, and therefore the coefficient of variation of data uncertainty is rather limited, varying from 4 to 10%. On the other hand, the coefficient of variation of the different allocation approaches can be determined, which is 21% in this study. This is thus larger than the variation caused by data uncertainty (as calculated with the 'traditional' approach). These two sources of variation are combined in Figure IV.2.4, in which the average value of different allocation approaches is chosen as the final carbon footprint, and where the uncertainty bars indicate the lowest (from energy subprocess allocation) and highest (from economic allocation) points within the 95% intervals. This is represented relative to the default carbon footprint of fossil fuel of 83.8g CO_2-eq/MJ (European Commission 2009). As such, it can be concluded that greenhouse gas emissions are saved in every scenario, but savings vary from 21% to 56% for the different allocation procedures with an average value of 35%. In the light of product policies, LCA practitioners should thus attempt to achieve consensus on handling these different sources of uncertainty (both in the datasets and in the models) and in the variation caused by value choices (system boundary, allocation, …). For the latter this can be avoided by making a specific rational choice, possibly per product category, or included by quantifying the variation.

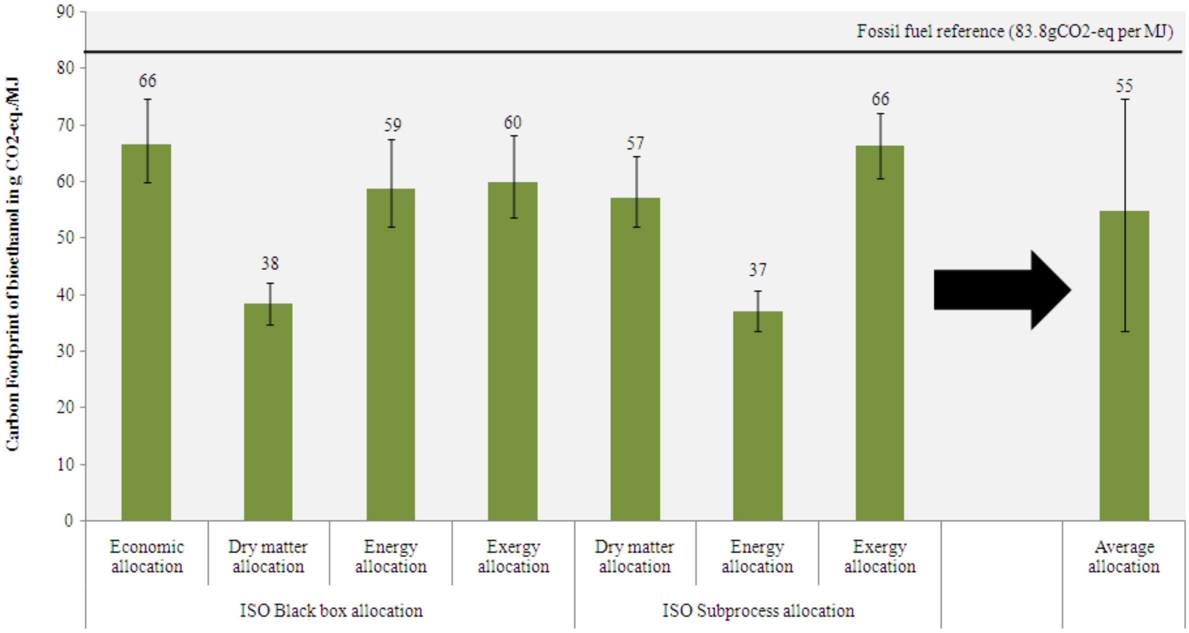

Figure IV.2.4: The Carbon Footprint of bioethanol calculated by using different allocation approaches with uncertainty and the average value with the combination of the decision rule variation and the data uncertainty

4. Conclusions

Since the beginning of LCA, this framework has faced a major methodological issue studying the impact of a functional unit on the natural environment. It is shown in this chapter that allocation is actually an essential methodological attribute in determining the goal and scope of the assessment. Therefore, the rationale to choose one specific allocation procedure should better be justified.

System expansion can be used in meso or macro scale assessments to study the impact of a certain basket of functions on the economy. This approach can be a very valuable contribution for policy makers and industry to analyze the environmental sustainability of certain product mixes and markets to which the products are delivered. On the other hand, several research questions, typical for a biorefinery, aim at product policy. In this case, allocation should be applied at the level where the partitioning actually occurs and furthermore, a fixed physical value might be preferred for this purpose. It is shown that the universal applicability of exergy is therefore an interesting attribute. Alternatively, it is also possible to consider allocation as a source of variation which can be combined with data uncertainty by taking the average value and the lower and upper boundaries of the uncertainty flags of the different approaches.

3. A conceptual life cycle sustainability indicator integrating environmental and socio-economic impacts of biorefineries

Redrafted from:

De Meester, S., Alvarenga, R.A.F., Dewulf, J. and Sanders, M. A conceptual life cycle sustainability indicator balancing anthropospheric and ecospheric impacts in an economic context. To be submitted to Environmental Science and Policy.

1. Introduction

Sustainable development is a hot topic. Many people seem to realize that rising ambitions and increasing population numbers both put unacceptable pressures on our planet and social structures. More sustainable alternatives have to be found to allow future generations to fulfill their needs and ambitions with the same potential as current and/or previous generations. As this seems obvious, the definition of ‘more sustainable’ is still not absolute and neither is the way to achieve it (Ness et al., 2007; Zamagni, 2012). In this context, sustainability assessments often follow the Triple Bottom Line in a life cycle perspective to combine a good performance on the social, economic and environmental dimension. These assessments have clearly shown that human activity, even when relying on renewable resources such as biomass, always has ecological and social impacts over the life cycle and so trade –offs seem unavoidable. That said, however, there typically is ample room to improve the existing situation. A lot of policy emphasis is currently being put on such assessment-guided, stepwise improvements. On the other hand one might point out that most global ecological impacts and social strains are still rising (UNEP, 2012). Despite huge progress in our understanding of ecological, social and economic dynamics, we seem unable to steer away from unsustainable social and ecological impacts and balance human development. To overcome this paradox, three major challenges in sustainability assessment should be addressed, namely aggregation, integration and measurement of value.

1.1. Aggregation issues

First, current economic policy is focused on growth, generally measured by the GDP indicator, as a central goal. This assumes an endless availability of natural non polluted resources, future substitutes and a perfectly inelastic labor supply (Töpfer, 2005). Such assumptions may have been less restrictive in earlier times, when economies could still increase their footprint without stepping on other people's toes or overstepping the planet's carrying capacity. The "go-west" mentality, where tightening environmental constraints could simply be avoided by moving on to the next resource (wood to peat to coal to oil to gas) and taking more and more marginal lands into production, is gradually coming to an end. As the limits are clearly reached, exponential economic growth as currently conceptualized is problematic; it implies that production increases in quantity, quality or variety, resulting in more life cycle chains and more related and potential sources of social and ecological impact. Innovation drives growth and profit drives innovation. But even if innovation increases resource efficiency and reduces environmental and social impacts at the micro-level, the process may well go at the cost of people and planet in the aggregate. This phenomenon is known as the Jevons paradox (Polimeni et al., 2008). The most obvious example is the use of natural resources: resource productivity (economic output per consumed resource) can be increased profitably by innovations that allow a more efficient use. As a consequence prices drop, resulting in more consumption and a rising overall resource use. The decoupling of economic value creation from resource use is thus 'relative' instead of 'absolute' (Eurostat, 2011; Hertwich et al., 2012; Jackson, 2009). Related to this are aggregate rebound effects indirectly driven by the income effects of such economic growth. When real income increases because of savings in one life cycle, this additional income will be spent on other and new products with higher income elasticities of demand. For example if a family saves on gas due to a more efficient boiler, money is saved to buy luxury goods such as a tablet pc. Attributional sustainability assessment, mainly performed on products and services (micro level) misses all these essential aspects occurring at the macro-level. For this reason, consequential assessments are gaining popularity. It should, however, be questioned whether this approach will help guiding society to sustainable development. The consequential approach is based on a lot of rather restrictive assumptions and uncertain parameters to predict the consequences of activities and functions. It differs only from attributional assessments in the fact that it includes additional, inherently uncertain and complex processes (Zamagni et al., 2012). It does not suggest if the assessed function itself is actually a step in the direction of sustainability without possible indirect consequences. The assumptions indeed face a high level of arbitrariness. A family with extra real income could buy a tablet pc, start traveling more, or do both or buy a tablet in one year and travel the next. And although conceptually a consequential assessment is a good approach to understand society better and to test some hypotheses, its uncertainty and arbitrariness can confuse decision makers more than help them.

1.2. Integration Issues

Second, the current way of life cycle sustainability assessment (LCSA) is based on the aforementioned Triple Bottom Line (Klöpffer, 2008):

$$LCSA = LCA + LCC + SLCA$$

With LCA the environmental Life Cycle Assessment, LCC economic Life Cycle Costing and SLCA Social Life Cycle Assessment. This is indeed a good starting point to realize that these three dimensions should be considered, but separating them is relatively artificial, since the ecosphere, econosphere and anthroposphere are obviously interconnected. The assessment of sustainable development focuses exactly on the interaction between these dimensions and should thus be more than adding together the three dimensions separately. Moreover, it is not trivial to value performance or costs in these three spheres in a common currency or unit and therefore we face a challenge in the measurement of value.

1.3. Measurement of value

Third, we fail to measure value adequately in our economic assessments. Traditional life cycle costing starts from an individual (company) perspective; the goal is to minimize the cost and maximize the profit margin of the system under study. This puts pressure on the other actors in the supply chain and thus may oppose sustainable development, which should aim at a fair distribution of wealth (Wood and Hertwich, 2012). For example lowering the cost also induces lowering the wages of employees or alternatively resulting in the necessity to increase labor productivity (by harder work or automation) or a movement of production to countries with lower wages, where accompanying working conditions are often worse. This is obviously not sustainable and therefore these issues have already raised discussion to the inclusion or exclusion of LCC in a sustainability assessments (Jørgensen et al., 2010; Klöpffer and Ciroth, 2011). Similar counteracting forces act also at the macro-level; as long as extracting and burning natural gas adds to GDP and spending time and effort on training young people reduces it, we clearly miss important elements in our assessments when we rely on GDP as our measure of success. A more fruitful approach would be to bring these elements into our traditional systems of assessments by not only quantifying and tracking the flows in the economic system (investment, income, transactions) but also quantify and link these flows to the capital stocks in the balance sheets. In this way, the burning of natural gas enters as a flow measuring the value of the service rendered, but at the same time a reduction of the natural capital is caused. And spending time and effort on teaching our children will be registered as a flow cost, representing the value of time spent, and an increase in human capital. For this purpose social assessment should also be rethought. Many social aspects, however, cannot be directly allocated to a production chain of one product or service as should be done in a 'traditional' life cycle approach. There is indeed a lack of a clear cause-and-effect chain for many possible impact categories, as they often depend on the surroundings with the related policy and the fulfillment of needs rather than on one specific technical system. It should be recognized that social sustainability assessment in the absence of a uniform and well-defined yardstick to measure social well-being, inevitably requires people to discuss and agree on the social sustainability of activities. This makes social sustainability assessment highly context specific. What is sustainable in one period and at one place, may be less sustainable at another place and time.

2. Methodological concept

The three pillar approach with life cycle assessment at the micro-level is thus useful, but has several shortcomings concerning measurement, aggregation and integration. Solving these problems is a very challenging task and will not be achieved in a few weeks or with one study. However, in the following, we propose a sustainability indicator for the assessment of products and services by building the concept for the indicator starting from tabula rasa and to open further discussion and improvement.

As a starting point we go back to the basic idea of sustainable development, where generally two perspectives are identified: the anthropocentric and ecocentric approach where the human’s and the earth’s wellbeing is respectively centralized (Rao, 2000). Considering this, an efficient economy that minimizes ecological impact whilst sustaining humans is essential.

The indicator should therefore be a ratio of human well-being or adequately measured by social value (satisfaction) creation delivered by a function, to the ecological burden of this function, measured by value destruction (capital creation or destruction) while accounting for viability in the economic system. The resulting framework for the indicator is represented in Figure IV.3.1, where the life cycle production chain of a product or service is embedded in economy and where the interactions with the ecosphere and sociosphere should be quantified and put in balance with the condition of the capital stock of that sphere. The ecological burden is based on the resource extraction and emission profile of the production chain in reference to the current condition and limits of the ecosystem resilience whereas the interaction with the sociosphere should also be quantifiable in a relevant and feasible way. For the latter, the two aspects that seem to fulfill these conditions and which can be linked to a technical production chain are labor aspects in the light of labor capital and satisfaction obtained from the final function delivered by the production chain versus the 'satisfaction stock'.

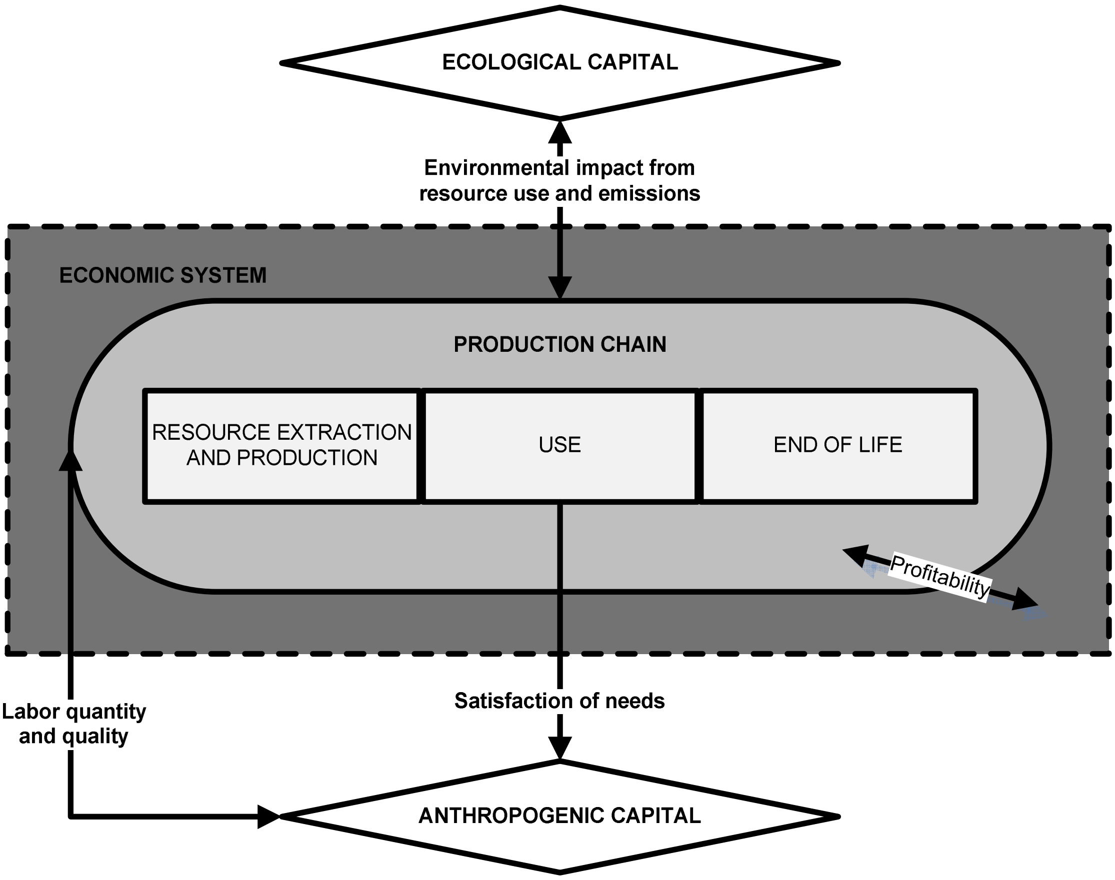

Figure IV.3.1: The conceptual framework of the indicator. The satisfaction of needs by a products or service and the positive and negative effects of labor quality and quantity are put relative to the environmental impact under the condition of profitability

3. From concept to practice

As a first condition for sustainable development, there is a need for economic profitability. Provided we keep track of value creation and value destruction accurately and we define profit as the net creation of value, we can consider profit as desirable outcome and suitable intermediary target for achieving economic sustainability. Profit in this sense, however, is a 'mean' rather than an 'end'. In this context, it is worth mentioning that traditionally measured economic growth does not necessarily contribute to average life satisfaction and that the link between financial wealth or income and happiness typically found to be concave or even non-linear and dynamic (Frey and Stutzer, 2002; Jackson, 2009). There are interfering aspects such as the relativity of wealth compared to others, the indifference at a certain level of welfare and a possible lower (time) freedom due to income duties (Kenny, 1999). For these reasons a traditional life cycle costing approach would be irrelevant in the assessment of sustainability as the aim of a production chain should be to deliver net value to humans, which can be measured as satisfaction, and not to gain as much private monetary profit as possible. However, whereas this traditional profit maximization might not be the overall goal, liquidity and solvability are still conditions for survival in the financial-economic system. Traditional profit defined as revenue minus costs will ensure such viability, but that could be accounted for by including a 'boolean' in the indicator where zero means 'not economically feasible' and 1 means that a 'threshold economic feasibility (ECF)' is reached. The definition of the latter would then be "sufficient income received above the break-even point with which a business can be sustained in competitive markets", thus including a certain profit margin that allows for necessary replacement investment, marketing, etc. This condition holds for well-implemented technologies and should thus not be applied on research or pilot scale assessments and could only obtain an intermediate value if the technology is supported by subsidies (e.g. 50% subsidies necessary for economic survival would result in a factor 0.5 instead of 1).

Taking this factor into account for economic feasibility, a balance should be made between the anthropocentric and ecological aspects of sustainable development. Two interactions with the anthroposphere are considered. First going deeper into satisfaction, this factor gives an indication on the potential wellbeing delivered by a product or service. The starting point chosen for this subindicator is Maslow's pyramid of human needs (Maslow, 1943), as it is assumed that the fulfillment of these needs would indeed result in satisfaction and thus 'social improvement' and in the same time it is possible to assign different product categories to the five levels of the pyramid:

1. Self-actualization: entertainment, beauty, travel, hobbies, …
2. Esteem: education, availability of information, …
3. Social: products and services enhancing social activities, including means of *basic* transportation and communication, …
4. Safety: hygienic aspects, pharmaceuticals, property, …
5. Physiological: food, water, sleep, clothing, …

A basic satisfaction factor based on the pyramid of Maslow (Satisfaction by the pyramid of Maslow, SPM) to account for the satisfaction flow caused by the product system could thus range from 1 to 5. A critique given on this hierarchy is that needs depend on the current satisfaction situation (capital). Modern utility theory indeed suggests that all people react differently according to a revealed preference, and that it is possible to identify a dependence with the amount of 'utils' a person already has (Binmore, 2007). This idea, in which we prefer the terminology satisfaction, holds for diverse regions and individuals, but the scale of the quantification depends on the level of the previous satisfaction (Harsanyi, 1955). For this purpose, we propose an *adjusted satisfaction factor* trying to incorporate aspects of fairness and the so-called 'preference drift' based on the surroundings (Frey and Stutzer, 2002).

The approach accounting for the current satisfaction capital is based on the Human Development Index (HDI). In this way, the utilitarian approach considering satisfaction of individuals is put in the perspective of the capability approach as proposed by Sen (1985). The latter serves as a weighting factor (w_{HDI}) to equalize opportunities to satisfaction for the world's population. In our approach, the HDI of 187 countries for which an average value (HDI_{av}) and standard deviation (SD) can be determined is used. As a result, countries can be grouped in five classes (Table IV.3.1). Different weighting factors can then be obtained for each value of Maslow's pyramid for the groups of countries, giving to the lower HDI countries higher values for the most basic products and lower values for the higher need levels whilst doing the opposite for the higher HDI countries. These weighting factors are then normalized, generating the adjusted satisfaction factor according to Table IV.3.2.

Table IV.3.1: Grouping of countries according to their HDI values

Group	Range of values for the HDI
Very High HDI	$HDI_{av} + SD < HDI$
High HDI	$HDI_{av} + 1/4\ SD < HDI \leq HDI_{av} + SD$
Average HDI	$HDI_{av} - 1/4\ SD < HDI \leq HDI_{av} + 1/4\ SD$
Low HDI	$HDI_{av} - SD < HDI \leq HDI_{av} - 1/4\ SD$
Very Low HDI	$HDI \leq HDI_{av} - SD$

Table IV.3.2: Adjusted satisfaction factors based on the HDI for five groups of countries

Basic satisfaction factor	Adjusted satisfaction factors				
	Very Low HDI	Low HDI	Average HDI	High HDI	Very High HDI
1	0.36	0.63	1.00	1.58	2.22
2	1.07	1.46	2.00	2.63	3.33
3	2.14	2.50	3.00	3.16	3.33
4	4.29	4.17	4.00	3.68	3.33
5	7.14	6.25	5.00	3.95	2.78

Footnote: The basic idea to create the adjusted satisfaction factors was to give countries with a very low HDI the double of the value given to average HDI countries for the *physiological* category of products and half of the value for the *self-actualization* category of products; while for countries with very high HDI the opposite; and in between groups of countries (e.g. low HDI) or in between category of products (e.g. *safety*), values should be in between. For instance, the satisfaction factor of *self-actualization* would be 0.5 for very low HDI, 0.75 for low HDI, 1.0 for average HDI, 1.5 for high HDI, and 2.0 for very high HDI. Since the sum of satisfaction factors should be 15 (as in the average HDI countries), those values were properly normalized, obtaining the adjusted satisfaction factor.

The second anthropogenic aspect that is considered is the labor associated with production. This concerns both quantity (L), the fact that a job is created or maintained, and secondly the quality of the job (JQ). Whereas the HDI weighting factor serves as an indication for macro-scale capability, the labor quantity is seen as relevant micro-scale feature of capability. The amount of working hours is not a direct goal as such, but it should rather allow people to have a 'threshold income' to be able to have opportunities in society, resulting in a certain degree of fairness and in a 'working' economy. This factor is normalized with the average amount of regional working hours (AL). The quality of jobs (JQ) includes different aspects accounting for the fact that it is 'pleasant' to be able to earn the necessary money and is normalized with the average job quality (AJQ) for that sector. Both these labor factors are weighted with the capital labor availability w_{UER} which is the unemployment rate of the studied country. The idea behind is that the amount of jobs is more significant if the unemployment rate is higher whereas the quality of the jobs is more important if the unemployment rate decreases.

The interactions with the anthropogenic capital should be put in perspective with the ecological impact. Accounting for the environmental impact can build on single score LCA practices to include the impact from resource use (R) and emissions (E). These impacts caused by the system under study are then normalized with an average value of its sector (AR and AE respectively) which can be obtained from extended input output tables. The normalized impact of resource use and emissions is weighted exponentially by the current status of the ecological capital (w_{EC}). By doing so, the ecological impacts gain importance if the earth's condition gets worse, thus allowing an increase in anthropogenic services if the ecosystem is recovering. The earth's carrying capacity is indeed an essential characteristic of long term sustainable development of society that may impose a certain restriction on human growth aspects such as overproduction and rebound effects. A potential suggestion in this light could be using the world ecological footprint approach (Global Footprint Network, 2012). The value could be quantified based on the current human ecological footprint (CHEF, in global hectares) and the similarly calculated resilience threshold footprint of the earth (RTF in global hectares):

$$w_{EC} = e^{\left(\frac{CHEF}{RTF}-1\right)}$$

Summarized, the proposed Indicator of Sustainable Development (ISD) is a conceptually developed ratio of human benefit and burden, quantified by satisfaction and work quantity and quality, and the ecological burden caused by resource use and emissions under the precondition of economic feasibility (ECF). Macro-economic weighting factors are added; a higher unemployment rate causes an increase in the importance of job quantity and a decrease of job quality whereas a higher world ecological footprint gives more weight to the environmental impact. The indicator is always positive (above zero), but should be maximized. It is thus aimed to be used for comparison between different options. The functional unit of this indicator is a monetary value of a product or service (e.g. 1€). This has two major advantages; first, different types of products and services can be compared based on a universal parameter that is tangible and that has direct interaction and thus possible influence on behavior of people. Second, it is a meaningful basis for decision makers (policy, company, family, …) as it is a return on investment type of indicator, where per invested flow of money the return in social value is balanced with the ecological burden. The indicator is thus able to give a direct guidance of sustainable development for investment over different product systems in a life cycle (n) and can be calculated by:

$$ISD = \frac{(SPM \times w_{HDI}) + \sum_n \left(\frac{L}{AL}^{1+w_{UER}} \times \frac{JQ}{AJQ}^{2-w_{UER}}\right)}{\sum_n \left(\frac{R}{AR} \times \frac{E}{AE}\right) \times w_{EC}} \times ECF$$

The parameters from this equation are summarized in Table IV.3.3 in which also possible data sources are proposed and a probable approximation range is given. Applying these ranges allows conducting a preliminary sensitivity check that gives possible values for the indicator. The indicator is constructed in such a way that it becomes 1 when taking the average of all parameters. Varying these factors simultaneously -50 to +50% from this average results in an ISD of 0.09 and 16.21 respectively for the 25th and 75th percentile boundary (Figure IV.3.2).

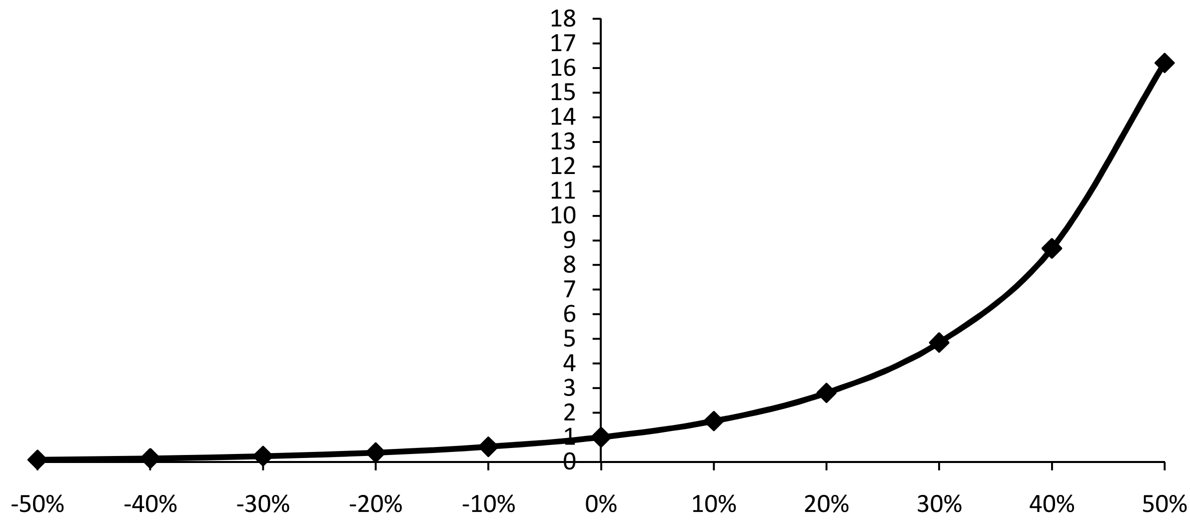

Figure IV.3.2: The sensitivity of the ISD by varying all parameters simultaneously from 0 to 50% of their median resulting in the most probable values in the 25th to 75th percentile of the ISD

Table IV.3.3: A summary of the used symbols with a definition, possible data sources and an approximate range of the values

Symbol	Definition	Possible data sources	Approximate range	Possible unit
SPM x w_{HDI}	Adjusted satisfaction factors	Table IV.3.2	0.4 - 7.1	Unitless
L/AL	Amount of working hours per euro (L) normalized by an average of the studied sector	Detailed assessments and input output tables	0.1 - 2.0	$\frac{h/€}{h/€}$
JQ/AJQ	Job quality normalized by an average of the studied sector	Detailed assessments, the social hotspots database (2012), the United Nations Economic Commission for Europe (2010)	0.1 - 2.0	Possible semi-quantitative score (e.g. Likert type)
w_{UER}	Weighting factor for labor capital stock	The unemployment rate in the country of implementation	0 - 1	Unitless
R/AR	Resource consumption impact per euro normalized by an average of the studied sector	LCA studies and input output tables	0.1 - 2.0	LCA endpoint unit, e.g. Recipe Pts/Pts
E/AE	Emission impact normalized per euro by an average of the studied sector	LCA studies and input output tables	0.1 - 2.0	LCA endpoint unit, e.g. Recipe Pts/Pts
w_{EC}	Weighting factor for the environmental impact	The Ecological Footprint versus earth's resilience	0.7 – 20.1	Unitless
ECF	Economic feasibility factor	ECF is a Boolean factor, except for subsidies, of which the values can be found in legislative documents	0 – 1	Unitless

Example of a sustainability assessment with the ISD

To clarify the results the ISD could generate, it is applied to a hypothetical case study where the sustainability is assessed in an average HDI country where € 1 is spent on a bread and a book both produced locally and an imported bread and a diamond ring, assuming that all these options are sufficiently profitable (Table IV.3.4).

The results suggest that locally produced bread in an average HDI country (e.g. Bolivia) has the best score on the ISD because it has a high satisfaction of needs, a good quantity and quality of jobs and a fair environmental. The imported bread has a relatively higher environmental impact and worse social conditions, and therefore scores worse than the book, which has an intermediate level of satisfaction, but has better working conditions and a relatively lower environmental impact. The diamond has the lowest score because of its lower level of satisfaction per euro spent, its worse working conditions and higher environmental impact.

Table IV.3.4: A hypothetical example to illustrate the potential operability of the ISD

	Local bread	Imported bread	Local book	Imported diamond ring
SPM x wHDI	5.0	5.0	3.0	1.0
L/AL	1.2	1.0	0.7	1.4
WUER	0.1	0.5	0.1	0.6
JQ/AJQ	1.3	0.9	1.5	0.2
R/AR	1.0	1.2	1.4	1.6
E/AE	1.0	1.4	0.8	1.6
wEC	1.6	1.6	1.6	1.6
EF	1.0	1.0	1.0	1.0
Numerator	7.9	6.9	5.8	2.8
Denominator	1.6	2.8	1.8	4.2
ISD	**4.8**	**2.5**	**3.2**	**0.7**

The numbers are currently hypothetical as this is a conceptual exercise, but more research could be done in choosing exact options.

4. Conclusion

In the transition to sustainable development, three main obstacles, namely aggregation, integration and measurement of value, were identified that counteract the stepwise improvement that would be expected from the broader implementation of sustainability assessments. This chapter suggests research could progress by elaborating a conceptual indicator for sustainable development that balances anthropospheric and ecospheric impacts in an economic context. The issue of aggregation is countered by using macro-economic weighting factors for micro-scale actions. Furthermore, integration and measurement of value could be solved by going back to the basics of sustainable development. As a starting point, a monetary value is proposed as the functional unit to allow fair comparisons and to give guidance for investment decisions. However, per invested money, traditional maximization of private profit is not a goal as such. Therefore, this factor is replaced by an economic feasibility factor aiming at a threshold profit margin allowing competitiveness without putting pressure on other actors in the supply chain. The anthropospheric and ecospheric endpoints are put relative to each other instead of separating them. In this way, it is an (ecological) cost – (human) benefit assessment, which fits into the basic concept of sustainable development. The environmental impact on resource use and emissions can be calculated with traditional life cycle assessment whereas the impacts on anthroposphere are subdivided in labor quantity, quality and satisfaction with the final product (per euro). These values are normalized with sectoral averages to account for improvement and decline compared to the current situation and are weighted with factors accounting for ecological and labor capital. While it is feasible to calculate results for the indicator without highly uncertain macro-economic projections, it gives a meaningful indication on the sustainability of human consumption accounting for several externalities that are inherent to human activity and which are currently often excluded from life cycle assessments. At the same time the results can be used to compare something relative to something else (the indicator does not deliver an ‘absolute’ physical value on a state). The approach presented is a proposition, which needs further discussion and elaboration, but aims at putting the basics of sustainable development back in the center of sustainability assessments rather than adapt sustainability assessment to our current economic models.

CHAPTER V: Conclusion and outlook

1. The sustainability of biorefineries

This goal of this work was analyzing the sustainability of biorefinery systems. For this purpose, the literature survey in chapter 2 indicated that the life cycle assessment framework is a valuable approach to account for complex interactions between production systems such as biorefineries and the natural environment. In chapter 3, the LCA methodology was therefore applied in biorefinery case studies.

In the first case study it was shown that biorefining feedstock into a wide range of products is a thermodynamically efficient (81%) way of processing molecules of bioresources for specific purposes in different segments of the market demand. On the other hand, it is demonstrated that replacing fossils requires a certain amount of inputs from the natural environment causing additional thermodynamic losses in the production chain (15.3%) based on the resource footprint of the Cumulative Exergy Extracted from The Natural Environment (CEENE) methodology. A scenario assessment demonstrated the resulting tradeoff between the Carbon Footprint of bioproducts and the Land, Water and Minerals Footprint; in the case study executed 27% fossil resources are saved at the cost of 93% extra land, water and mineral input from the natural environment. This means that replacing 1kg of crude oil by wheat based bioethanol requires approximately 10 m^2 of land for one year, 36 L water and 0.0077 kg minerals. Constructing a resource footprint thus allows to have a more balanced overview on the cost of saving fossil resources and lowering GHG emissions.

Thinking of the vast amounts of oil that are used, arable land use and the resource footprint of biomass in general poses an obvious restriction on the growth of the biorefinery sector. Therefore, the available biomass should be maximally valorized. In a second case study, anaerobic digestion of several types of biomass is analyzed. The valorization of energy crops such as silage maize, sugar beet and grass, is compared to the valorization of farm residues (cow manure & corn stover) and domestic organic waste. It is shown that the energy crops and farm residues are converted with a high rational exergy efficiency compared to waste because the latter contains more difficult molecules to convert such as lignocelluloses. This type of biomass therefore requires more pre- and post-treatment. From a life cycle perspective, all options are environmentally competitive to national grid electricity inducing a resource saving of over 90% in most impact categories. Not using the heat however, results in a poorer performance (-32%) whereas the valorization of organic waste (domestic and agricultural residues) avoids land resources and is therefore the best option to use as biofeedstock. The use of digestate as a fertilizer is beneficial for resource use, since it contains nutrients such as nitrogen, phosphorus, potassium and trace elements. Recycling these nutrients by using digestate as a fertiliser, is a sound strategy to become partially independent from imported minerals. However, nutrient leaching and ammonia emissions can increase by using digestate instead of mineral fertilizers, but these can be reduced by 50% by a better agricultural practice.

2. The assessment methodology

Sustainable development is a holistic concept, and its assessment is a difficult task. The required life cycle assessment framework is a useful approach to gain insight in different types of interactions between the technosphere, ecosphere and possibly the anthroposphere. Nevertheless, due to its complexity, sustainability assessment is far from a finished research area. Many examples with a very high relevance can be determined in the sector of biorefineries such as the assessment of biodiversity, long term soil fertility, erosion, invasive species, risk of diseases, further regionalization, etc. Another example is the fact that it is not sufficiently possible to assess the advantage of biodegradation, as we do not know how to quantify the impact of a material such as a plastic that is thrown away in nature (e.g. the plastic soup in the ocean). Furthermore, improvement could be made in the cause-effect chain of endpoint modelling and in the quantification of uncertainty.

Whereas we acknowledge these potential interesting research areas, the methodological part of the dissertation has focused on the inventory collection phase, on the life cycle assessment goal and scope and on quantifying the sustainability concept in general.

Inventory modelling is indeed an extremely relevant part of the assessment, as the value of the result is directly linked to the quality of the data. This aspect is even more important when analyzing novel technologies because in this case often no direct data source is available. This impedes prospective assessments and therefore the relevance of LCA in general. For this purpose, this work has elaborated engineering modules for 22 processes commonly applied in industry in order to use parameters and formulas to obtain mass and energy balances of these processes. The approach proved to be useful and relatively accurate on a process basis. Nevertheless it is a very challenging task and requires further elaboration and as indicated, a certain degree of caution is crucial. Apart from the need of including more processes, it is for example required to use heat integration in order to avoid overestimation of total heat use. Furthermore, more rule of thumb values should be acquired to estimate supporting unit operations such as pumping and ventilation.

Another methodological aspect studied is the allocation procedure which is very relevant in the sector of multipurpose biorefineries. It is illustrated that allocation is more than an arbitrary step in the assessment of sustainability, but that is rather a methodological attribute that has a strong link to the goal and scope of a study. When relying on system expansion, the scope changes from one specific functional unit to an economy wide assessment with a whole basket of functions, whereas applying a partitioning approach is useful in product specific assessments. The first is therefore useful to analyze scenarios and establish links between product systems and sectors, whereas the second can be used to determine the impact of one product or service as such which might be required in product policy. Within the partitioning approach, several options can be chosen, but a fixed physical parameter for allocation seems more appropriate to fulfil the goal of supply chain improvement. In this case the concept of exergy, based on the second law of thermodynamics has useful properties as a universally applicable physical value for mass and energy flows.

In the last part of the methodological chapter of this dissertation it is chosen to broaden the assessment in scale and scope. For this purpose the concept of sustainable development is revisited in the context of the actual goal of sustainability analysis. As a result, an indicator of sustainable development is constructed that balances an ‘anthropospheric return’ on an ‘ecospheric investment’. The former is quantified as satisfaction obtained by a final function and labor quantity and quality associated with a production chain whereas the latter relies on LCA practices. This indicator uses weighting factors based on macro-scale sustainability conditions such as the human development index of countries, unemployment rates and the worldwide ecological footprint. As such a link between bottom-up and top-down sustainability assessments can be made. While probably not being the final solution, this type of work is highly required in the future because:

- If only top-down approaches are used, the distance between policy and practice may be too large for practical implementation of improvement strategies
- If only bottom-up approaches are applied, this is like rearranging the deck chairs on the titanic without changing track

The integration of both different scales and different research areas is one of the main challenges for the future. Coordination is therefore required to implement sustainable development and its assessment as the link between different research areas and decision makers.

3. Outlook

Based on research performed in this manuscript it can be stated that the 'easy' welfare creation caused by the use of fossil resources is gradually coming to an end. It seems unlikely that mankind will ever find a source of exergy that is so easily and constantly available. Many resource options and conversion technologies will need to be researched in the future, however, unlike most other renewable technologies, biomass is a source of carbon and will therefore take an indispensible place in future developments. Applying life cycle assessment shows that the valorization of biomass indeed saves fossils in all studied systems of this dissertation. On the other hand, it is clear that each offset by biomass of fossils and related greenhouse gas emissions indirectly goes at the cost of other resources such as water, land and minerals and that biomass is a precious resource. It is therefore necessary to make a balance between environmental burden and services delivered by the resources. Apart from the optimization of supply chains, also strategic choices are necessary concerning the use of biomass for food, feed, fuel or material purposes, in which life cycle assessment can give guidance on the environmental sustainability of these different options.

It seems obvious that a strong worldwide environmental policy is desired for biomass cultivation and processing. From a theoretical viewpoint the only way to obtain a sustainable society is a stepwise procedure that is probably valid for all other materials as well:

- First it is required to determine the resilience of the earth. For each type of resource and emission a maximum allowable limit should be determined that guarantees the long term health of the planet
- Second a uniform life cycle assessment of all products and services that can possibly be delivered to society should be performed whilst maintaining a closed mass and energy balance

- Third, the population numbers should be checked
- Fourth, based on the limitation of earth and on the population number, a choice should be made which products and services can be delivered and how these means are divided
- And fifth, if mankind wants a higher average standard of living, population numbers should decrease or more environmentally benign production chains should be developed

A specific simplified procedure could be designed for biomass based on a possible cascade pyramid:

- Biomass for food (including animal feed)
- Biomass as material (excl. food and feed) resource
- Biomass as energy resource

A first step is the collection of an inventory of all arable land and the potential yields that can be attained without degrading other ecosystem functions. Subsequently, one can determine the food requirement mix of the world population. The remaining biomass, including food wastes, can then be used for the replacement of fossils as material or energy resource. This can be summarized as follows:

$$BRF = HB - FC \times HP$$

With BRF the biomass available for fossil resource replacement (as material or energy), HB the total worldwide harvested biomass, FC the food and indirect feed consumption per capita and HP the human population. The biomass fraction available for energy (BFE) can then be determined by subtracting the biomass required as material resource (BFM):

$$BFE = BRF - BFM$$

Life Cycle Assessment takes an indispensible place in this procedure. It can be used top-down to quantify market mechanisms, indirect impacts and boundary conditions such as water consumption, soil depletion, air and water emissions, etc. that should be quantified to link products and services and their respective chains to the earth's resilience. Furthermore, a bottom-up life cycle assessment can be used in product policies to compare production chains and in the search for improvement potential along supply chains.

For example if biomass would be the only material source, it would have to provide all non recycled molecules delivered to society (MP), but it would also include all material losses (ML) in the supply chain. In this case:

$$BFM = MP + ML$$

Obviously ML should be minimized, for which a life cycle assessment can give valuable insight in possible supply chain improvements.

Summary

Fossil resources are gradually depleting and becoming more expensive. Therefore, new ways to fuel our economy should be sought. Being a renewable carbon source, biomass will take a key role in the transition to a more sustainable economy. However, while potentially renewable, biomass relies on an intensive cultivation step and it will not be able to deliver a constant and endless supply without inducing other harmful effects. Therefore sustainability assessments of biorefineries are highly relevant.

After an introductory first chapter, the sustainability concept and assessment methodologies are studied in chapter two. Based on this information, the life cycle framework is applied in chapter three, in which it is shown that a food and feed company processing wheat can switch to a fossil fuel replacing biorefinery without inducing efficiency losses. On the other hand, the replacement of fossil fuels goes at the cost of other resources such as land, water, minerals, etc. A profound study of the supply chain of different sources of biomass illustrates that the valorization of domestic organic waste and farm residues is an environmentally benign opportunity. These types of biomass however, have lower conversion efficiencies compared to agricultural crops such as silage maize because they often contain more difficult molecules to process such as lignocelluloses requiring more pre- and post-treatment. It is demonstrated that these different types of organic resources can be efficiently converted to a highly energetic biomethane by anaerobic digestion while maintaining nutrients in the digestate, which can be used as fertilizer. Additional emissions causing acidification and eutrophication should however be avoided by good agricultural management.

The fourth chapter of this dissertation focuses on methodological development. The quantification of sustainability is a complex task and therefore more research is required to improve assessment techniques. A first identified bottleneck is the acquirement of reliable data. While this is the key to obtain useful results from a life cycle study, it is especially difficult to gather mass and energy balances of future production processes. For this purpose, engineering

modules are developed of 22 processes that are commonly used in industry which can be used in prospective sustainability assessments. Although challenges are identified, an application in a case study illustrated the operability and reliability of the approach. The second part of this chapter focuses on the allocation procedure of LCA. It is illustrated that this methodological attribute should be linked to the goal and scope of the assessment. System expansion can give interesting insights in economy wide assessments to assess different product mixes and markets, whereas partitioning is a useful approach in product policies and supply chain improvement. For the latter, exergy is identified as a useful parameter to quantify the physical value of both mass and energy. In a last part of the methodological chapter, an indicator of sustainable development is proposed that focuses on the broader concept of sustainable development. The indicator weighs the antropospheric benefit, quantified as satisfaction by a product or service and the labor quality and quantity, with the ecological burden, quantified as resource and emission impact. These factors are weighted with macro-scale aspects such as the human development index, unemployment rate and the world's ecological footprint.

Overall, it can be concluded that society will have to take better care of its available resources. Biorefineries can have a role in this development by optimally utilizing the available biomass. However, a strong policy is needed that analyzes supply and demand interactions and related impacts such as land use, water use and field emissions. Life cycle assessment will take an essential role in these developments, both in a top-down perspective by analyzing direct and indirect effects of product mixes and markets, as in a bottom-up approach by analyzing and optimizing production chains. On the other hand, more collaborative research is required to better understand different aspects of sustainable development and to search for better ways for a proper assessment of different scopes and scales.

Samenvatting

Door de dalende beschikbaarheid van goedkope fossiele brandstoffen en door de opwarming van de aarde, is het noodzakelijk een nieuwe en duurzame motor voor de economie te zoeken. In deze transitie kan biomassa een belangrijke bron van hernieuwbare koolstof worden. Het verkrijgen van deze grondstof hangt echter samen met een intensieve en oppervlakte afhankelijke landbouw stap, waardoor er geen eindeloze voorraden beschikbaar zullen zijn. Bovendien zijn er in de productieketen van biomassa ook verschillende types emissies mogelijk. Een grondige duurzaamheidsanalyse is dus noodzakelijk in deze opkomende sector.

In dit doctoraatswerk wordt eerst het concept duurzame ontwikkeling uitgediept en worden daarna de bijhorende kwantitatieve meetmethoden geanalyseerd. Op basis van deze informatie worden levenscyclusanalyses uitgevoerd en wordt enerzijds aangetoond dat een bedrijf uit de voedingssector zich op performante wijze kan omschakelen tot een bioraffinaderij die ook bioethanol produceert. Anderzijds blijkt dat het vervangen van fossiele brandstoffen ten koste gaat van andere grondstoffen zoals land, water, mineralen, enz. Een diepere studie van de productieketen van de biomassa toont aan dat het valoriseren van organische afvalstromen een waardevolle aanpak is. De conversie van dit type materiaal is nochtans vaak minder efficiënt dan de efficiëntie van het verwerken van landbouwgewassen zoals maïs, aangezien zij een groter aandeel moeilijker om te zetten moleculen bevatten zoals lignocellulose. Hierdoor is dan ook vaker een intensieve voor- en nabehandeling noodzakelijk, maar dit wordt gecompenseerd doordat er geen noodzaak is aan extra landbouwactiviteiten. Ook wordt geconstateerd dat anaerobe vergisting een efficiënte technologie is voor het omzetten van verschillende soorten organisch materiaal tot een hoog calorisch biomethaan. Bovendien worden nutriënten die kunnen gerecycleerd worden als meststof behouden in het digestaat. Hierbij is een goede toepassing in de landbouw wel noodzakelijk voor het vermijden van extra emissies die verzuring en eutrofiëring veroorzaken.

Hierna focust dit doctoraatswerk op de methodologische ontwikkeling van duurzaamheidsanalyse. Eerst wordt onderzoek gedaan naar het verbeteren van de data-inventarisatie in de levenscyclusanalyse. De resultaten van een LCA studie zijn namelijk maar van waarde als er gewerkt wordt met betrouwbare data, wat zeker relevant is bij het bepalen van de duurzaamheid van toekomstige technologieën waarvoor vaak geen gedetailleerde data beschikbaar is. Hiervoor zijn in dit doctoraatswerk op basis van ingenieursberekeningen 22 modules uitgewerkt voor frequent gebruikte industriële processen, wat toelaat om de massa- en energiebalans van productieketens te verzamelen. De aanpak werd toegepast in een case en er werd aangetoond dat de modules, rekening houdend met hun restricties, bruikbaar kunnen zijn bij het analyseren van de duurzaamheid van toekomstige productieketens. Hierna wordt het belang van de allocatiemethode bestudeerd en wordt de link tussen deze methodologische keuze en het doel en de reikwijdte van de studie aangetoond. Systeemexpansie biedt hierbij nuttige informatie over de duurzaamheid van verschillende product mixen en markten. De verdelingsmethoden daarentegen, hebben hun nut in beleidsstrategieën voor producten en in de optimalisatie van productieketens. Voor deze laatste toepassing blijkt dat het concept exergie door zijn fysische relevantie en universele toepasbaarheid erg bruikbaar is als allocatiemethode.

In het laatste deel wordt een indicator ter kwantificatie van duurzame ontwikkeling uitgewerkt die de anthroposferische winst, uitgedrukt als tevredenheid met een product of dienst en de kwaliteit en kwantiteit van arbeid, uitdrukt tegenover ecologische belasting, gemeten als impact door emissies en grondstofextractie. Door het gebruik van onder andere de Human Development Index, werkloosheidscijfers en de ecologische voetafdruk van de totale bevolking worden ook macro-schaal aspecten mee in rekening genomen.

Als algemene conclusie kan gesteld worden dat de maatschappij anders en beter zal moeten omgaan met zijn mogelijkheden. Bioraffinaderijen zullen een belangrijke rol spelen door het optimaal verwerken van biomassa tot finale producten. Eén van de belangrijkste aspecten zal echter zijn om een sterk beleid te ontwikkelen betreffende de mogelijkheden van biomassa, waarbij rekening gehouden dient te worden met neveneffecten zoals het gebruik van extra land en water en verschillende types emissies tijdens de landbouw. Levenscyclusanalyse kan in deze ontwikkelingen een belangrijke rol spelen. Eerst en vooral kan in een top-down perspectief geanalyseerd worden welke directe en indirecte effecten zich voordoen van verschillende producten en afzetmarkten. Bovendien kan een analyse vanuit een bottom-up perspectief bijdragen aan procesanalyse, procesoptimalisatie en product specifiek beleid.

In al deze ontwikkelingen is het noodzakelijk om meer collectief onderzoek te organiseren om een beter vat te krijgen op de alle mogelijke aspecten van duurzaamheid op verschillende niveaus en op verschillende gebieden.

Curriculum Vitae

Personalia

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Education

- 2003-2008: Master in Bioscience Engineering: Environmental Technology. Cum Laude. Faculty of Bioscience Engineering, Ghent University

  Master thesis: Occurrence and potential effects of microplastics in the Belgian Coastal area. Laureate of the encouragement award for marine sciences, VLIZ

- 1997-2003: Latin Maths, Koninklijk Atheneum, Sint-Niklaas

Professional activities

- 2012 - … Project Manager, OWS
- 2008 - … Doctoral Research in Applied Biological Sciences. Environmental Organic Chemistry and Technology Research Group (EnVOC), Faculty of Bioscience Engineering, Ghent University

  Title: Life Cycle Assessment in biorefineries: case studies and methodological development.

  Projects:

  - FP7 PROSUITE: Prospective sustainability assessment of technologies

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Teaching and tutoring experience

- 2008-... Tutor of 9 thesis students
  - The environmental impact of bioethanol production in a multi-output plant
  - LCA of Pangasius production in the Mekong delta: a cradle to farm gate study
  - LCA of Pangasius production in the Mekong delta: a farm gate to market study
  - Duurzaamheidsanalyse van anaerobe vergisting als technologie voor de valorisatie van biomassa
  - The use of engineering modules for the data inventory collection in prospective sustainability assessments
  - De duurzaamheid van algen als grondstof in de bioraffinaderij
  - Een LCA gebaseerde vergelijking tussen verwerkingsscenario's van organisch afval met een focus op compostering en pyrolyse
  - Gate to gate analysis of an IB/PIB plant
  - An assessment of the production of BSC: traditional production versus microreactor technology
- 2009-2010: Teaching exercises Analytical Organic Chemistry
- 2009-2012: Teaching exercises Process Engineering

Workshops and courses

- 2009: Sustainability and product efficiency in the chemical industry
- 2010: Bilan Carbone
- 2010: Superpro Designer
- 2011: Ecoinvent and Eco-editor

- 2012: Ecolabels
- 2012: Uncertainty in LCA
- 2012: LCA of solid waste

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Appendix

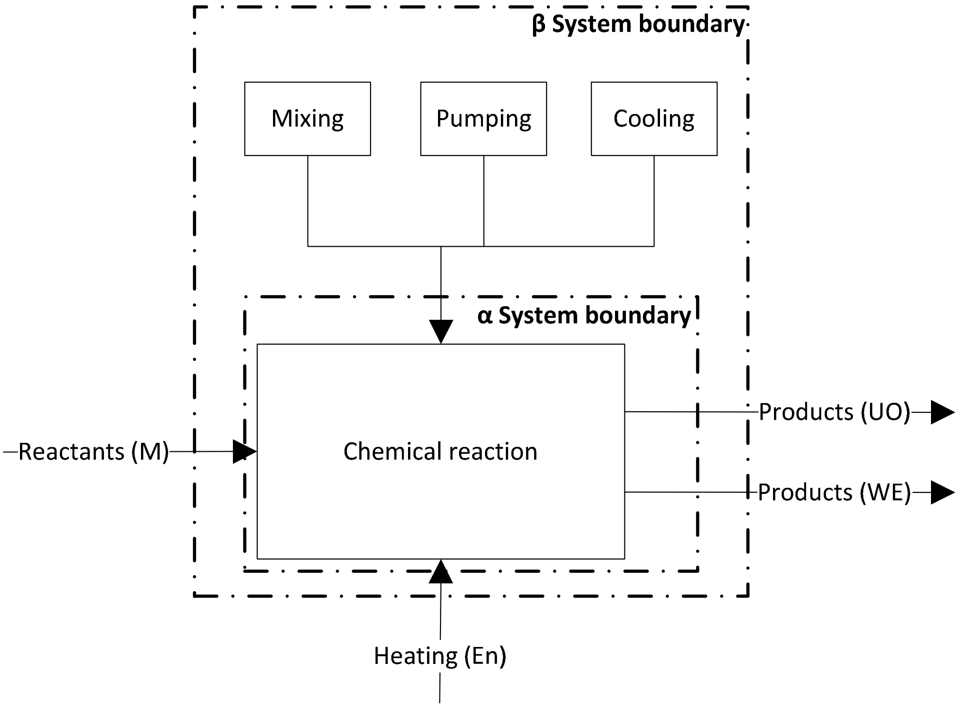
1. Reactions

1.1. Chemical reactions

Chemical reactions, are modelled with the thermodynamic equilibrium model. This is a very useful approach for generic modelling, since it is stated that this approach is independent of reactor design (Puig-Arnavat et al., 2010). However, for each specific case, several assumptions will have to be made. Most importantly: a thermodynamic equilibrium should be reached, which is not always the case. Therefore, residence time in the reactor should be high enough. On top of this, the process is assumed to be adiabatic (no heat losses), the conditions in the reactor should be constant without spatial variation and gaseous products are assumed to be ideal. The model does not include effects with byproducts such as tar, ash, micro-organisms, etc. However, for the latter the amount of such byproducts formed can be deducted from the original amount of reactants if this quantity is known.

System boundary description

The α system boundary for this BUO includes the reaction of the reactants to products in gas or liquid (including slurries) state in any type of vessel that allows a thermodynamic equilibrium. It is valid over a broad temperature range, as long as the coefficients for the heat capacity calculations remain valid; often between 200 and 1500K. Apart from the quantity of output products (useful (UO) and wastes (WE)), the module calculates the amount of heating or cooling energy, if required (in MJ). Possible SUO are mixing, pumping and cooling.



Calculation algorithm

Three type of equations are used to solve chemical reactions of which the reactants and reaction products are known. Firstly an elementary balance can be performed. If this is not sufficient, extra equations can be added by considering the thermodynamic equilibrium of the different reaction mechanisms. The third type of equation is solving the enthalpy balance of the reaction, which can be used to obtain additional stoichiometric information or to have an estimate of temperature. The three types of equations are elaborated below:

Elementary balance

The thermodynamic equilibrium links input and output flows to each other by means of an equilibrium constant (Coker, 2001):

$$aA + bB \leftrightarrow cC + dD$$

$$K = \frac{A^a \times B^b}{C^c \times D^d}$$

The equilibrium constant should thus be calculated with the Gibbs free energy of reaction, the temperature and the gas constant:

$$\ln K = -\frac{\Delta G_r}{RT}$$

The temperature dependent Gibbs free energy of reaction ΔG_r in its turn is obtained with the enthalpies and entropies of the different products and reactants:

$$\Delta G_r = \Delta H_{rT} - T\Delta S_{rT}$$

With ΔH the temperature dependent heat of formation, and ΔS the temperature dependent entropy. This equation requires the heat of formation ΔH_r that can be obtained by:

$$\Delta H_{rT} = \Delta H_{rT_0} + \Delta H_{products} - \Delta H_{reactants}$$

Without phase changes the enthalpy difference between the products and reactants can be based on the heat capacity:

$$\Delta H_{products} - \Delta H_{reactants} = \int_{T_0}^{T} \Delta c_p \times dT$$

With T the actual temperature and T_0 the reference temperature (298K).

$$\int_{T_0}^{T} \Delta c_p \times dT = \Delta a \times (T - T_0) + \frac{\Delta b}{2} \times (T^2 - {T_0}^2) + \frac{\Delta c}{3} \times (T^3 - {T_0}^3) + \frac{\Delta d}{4} \times (T^4 - {T_0}^4)$$

With a, b, c and d the regression coefficients of the heat capacity temperature dependence equation, which can be found for many chemicals in 'The Chemical Properties Handbook' (Yaws, 1998). Thus the heat of formation ΔH_r is obtained from:

$$\Delta H_{rT} = \Delta H_{rT_0} + \int_{T_0}^{T} \Delta c_p \times dT$$

Where the standard heat of reaction (ΔH_{rT_0}) is determined by:

$$\Delta H_{rT_0} = \sum \alpha_p \times \Delta H_{products\ at\ T_0} - \sum \alpha_r \times \Delta H_{reactants\ at\ T_0}$$

With α_p and α_r the stoichiometric coefficients. The ΔH_r factor can also be used to calculate heating or cooling requirements of the reaction.

Similarly, the entropy balance can be calculated by:

$$\Delta S_{rT} = \Delta S_{rT_0} + \int_{T_0}^{T} \frac{\Delta c_p}{T} \times dT$$

With:

$$\int_{T_0}^{T} \frac{\Delta c_p}{T} \times dT = \Delta a \times \ln\frac{T}{T_0} + \Delta b \times (T - T_0) + \frac{\Delta c}{2} \times \left(T^2 - {T_0}^2\right) + \frac{\Delta d}{3} \times \left(T^3 - {T_0}^3\right)$$

As a third equation, the enthalpy balance of the reaction can be formulated:

$$aH_A + bH_B = cH_C + dH_D$$

This BUO is summarized in Table A.1.

Input values required	DATAPHYSCHEM	Output
Flow rate and type of feed Reaction products Estimated temperature	Elementary compositions Standard enthalpy and entropy of products and reactants Heat capacity coefficients	Quantity and temperature of inputs or outputs (e.g. emissions) Heating or cooling requirement

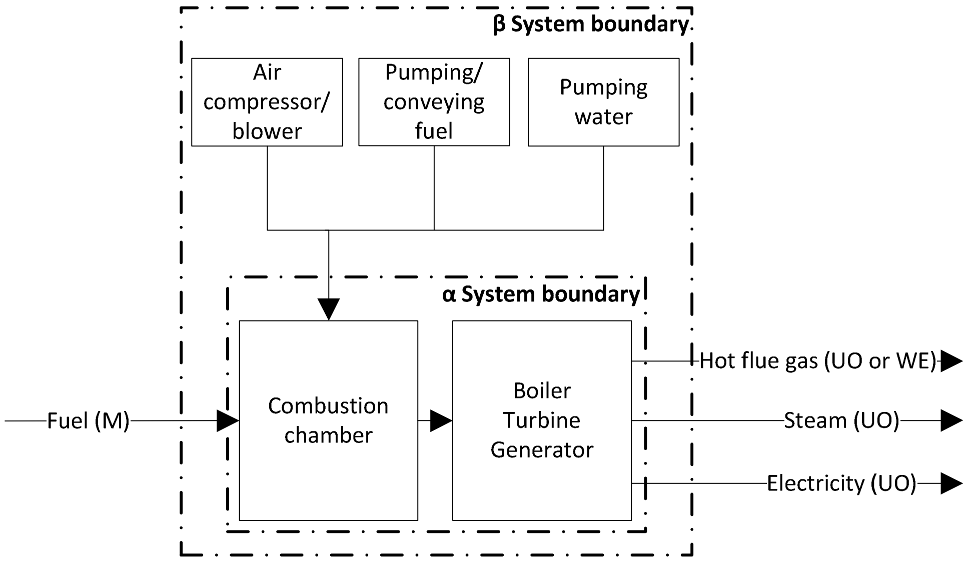
Table A.1: Summary of the BUO chemical reactions

1.2. Incineration for heat and power

Incineration is a technology which is typically used to gain energy from different types of resources by oxidation. The engineering module calculates the energy in the form of heat, electricity or a combination, generated in different types of industrial combustion configurations. In the first step, the Lower Heating Value (LHV) of the energy source(s) is calculated, whilst in the second step efficiencies to convert LHV to electricity (and steam) are accounted for. Other calculated outputs are: the auxiliary power needed, ash production and emission and a rough estimation of the other main flue gas components H_2O, CO_2, NO_x, SO_2, P_2O_5.

System boundary description

The BUO “incineration for heat and power” includes the reaction of the incoming fuel in an industrial combustion chamber, and the optional conversion of the flue gas to steam and electricity in a boiler and/or turbine and generator. A certain amount of power is needed to support the combustion process in the β system boundary. Literature numbers found vary from 2%(Henderson, 2004) to 6% (Bedi) of total feed LHV. A value of 3% is chosen (Kehlhofer et al., 2009) which can be subtracted from LHV before calculating the energy output if no better data for the SUO is available.



Calculation algorithm

The produced electricity (P_e) and heat (P_h) are obtained by multiplying the LHV of the fuel with their respective efficiency factor:

$$P_e = LHV_{fuel} \times eff_e$$

$$P_h = LHV_{fuel} \times eff_h$$

The included setups and the electricity and heat efficiency can be found in Table A.2 taken from DATABUO.

Name of the setup	Electrical efficiency (eff_e)	Steam/heat efficiency (eff_h)
Steam boiler	0	90
Small burner for electricity (all inputs)	30	0
Large burner for electricity (all inputs)	40	0
Efficient burner for electricity with combined cycles (fossils, non gas)	50	0
High Efficient burner for electricity with combined cycles (gas)	60	0
CHP (all inputs)	25	45
Efficient CHP (fossils, non gas)	30	55
High efficient CHP (gas)	40	50

Table A.2: Included setups of the BUO incineration for heat and power

For fossil fuels standard LHV's are available in a database, whilst for organic chemicals (e.g. waste solvents) standard net enthalpies of combustion are documented in literature. These values can be found in DATAPHYSCHEM.

Since the composition of coal and biomass can differ substantially, the LHV should in best case be calculated specifically per fuel, which is done by obtaining the HHV (Higher Heating Value) based on the ultimate analysis of the fuels. For different types of coal the Milne equation can be used (Institute of Gas Technology, 1978; Hoinkis & Lindner, 2007):

$$HHV_{dry} = 0.341 \times C + 1.322 \times H - 0.12 \times O - 0.12 \times N + 0.0686 \times S - 0.0153 \times ash$$

Where C, H, O, N, S and ash are the elementary compositions on a weight basis.

For biomass this can be calculated with the most appropriate equation for biomass ($R^2 = 0.834$) (Sheng & Azevedo, 2005):

$$HHV_{dry} = -1.3675 + 0.3137 \times C + 0.7009 \times H + 0.0318 \times O^{*}$$

Where:

$$O^* = 100 - C - H - ash$$

The database contains default elementary compositions (based on dry weight) for different types of coal and biomass. The LHV is in both cases calculated by (Phyllis; Fowler et al., 2009):

$$LHV_{dry} = HHV_{dry} - 2.442 \times 8.936 \times H/100$$

The LHV_{wet} can be correlated to the LHV_{dry} by:

$$LHV_{wet} = LHV_{dry} \times (1 - MC) - 2.442 \times MC$$

With MC the Moisture Content of the wet feed in wt%. The LHV_{wet} value in MJ/kg is then multiplied with the feed flow in kg/s to give the total LHV_{wet} in MW. If the energy source is a mixture of fuels, it is assumed that the LHV can be added linearly for input mixtures. For example for two input streams x and y:

$$LHV_{tot} = LHV_x \times flow_x + LHV_y \times flow_y$$

Based on elementary composition, either from the database DATAPHYSCHEM or from the user, a rough calculation can be made to estimate the main flue gas components H_2O, CO_2, NO_x, SO_2, P_2O_5. A complete oxidation of the basic components is assumed for simplicity and the emissions are expressed in kg/s.

Thus making a mass balance:

1kg H → 9kg H_2O

1kg C → 3.67kg CO_2

1kg N → 3.29kg NO_x

1kg S → 2kg SO_2

1kg P → 2.29kg P_2O_5

CO formation depends on local temperature differences in the combustion chamber and therefore it is very difficult and data intensive to make generic models for CO formation

(Velicu and Koncsag, 2009). For the mass balance, NO_x is calculated as NO_2. The main NO_x component formed at the incineration is NO, but this is instable and will react further with oxygen to NO_2 when released in air. Only fuel NO_x is considered: the Zeldovich mechanism accounting for thermal NO formation from N_2 originating from fuel or air is not considered, because of uncertainties in the currently existing models and high required input data (the reactions depend amongst others on residence time, local oxygen concentrations and local temperature) (Schwerdt, 2006).

Ash production is calculated for biomass and coal based on data from the ultimate analysis in the database (DATAPHYSCHEM). Of this ash content, 98% is retained, whilst 2% is emitted in the case an ash filter installation (Röder et al., 2004). If this is not the case, 80% is retained, and 20% is emitted (Schobert, 2002). To predict the amount of air required, potentially useful for SUO operations, the relationship of Borman and Ragland (1998) can be used which states that the air fuel ratio is equal to a + 0.25b-0.5c if the fuel has a composition of $C_aH_bO_cN_d$.
A summary of this module can be found in Table A.3.

Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow rate and composition of feed Type of energy generation setup Ash filter; yes/no	Efficiencies Ash retention	Enthalpies of combustion Ultimate analysis of the fuel	Fuel requirement Energy output Emissions and ash production

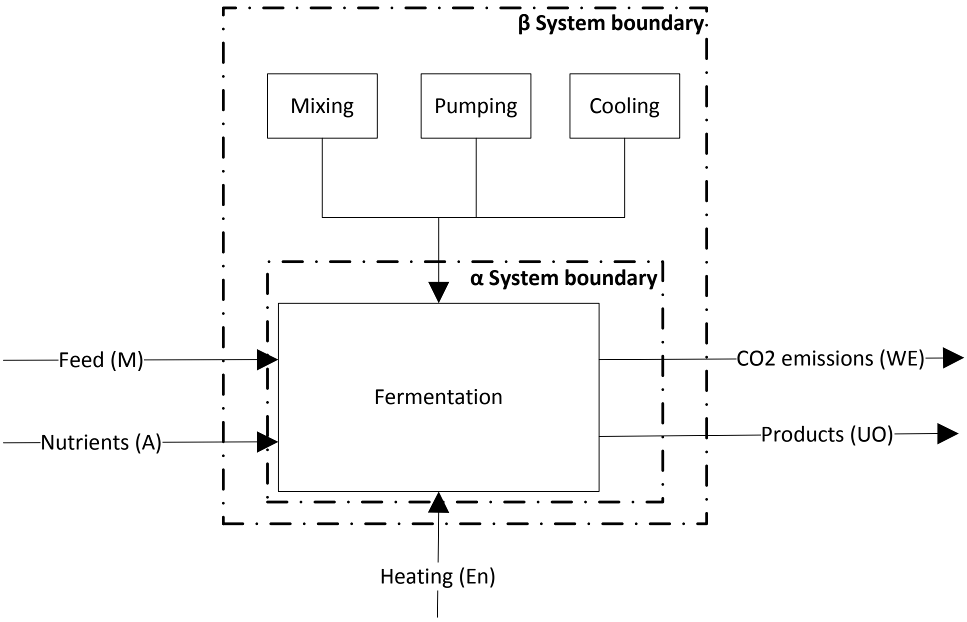
Table A.3: Summary of the BUO incineration for heat and power

1.3. Fermentation

The BUO fermentation includes the conversion of a starch/glucose feed stream to a product/water/rest products/biomass mixture and optionally a CO_2 gas stream. Calculations are based on default reactions, which can be complemented with extended Haldane kinetics if reactor volume or time is required.

System boundary description

The α system boundary includes only the conversion of the feed stream in the fermenter. The module is also able to calculate the mixing time and the potential need of cooling or heating, which can be used to calculate the UPR of the SUO in the β system boundary. Most relevant SUO are thus mixing, pumping and heating/cooling.



Calculation algorithm

If the feed stream is starch, it is assumed to be completely hydrolysed according to:

$$(C_6H_{10}O_5)_n + n\ H_2O \rightarrow n\ C_6H_{12}O_6$$

This means that the mass of starch should be multiplied with 180/162 to include the additional water in the final mass of glucose. The glucose available is then fermented to an end product according to one of the reactions in Table A.4, depending on the reaction conditions and type of micro-organism used:

Product	Reaction products	Product yield; $Y_{P/S}$ (g product /g substrate)	
		C	F
Ethanol	$C_6H_{12}O_6 \rightarrow 2\ C_2H_6O + 2\ CO_2$	0.46	0.47
PDO (1,3 – Propanediol)	$C_6H_{12}O_6 +\ 0.31\ O_2 \rightarrow 1.42\ C_3H_8O_2 + 1.73\ CO_2 + 0.32\ H_2O$	0.41	0.54
ABE (butanol)	$C_6H_{12}O_6 \rightarrow 0.20\ C_3H_6O + 0.82\ C_4H_{10}O + 0.08\ C_2H_6O + 1.50\ CO_2 + 12\ H_2$	0.42	0.50
Acetic acid	$C_6H_{12}O_6 \rightarrow 3\ C_2H_4O_2$	0.50	0.90
Acrylic acid	$C_6H_{12}O_6 \rightarrow 2\ C_3H_4O_2 + 2\ H_2O$	0.72	
Lactic acid	$C_6H_{12}O_6 \rightarrow 2\ C_3H_6O_3$	0.93	0.95
Succinic acid	$C_6H_{12}O_6 + 2\ CO_2 + 4\ H \rightarrow 2\ C_4H_6O_4 + 2\ H_2O$	0.88	1.01
Adipic acid	$3\ C_6H_{12}O_6 + 7\ O_2 \rightarrow 2\ C_6H_6O_4 + 6\ CO_2 + 12\ H_2O$	0.17	0.47
Citric acid	$C_6H_{12}O_6 + 0.5\ O_2 \rightarrow C_6H_8O_7 + 4\ H$	0.86	0.96

Table A.4: Stoichiometric fermentation reactions and current and future product yields per substrate consumed (Patel et al., 2006)

*C = Current, F = Future potential yield

The generic reaction which occurs when 1 mole of substrate is consumed includes the formation of the product(s) and the production of biomass:

$$\mathrm{C_6H_{12}O_6} + \mathrm{u\ O_2} + \mathrm{w}\ CO_2 + (\mathrm{B} \times \mathrm{m})\mathrm{N\ source} + (\mathrm{B} \times \mathrm{n})\mathrm{S\ source} + (\mathrm{B} \times \mathrm{o})\mathrm{P\ source}$$

$$\rightarrow \frac{\mathrm{Y}_{\frac{\mathrm{P}}{\mathrm{S}}} \times \mathrm{MM_{glu}}}{\mathrm{MM_{prod}}}\ \mathrm{C_aH_bO_cN_d} + B\ \mathrm{C_1H_yO_zN_mS_nP_o} + \mathrm{R\ rest\ products}$$

Where R is the amount of moles carbon in the reaction specific rest products, which can be found in the reaction equations of Table A.4, and B is the amount of moles of biomass which is formed per mole of substrate consumption and which is based on the carbon balance:

$$B = 6 + w - R - a \times \frac{Y_{\frac{P}{S}} \times MM_{glu}}{MM_{prod}}$$

$Y_{P/S}$ is the yield of product per substrate (g/g) and can be found in Table A.4. The elementary balance of hydrogen and oxygen is not checked due to the complexity of bacterial growth, but standard values of bacterial composition can be found in Table A.5 (Harding, 2008). Based on these compositions, the amount of nitrogen, sulphur and phosphorus nutrients to be added in the fermenter can be calculated.

Organism	C	H	O	N	S	P
Aerobacter aerogenes	1	1,83	0,55	0,25		
Aspergillus niger	1	1,74	0,711	0,117		
Azohydromonas lata	1	1,76	0,48	0,19		
Candida sp.	1	1,84	0,52	0,16		
Escherichia coli	1	1,77	0,49	0,24		
Klebsiella sp.	1	1,75	0,43	0,23		
Paracoccus denitrificans	1	1,66	0,49	0,2		
Pseudomonas C12B	1	2	0,52	0,23		
Saccharomyces cerevisiae	1	1,76	0,53	0,17	0,005	0,01
Other	1	1,82	0,53	0,2		

Table A.5: Elemental formula for micro-organisms (Harding, 2008)

The total output mass flow (kg/s) of end product formed is:

$$M_{prod} = Y_{P/S} \times S_{in}$$

In continuous mode, the enthalpy change of the reaction allows the calculation of amount of cooling or heating medium required to maintain a certain temperature. For example for ethanol fermentation by Saccharmoyces cerevisiae, following reaction enthalpy can be used:

$\Delta H = -120{,}6 kJ/mol$ (Chongvatana, 2007-2008)

To determine the reaction time, and thus reactor volume, necessary for the fermentation, Haldane kinetics with product inhibition can be used. The rate of biomass formation (r_b) can be calculated by multiplying the biomass concentration (B) with the specific growth rate, μ (h^{-1}) (Ghose & Tyagi, 1979):

$$r_b = B \times \mu$$

The latter can be determined by:

$$\mu = \mu_{max} \times \frac{C_{S_{un}}}{K_S + C_{S_{un}} + \frac{C_{S_{un}}^{\ 2}}{K_i}} \times \left(1 - \frac{P}{P_{max}}\right)^{\alpha}$$

In this equation K_s is the Monod constant (g/L), K_I the inhibition constant (g/L), μ_{max} the maximum specific growth rate (h^{-1}), P the ethanol concentration in the fermentor (g/l), α the product inhibition constant, P_{max} the maximum ethanol concentration (g/l) and C_{Sun} = substrate concentration (g/L). Assuming a perfectly mixed fermenter implies that the concentration in the tank is the same as the concentration in the outlet flow. In a continuous reactor, this can be determined by:

$$C_{S_{un}} = \frac{S_{un}}{S_{un}/\rho_{un} + M_{H_2O}/\rho_{H_2O} + M_{prod}/\rho_{prod} + M_B/\rho_B + M_{rest\ prod}/\rho_{rest\ prod}}$$

With M and ρ the mass and density (kg/l) of the unused product (un), the water (H_2O), the end product (prod), the biomass (B) and the rest products respectively and assuming that density can be added linearly.

These kinetics can be simplified to

$$\mu = \mu_{max}$$

in the case that substrate and product inhibition are negligible, and if substrate concentration is high in comparison to the Monod constant. However in industrial practice this might not always be the case, since it is the goal to consume as much as the substrate as possible to form high concentrations of end products. Furthermore, the product inhibition factor $\left(1 - \frac{P}{P_{max}}\right)^{\alpha}$ and substrate inhibition $\frac{{C_{S_{un}}}^2}{K_i}$ factor can be neglected if no influence of product and substrate concentration is expected. Based on these reaction rates, the residence time in the reactor can be estimated.

A summary of this BUO can be found in Table A.6.

Input values required	DATABUO	DATAPHYSCHEM	Output
Fermentation reaction Type of micro-organism Mass and composition of input flow	Yield coefficient Kinetic parameters Reaction enthalpy (preferably entered by user)	Composition of feed streams	Mass input and output (including nutrients and emission) Heating and cooling required

Table A.6: Summary of the BUO fermentation

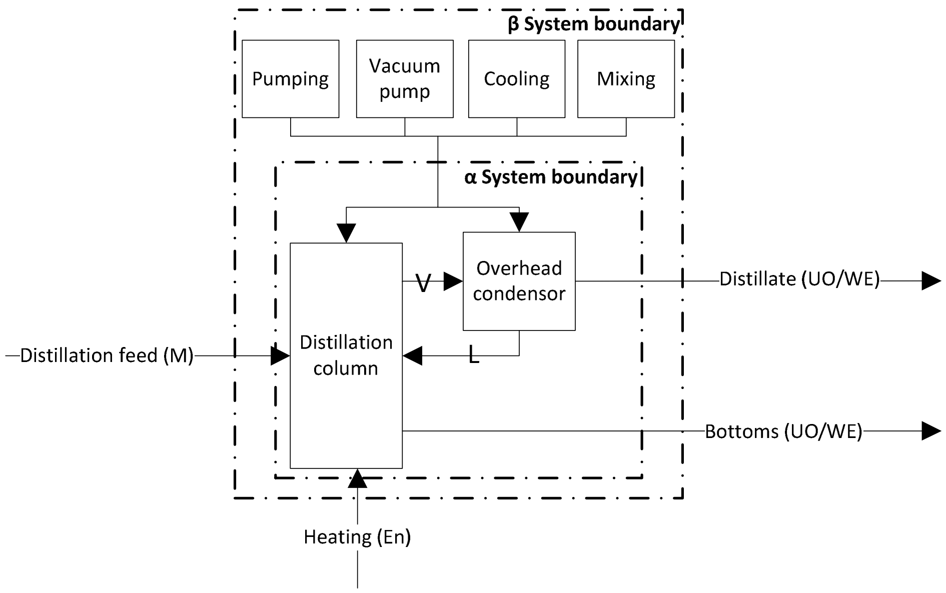
2. Separation processes

2.1. Binary distillation

Distillation is used as a separation process based on different boiling points. In contrary to evaporation, all components are appreciably volatile. Furthermore, the vapour phase is condensed in an overhead condenser, optionally with a reflux, the latter returning a part of the condensed vapour to the distillation column.

System boundary description

The BUO can be used for non extractive binary distillations with or without reflux. It calculates the heat required for the evaporation process (often in a reboiler) and the cooling energy required in the condensation (incl. reflux). This is valid over a broad temperature range, as long as the coefficients for the heat capacity calculations remain valid. Pumping operations for the different liquid and gas streams, vacuum pumps and possible mixing operations are not included in the α system boundary. Furthermore, cooling (in the condenser) should be added as a SUO in the β system boundary.



Calculation algorithm

The general equation for calculating the energy requirements of a distillation is very similar to the equation for an evaporation, but includes the fraction of reflux that has to be added to the enthalpy of vaporization:

$$q = \left((1 + RR) \times \left(m_f - m_b\right) \times \lambda_v + m_f \times c_p \times \left(T_b - T_f\right)\right) \Big/ \eta$$

With m_f and m_b the mass of the feed and the bottoms respectively, λ_v the latent heat of the vapor, c_p the mean heat capacity of the feed, T_b the pressure dependent boiling point of the vaporized component and η an efficiency factor, typically 0.9, accounting for heat losses.

The Reflux Ratio (RR, or L/D) can be calculated based on the minimum reflux ratio (RR_{min}) with a rule of thumb (Perry & Green, 1999):

$$RR = 1.35 \times RR_{min}$$

Assuming negligible holdup of liquid on the trays, in the column, and in the condenser, the minimum reflux ratio can be obtained by:

$$R_{min} = (L/D)_{min} = \frac{\frac{y_d - y_{pi}}{x_d - x_{pi}}}{1 - \frac{y_d - y_{pi}}{x_d - x_{pi}}}$$

With y_{pi} and x_{pi} the initial molar fraction of the more volatile component and y_d and x_d the molar fraction of the more volatile component in the distillate in the vapour phase and liquid phase respectively. Where x_d and y_d are equal assuming a total condensation (Figure A.1 (Perry & Green, 1999)).

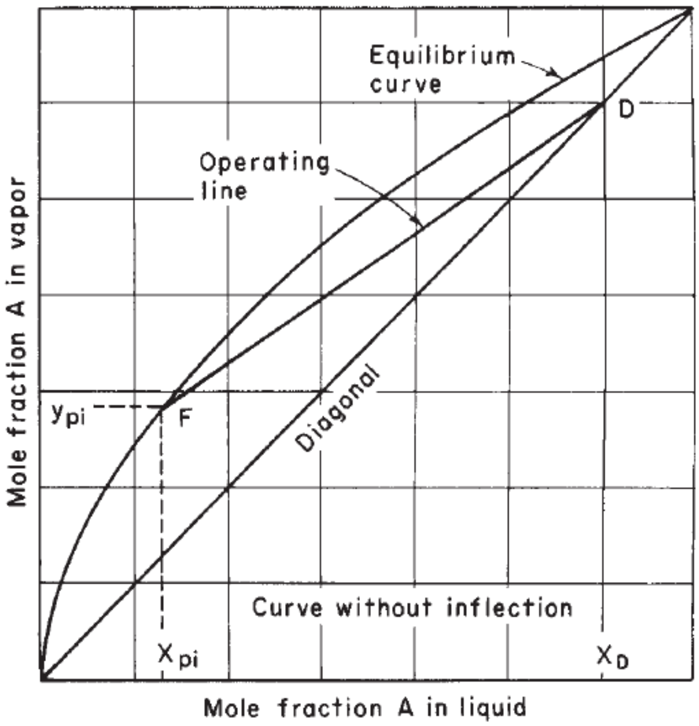


Figure A.1: Determination of the minimum reflux ratio from the Equilibrium curve and operating line in a distillation. Point D is the composition of the distillate, whilst point F is the composition of the feed (Perry & Green, 1999)

Assuming that the vapor is cooled to obtain a phase change, the cooling duty for the condensation (q_c) of is:

$$q_c = (1 + RR) \times \left(m_f - m_b\right) \times \lambda_v$$

Aforementioned theory is generally applicable, however does not include the specific cases of azeotropes. A frequently used example is the case of an ethanol – water – biomass mixture obtained after a fermentation. Table A.7 gives a summary of this BUO

Input values required	DATAPHYSCHEM	Output
Composition feed Compositions distillate	Heat capacities Enthalpy of vaporization Pressure dependent boiling temperature	Heating and cooling required Temperatures

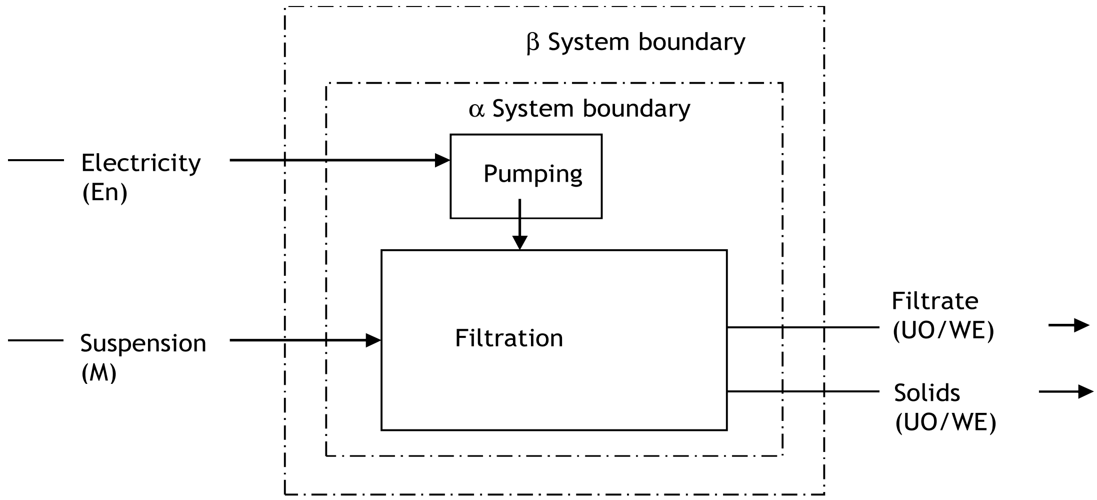
Table A.7: A summary of the BUO binary distillation

2.2. Filtration

In chemical processes, filtration is the mechanical or physical operation which is used for the separation of solids from fluids (liquids or gases) by leading them through a medium that allows only the fluid to pass and that retains oversize solids. As a filtration medium, normally a solid sieve or a membrane (surface filter) is applied although filtration can also occur through a bed of granular material (depth filter). Fluids flow through a filter due to a difference in pressure – fluids flow from the high pressure side to the low pressure side of the filter, leaving solids behind. The application of gravity is the simplest way to achieve this, but in the laboratory, pressure in the form of compressed air on the feed side or vacuum on the filtrate side may be applied to enhance the filtration process. In industry, when a reduced filtration time is important, the liquid may flow through a filter by the force exerted by a pump.

System boundary description

The α system boundary for this BUO includes the filtration of a suspension and the pumping operation applied to create a pressure difference. Depending on the requirements, either the filtrate or the solids are the useful output.



Calculation algorithm

The power for filtration (P_f in W) is calculated according to (Harding, 2008):

$$P_f = \frac{\Delta P \times Q}{eff.}$$

In which:

ΔP = Pressure difference across the filter (Pa)

Q = Flow through the filter (m^3/s)

eff. = Pumping efficiency (dimensionless)

Alternatively, rule of thumb values for different type of filtration can be used, which can be found in Table A.8 (Patel et al., 2006).

Type of membrane filtration	Unit	Value range	Chosen value
Microfiltration	kWh/m^3 permeate	1.2-2.6	2
Ultrafiltration	kWh/m^3 permeate	3.5-16	5
Diafiltration	kWh/m^3 permeate	5	5
Nanofiltration	kWh/m^3 permeate	1-7	7

Reverse osmosis	kWh/m^3 permeate	2.5-10	9

Table A.8: Default electricity consumption values for different types of filtration

A summary of this BUO can be found in Table A.9.

Input values required	DATABUO	DATAROT	Output
Flow of fluid Pressure difference if available	Pumping efficiency	Default electricity consumption	Electricity use

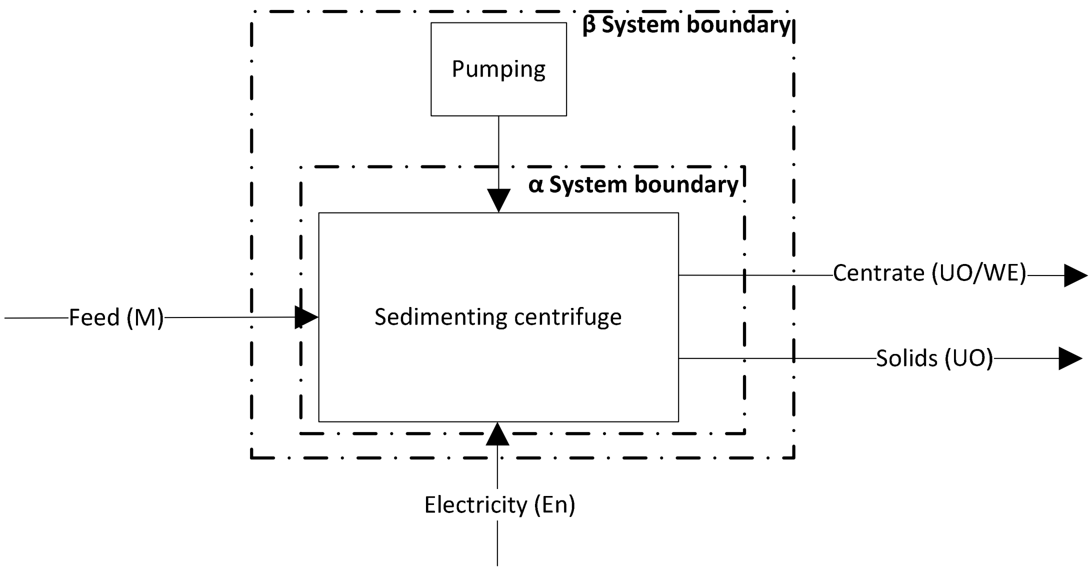
Table A.9: A summary of the BUO filtration

2.3. Sedimenting Centrifuges

Sedimenting centrifugation is a broadly used, but energy intensive equipment to separate solids from liquids based on a difference in density, without using a filter (Perry & Green, 1999).

System boundary description

This BUO focuses in the α system boundary on the electricity use of the sedimenting centrifuges. Data is available for tubular, disk, disk with nozzle discharge and decanters/helical conveyors. Necessary pumping operations are situated in the β system boundary. An approximation can be made of the separation efficiency, to serve as input for further BUO.



Calculation algorithm

Due to the complexity of the process, where the settling speeds and power consumption depends heavily on type of centrifuge and particle size and shape of the solids, it is very difficult to obtain one generic equation. Therefore, the power consumption is modelled by using default powers of different types of equipment, which can be taken from DATABUO (Table A.10 (Perry & Green, 1999)).

Type	Bowl diameter (cm)	Typical speed (r/min)	Maximal centrifugal force x gravity	Liquid throughput min (l/s)	liquid throughput max (l/s)	Solids throughput min (kg/s)	Solids throughput max (kg/s)	Typical motor size (kW)
Tubular	4.45	50000	62400	0.003	0.016			[1]
	10.48	15000	13200	0.006	0.630			1.5
	12.70	15000	15900	0.013	1.260			2.2
Disk	17.78	12000	14300	0.006	0.630			0.2
	33.02	7500	10400	0.315	3.150			4.5
	60.96	4000	5500	1.260	12.600			5.6
Disk; nozzle discharge	25.40	10000	14200	0.630	2.520	0.028	0.278	14.9
	40.64	6250	8900	1.575	9.450	0.111	1.111	29.8
	68.58	4200	6750	2.520	25.200	0.278	3.056	93.3
	76.20	3300	4600	2.520	25.200	0.278	3.056	93.3
Decanter / Helical conveyor	15.24	8000	5500		1.260	0.008	0.069	3.7
	35.56	4000	3180		4.725	0.139	0.417	14.9
	45.72	3500	3130		6.300	0.278	0.833	37.3
	60.96	3000	3070		15.750	0.694	3.333	93.3
	76.20	2700	3105		22.050	0.833	4.167	149.2
	91.44	2250	2590		37.800	2.778	6.944	223.8
	111.76	1600	1600		44.100	2.778	6.944	298.4
	137.16	1000	770		47.250	5.556	16.667	186.5

Table A.10: Typical centrifuge configurations and power (pw) (Perry & Green, 1999)

[1] Turbine driven, 372kPa necessary (steam or air compressor)

Alternatively for yeast and bacteria a rule of thumb value can be used. The values for yeast centrifugation range from 0.7-2.5 kWh/m3 of feed. The recommended value was determined at 1.5 kWh/m3 of feed. The values for bacteria centrifugation range from 6.2-25 kWh/m3 of feed. The recommended value was determined at 7 kWh/m3 of feed.

A summary of the BUO sedimenting centrifuges can be found in Table A.11.

Input values required	DATABUO	DATAROT	Output
Type of centrifugation equipment Liquid/solid throughput	Centrifuge power Rotational speed Bowl diameter	Default values for yeast and bacteria	Electricity use

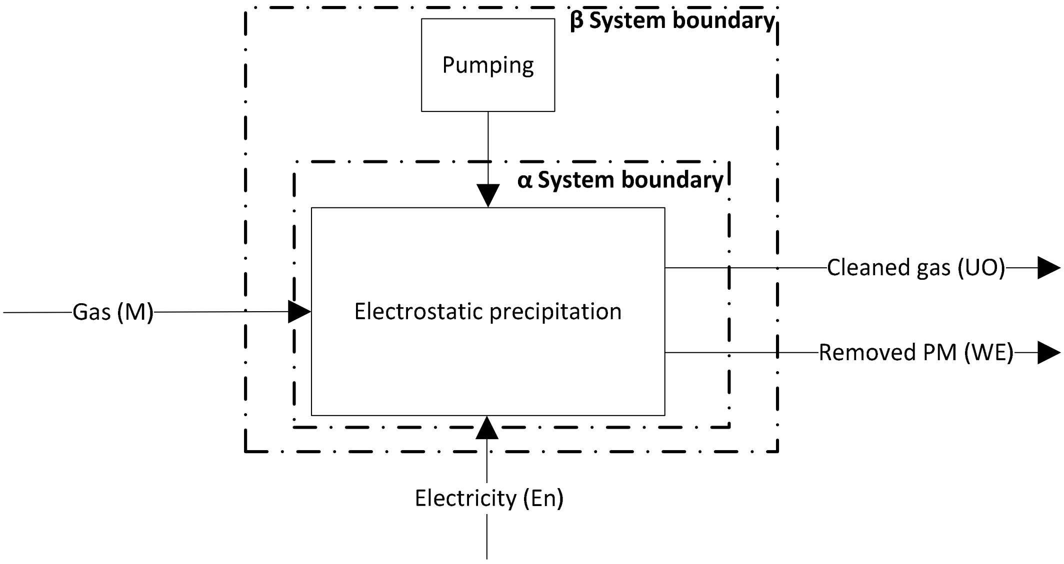
Table A.11: A summary of the BUO sedimenting centrifuges

2.4. Electrostatic precipitation (ESP)

Electrostatic precipitators use an induced electric charge to separate solids from a gaseous stream.

System boundary description

This BUO includes the electricity used for the corona generation and is valid for gas velocities between 0.5 and 3m/s. The module is aimed at dry electrostatic precipitation of particulate matter from 0.01 to 10µm. It does not include pumping operations.



Calculation algorithm

The electrical corona produced requires a certain amount of power, which can be calculated by (University of Florida, Environmental Engineering Sciences, Aerosol & Particulate Research Lab, 2011):

$$P = -19.42 \times Q \times ln(1 - \eta)$$

P is the Power (in W), Q is the volumetric gas flow (in m³/s) and η is the efficiency of the precipitation in %.

A summary of the BUO electrostatic precipitation can be found in TableA.12.

Input values required	DATABUO	DATAPHYSCHEM	Output
Gas flow rate + composition Efficiency of solids removal	-	-	Electricity use Mass of solids precipitated

Table A.12: A summary of the BUO electrostatic precipitation

2.5. Electrodialysis

Electrodialysis is a separation technique that uses an applied electric potential difference for the transportation of salt ions from one solution to another through ion-exchange membranes. This is done in a configuration called an electrodialysis cell. The cell consists of a feed (dilute) compartment and a concentrate (brine) compartment formed by an anion exchange membrane and a cation exchange membrane placed between two electrodes. Under the influence of an electrical potential difference, negatively charged ions in the dilute stream migrate towards the positively charged anode. These ions pass through positively charged anion exchange membrane, but are prevented from further migration toward the anode by the negatively charged cation exchange membrane and therefore stay in the concentrate stream, which becomes concentrated with the anions. The positively charged species in the dilute stream migrate toward the negatively charged cathode and pass through the negatively charged cation exchange membrane. These cations also stay in the concentrate stream, prevented from further migration toward the cathode by the positively charged anion exchange membrane. Anion and cation migration is enabled by an electric current that flows between the cathode and anode. A schematic example of an electrodialysis process is given in Figure A.2 for NaCl concentration. Only an equal number of anion and cation charge equivalents are transferred from the dilute stream into the concentrate stream, maintaining the charge balance in each stream. The overall result of the electrodialysis process is an ion concentration increase in the concentrate stream with a depletion of ions in the dilute solution feed stream (American Water Works Association, 1995).

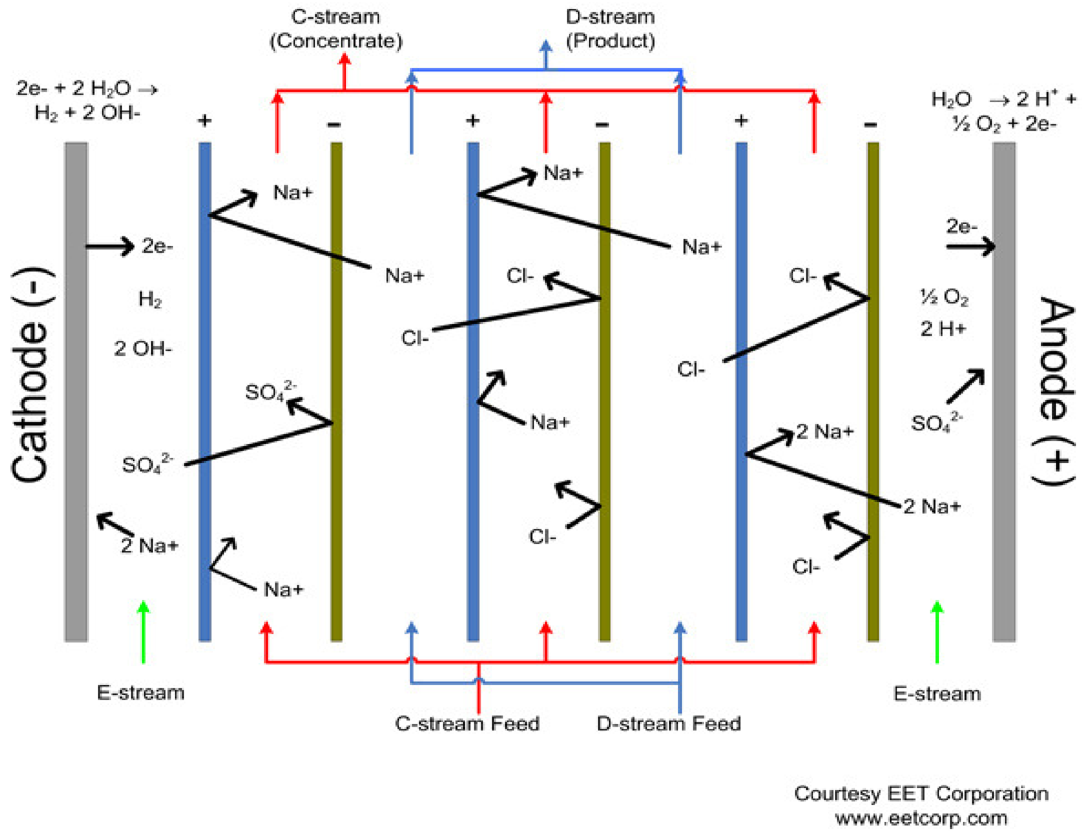
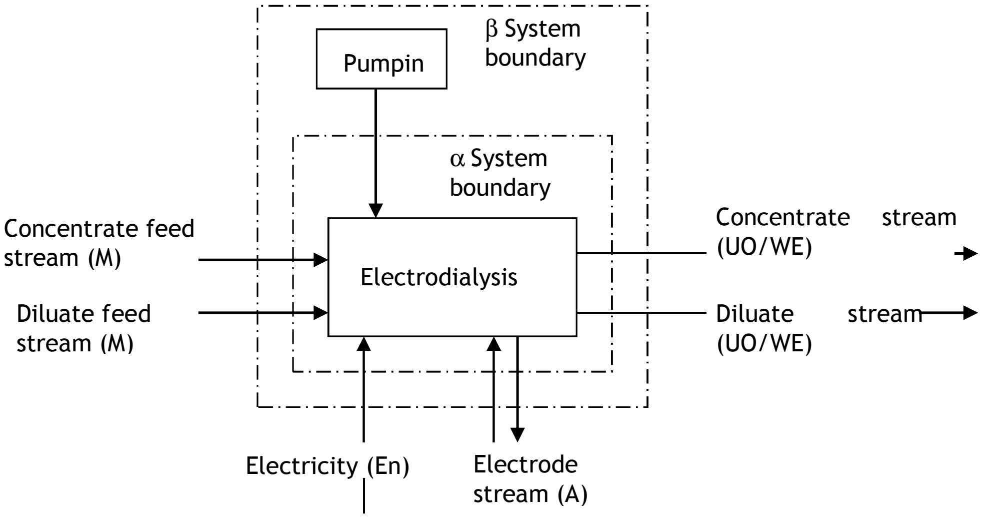


Figure A.2: Example of an electrodialysis process (Wikipedia)

This basic engineering module calculates the energy requirements for the electrodialysis process.

System boundary description

The α system boundary of this process includes the electrodialysis process in which ions are shifted from a diluate stream to a concentrate stream. Either the diluate stream is the useful output (if the aim is to get rid of certain substances in a liquid) or the concentrate stream is the useful output (if the aim is to concentrate certain substances in a liquid). There is an additional flow, i.e. the electrode stream. The electrode stream flows past each electrode in the stack. This stream may consist of the same composition as the feed stream or may be a separate solution containing different compounds. Depending on the stack configuration, anions and cations from the electrode stream may be transported into the concentrate stream, or anions and cations from the diluate stream may be transported into the electrode stream. In each case, this transport is necessary to carry current across the stack and maintain electrically neutral stack solutions. The β system boundary includes pumping requirements for the transport of the streams.



Calculation algorithm

The electricity requirement for electrodialysis is calculated according to (Perry & Green, 1999):

$$E_{ed} = \frac{U \cdot F}{\eta_I \cdot n}$$

In which:

E_{ed} = Energy consumption (J/ mol equivalent salt shifted)

U = Applied voltage (V)

F = Faraday constant (= 96485.34 Amp.s/mol)

η_I = Current efficiency (dimensionless)

n = number of cell pairs (dimensionless)

The energy consumption is expressed per mol equivalent salt shifted. An equivalent stands for a unit of charge. This means that, e.g., 1 mol SO_4^{2-} equals 2 mol equivalents. And likewise, the shift of 1 mol H_2SO_4 equals 2 mol equivalents. The meaning of expressing shifts per equivalent appears from the following formula for current efficiency:

$$\eta_I = \frac{N_i \cdot F}{n \cdot I} = \frac{Q_p\left(c_i - c_i^0\right)F}{n \cdot I}$$

In which:

N_i = Flow of ionic substance i formed from the splitting operation (mol eq/s)

I = Current intensity through the stack (A)

Q_p = Volumetric flow of the product (m^3/s)

c_i = Concentration of ionic substance i in the product stream (mol eq/m^3)

c_i^0 = Concentration of ionic substance i in the inlet stream (mol eq/m^3)

The current efficiency basically determines the amount of coulombs shifted per coulomb applied by means of external power. The amount of coulombs shifted is determined by the charge of the ions. Each coulomb originates from 1 charge equivalent of an ion. It is represented by the numerator and expressed in Amp.s/s = Coulomb/s. The amount of Coulombs externally supplied is determined by the denominator and is expressed in Amp which is also Coulomb/s.

Alternatively, literature values can be found in the BREW study (Patel et al., 2006 for different electrodialysis processes. The energy consumption ranges from 0.07-0.34 kWh/mol eq. The recommended value in this study is to use 0.1 kWh/ mol eq. The respective equivalent value from the example above is 0.2 kWh/mol. The difference to the generic value according to the BREW study (factor of 2) may be explained primarily by a rather low current efficiency in the lab-scale process (44%). Table A.13 summarizes this BUO.

Input values required	DATAPHYSCHEM	Output
Applied voltage Number of cell pairs Current intensity through the stack Volumetric flow of the product Concentration of ionic substance i in the product stream Concentration of ionic substance i in the inlet stream	Faraday constant	Electricity use

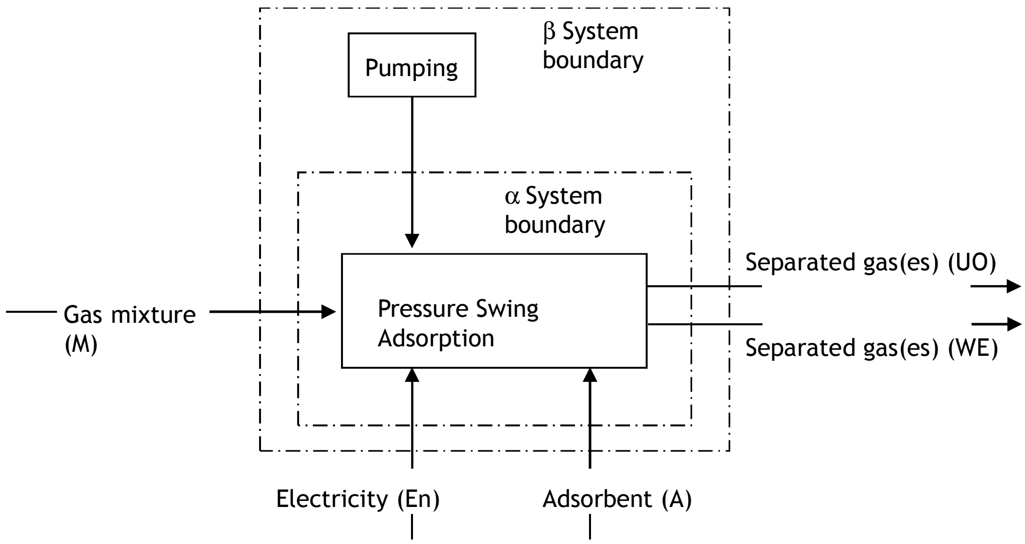
Table A.13: A summary of the BUO electrodialysis

2.6. Pressure swing adsorption

Pressure swing adsorption is a technology that is used for the separation of gas species from a mixture of gases under pressure. It is based on the species molecular characteristics and affinity for an adsorbent material. Pressure swing adsorption processes rely on the fact that under pressure, gases tend to be attracted to solid surfaces, or 'adsorbed'. Special adsorptive materials are used as a molecular sieve, for example 'zeolites'. The process then swings to low pressure to desorb the adsorbent material. This basic engineering module calculates the energy required to separate a gas from a gas mixture by pressure swing adsorption.

System boundary description

The α system boundary of this process includes the separation of (a) gas(es) from a gas mixture by means of pressure swing adsorption. Either removed gas(es) or the remaining gas mixture can be the useful output product. For this process, energy in the form of electricity is needed as well as adsorbent material. The adsorbent material can be reused many times however. In the β system boundary, some pumping is required to transport the gases.



Calculation algorithm

An extensive theoretical analysis of a pressure swing adsorption process is given by Huang et al. (2008). The power requirements of a pressure swing adsorption process are calculated according to:

$$P = \frac{\gamma}{\gamma - 1} \cdot R_g \cdot T_{feed} \left[\left(\frac{p_{feed}}{p_{atm}} \right)^{\frac{(\gamma-1)}{\gamma}} - 1 \right] \pi \cdot r_{bed}^2 \cdot u_{feed} \cdot c_{feed}$$

In which:

P = Power (W)

ζ = Ratio of heat capacities, c_p/c_v (dimensionless)

R_g = Ideal gas constant, i.e. 8.314 J $mol^{-1}K^{-1}$

T_{feed} = Temperature of the feed (K)

p_{feed} = Pressure of the feed (bar)

p_{atm} = Atmospheric pressure, i.e. 1.013 bar

r_{bed} = Column radius (m)

u_{feed} = Interstitial gas velocity (m/s)

c_{feed} = Concentration of the feed stream (mol/m^3)

The ratio of the heat capacities for various gases can be found in DATAPHYSCHEM or in chemical handbooks (White, 1999; Lange and Dean, 1973).

The interstitial gas velocity is calculated with:

$$u_{feed} = \frac{Q}{A \cdot \varepsilon}$$

In which:

Q = Volumetric flow rate (m^3/s)

A = Cross sectional area of the bed (m^2)

ε = Void fraction of the bed, i.e. ratio of the void volume to the total volume of the bed

The concentration of the feed stream (all compounds) is calculated based on the ideal gas law:

$$c_{feed} = \frac{p_{feed}}{R_g \cdot T_{feed}}$$

If the flow rate of the separated gas is known, the total energy requirements (in J/kg) can be calculated:

$$E = \frac{P}{v}$$

In which:

E = Energy use (J/kg)

P = Power (W)

v = Flow rate separated gas (kg/s)

A summary of the BUO pressure swing adsorption can be found in Table A.13

Input values required	DATAPHYSCHEM	DATABUO	Output
Temperature of the feed Pressure of the feed Column radius Interstitial gas velocity Concentration in feed Flow rate separated gas	Atmospheric pressure Ratio of heat capacities	-	Electricity use

Table A.13: A summary of the BUO pressure swing adsorption

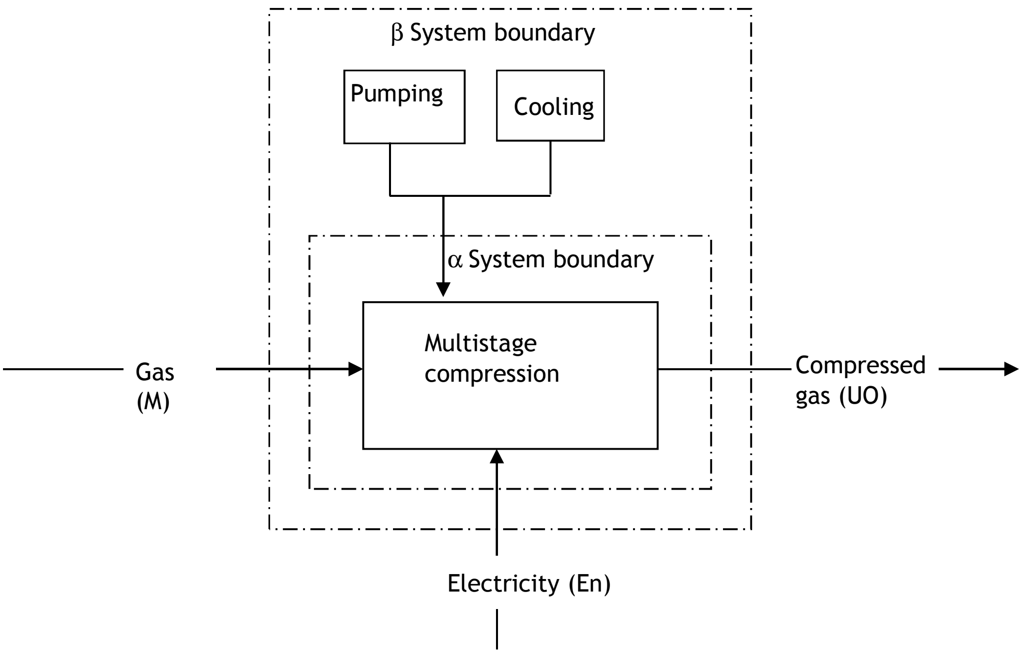
3. Physical mechanical processes

3.1. Mechanical Compression- Multi stage

In multistage compression, the pressure to which gases can be compressed is much higher than when using single stage compression. Another reason for applying multistage compression is that the same compression task can be realized with lower energy use. Multistage compression is a sequence of compressions. After each compression stage the heat that is generated in the compression is removed by cooling, making multistage compression less adiabatic and more isothermal. The choice of the compressor type for each compression step depends mainly on the flow rate and the differential pressure (Damen, 2007). The theoretical energy requirements can be estimated, however. This basic engineering module calculates the estimated energy requirements for multistage compression of gases.

System boundary description

The α system boundary of this BUO includes the multistage compression of a gas. Electricity is needed for the compressor. The β system boundary includes the pumping and cooling requirements and is therefore not directly included in the calculation algorithm.



Calculation algorithm

For a multistage compression with n stages, power requirements are given by following equation (Diomedes Christodoulou, 1984):

$$W = \frac{ZRT_1}{M}\frac{n\gamma}{\gamma - 1}\left[\left(\frac{p_2}{p_1}\right)^{\frac{\gamma-1}{n\gamma}} - 1\right]$$

In which:

W = Specific compression work (J/g or kJ/kg)

Z = Compressibility factor (Dimensionless)

R = Universal gas constant i.e. 8.314 J $mol^{-1}K^{-1}$

T_1 = Suction temperature (K)

n = Number of stages (Dimensionless)

ζ = Ratio of heat capacities, c_p/c_v (dimensionless)

M = Molar mass (g/mol)

p_1 = Suction pressure (MPa)

p_2 = Discharge pressure (MPa)

Since this is the theoretical power use of the multistage compression process, a correction has to be made for efficiency losses:

$$P = \frac{W}{\eta_{is}\eta_m}$$

In which:

P = Power requirements (kJ/kg)

η_{is} = Isentropic efficiency (Dimensionless)

η_m = Mechanical efficiency (Dimensionless)

A summary of the BUO mechanical compression – multi-stage can be found in Table A.14

Table 1: A summary of the BUO Mechanical compression - multi -stage

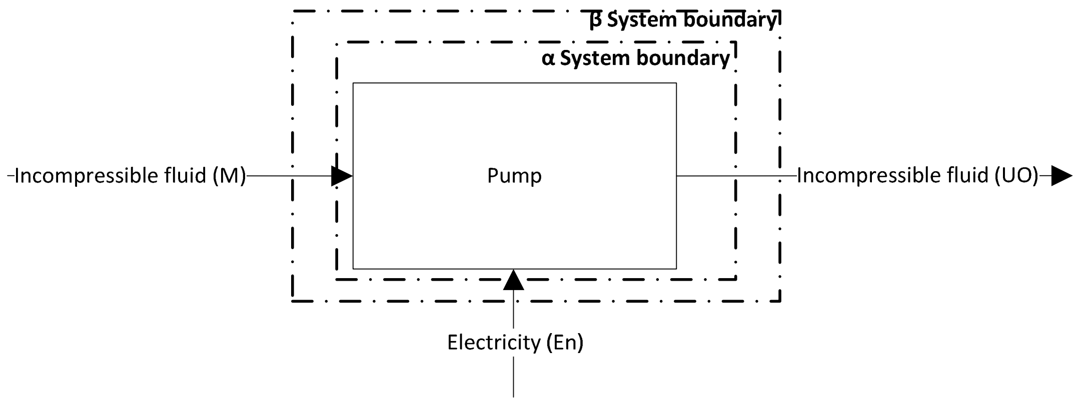
Input values required	DATAPHYSCHEM	DATABUO	Output
Suction temperature Number of stages Suction pressure Discharge pressure	Universal gas constant Specific heat ratio Molar mass	Compressibility factor Isentropic efficiency Mechanical efficiency	Electricity use Properties of output streams

3.2. Pumping incompressible fluids

This module includes the pumping of incompressible fluids. Whilst in principle all fluids are compressible, the compressibility of liquids is low, and for gases, incompressibility is often used as an approximation at lower speeds.

System boundary description

The electricity use is calculated to pump an incompressible fluid over a certain distance and height. The calculation algorithm can be used for centrifugal, axial, rotary and reciprocating pumps, for Newtonian and Power law fluids. Herschel – Bulkley can also be chosen, but larger errors are expected, due to limited knowledge of their behaviour in different pipe configurations. Numerous assumptions are made in the equations: constant fluid density, the absence of thermal energy effects; single phase, uniform material properties and uniform equivalent pressure (Valentas et al., 1997).



Calculation algorithm

The starting point to estimate the pump power is to determine the type of fluid. Three different types of fluids are considered depending on the relation between the shear stress (σ) and the shear rate (γ):

Newtonian fluids: $\sigma = \mu \times \gamma$

Power law fluids: $\sigma = K \times \gamma^n$

Herschel – Bulkley fluids: $\sigma = \sigma_0 + K \times \gamma^n$

With μ the viscosity, K the consistency index, n the flow behavior index and σ_0 the yield stress. Often the Newtonian equations are used, but in many real cases such as different types of slurries the Newtonian theory is not applicable. Even fibrous slurries such as fermentation broths, fruit pulps, crushed meal animal feed, tomato puree, sewage sludge, and paper pulp, which may not contain a high percentage of solids may flow as non-Newtonian regimes (Abulnaga, 2002). Because of its ease of use, the empirical Power Law is often used (Rao, 1999).

Pump power

The basic equation to estimate pump power for transporting incompressible fluids is:

$$P_n = \frac{H \times Q \times \rho \times g}{eff.}$$

P_n = pump power output in W, H the total dynamic head in Nm/kg, Q the capacity in m³/s, ρ the density (kg/m³), g the gravity constant and eff. the efficiency of the pump (Perry & Green, 1999).

The main bottleneck for the calculation of the necessary power is thus determining the dynamic pump head to displace the fluid. This factor depends on the conditions at starting and end position, on the flow rate, on the type and configuration of the pipes used, and on the type of fluid that is pumped. The dynamic head can be obtained from the Bernoulli equation: (Valentas et al., 1997).

$$H = \Delta z + \frac{\Delta p}{\rho \times g} + \frac{\Delta u^2}{g \times \alpha} + h_w$$

With Δz the difference in height between the starting and end position, which equals zero in closed systems. Δp is the pressure difference between initial and end situation, α is the correction factor for velocity distribution in the pipe and h_w is the resistance head.

Velocity head

The difference in velocity is represented by Δu, where the velocity behind the pump can be calculated based on the flow rate and the cross sectional area of the pipes (A):

$$u = \frac{Q}{A}$$

According to www.cheresources.com liquid transport pipes should be sized according to:

$$u = \left(1.524 + \frac{D}{0.9144}\right) m/s$$

With D the diameter of the pipe (in m).

For circular pipes:

$$A = \pi \times \frac{D^2}{4}$$

Merging these equations delivers a link of flow (in m³/s) and diameter (in m):

$$Q = \pi \times \frac{D^2}{4} \times \left(1.524 + \frac{D}{0.9144}\right)$$

$$Q = 1.197D^2 + 0.859D^3$$

This can be solved if the flow is known.

α is the correction factor for velocity distribution in the pipe. For the turbulent flow this is always approximated as 2, whilst for laminar flow it depends on the type of fluid (Ibarz and Barbosa-Cánovas, 2003):

Newtonian fluids: α=1

Power law fluids (using the flow behavior index n)

$$\alpha = \frac{2 \times (2n + 1) \times (5n + 3)}{3 \times (3n + 1)^2}$$

Herschel – Bulkley fluids: The correction factor can be deducted from Figure A.3:

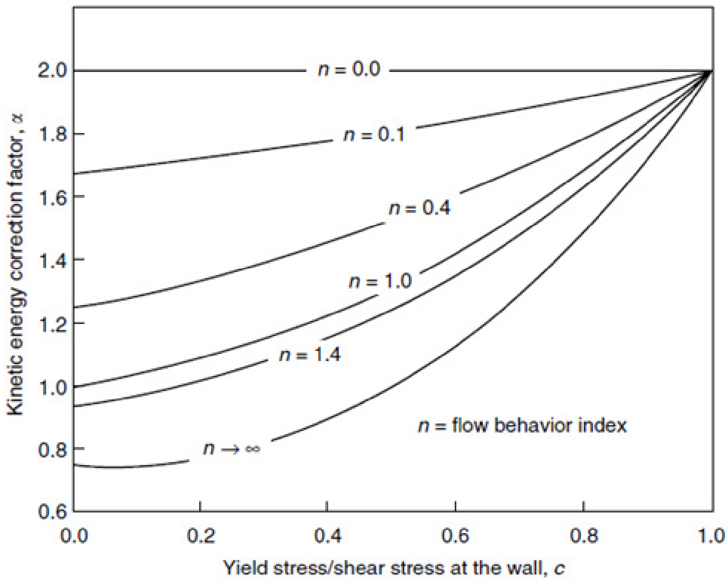


Figure A.3: The kinetic energy correction factor for Herschel-Bulkley fluid foods (Valentas et al., 1997)

The dimensionless yield stress (c):

$$c = \frac{\sigma_0}{\sigma_w} = \frac{\sigma_0}{(\frac{D \times \Delta P}{4L})} = \frac{\sigma_0}{f \times \rho \times \frac{u^2}{2}}$$

σ_0 = the yield stress, σ_w the shear stress at the wall and $\Delta P/L$ the pressure drop per unit of length.

Resistance head

h_w is the resistance head (m), which consists out of a basic friction resistance, with f the fanning friction factor, and a factor k_f accounting for supplementary losses, with b the amount of fittings, valves, elbows,...

$$h_w = \frac{2f \times u^2 \times L}{D} + \sum_{1}^{b} \frac{k_f \times u^2}{2 \times \alpha}$$

This resistance factor depends heavily on the flow regime. Therefore the Reynolds number has to be determined, which can be calculated for Power Law fluids by:

$$Re_G = \frac{d^n \times u^{2-n} \times \rho}{8^{n-1} \times K} \times \left(\frac{4n}{1+3n}\right)^n$$

For fluids without yield stress, the critical Reynolds number is determined with:

$$Re_C = \frac{6464n}{(1+3n)^2 \times \left(\frac{1}{2+n}\right)^{\frac{2+n}{1+n}}}$$

When the magnitude of n < 1 the fluid is shear-thinning or pseudoplastic, and when n > 1 the fluid is shear thickening or dilatant in nature (Rao, 1999). For the special case of a Newtonian fluid (n = 1), the consistency index K is identically equal to the viscosity of the fluid. Thus for Newtonian fluids this becomes:

$$Re = \frac{\rho \times u \times d}{\mu}$$

And the critical Reynolds number is 2100, meaning that a Reynolds numbers lower than this value are laminar. Reynold numbers above 4000 are situated in the turbulent region. For the intermediate region (2100<Re<4000), it is impossible to obtain the pumping equations, thus an approximation should be made. Often Reynolds numbers above the critical number (2100 for Newtonian fluids) are assumed to be in the turbulent region.

When a fluid has a non negligible yield stress, the Herschel – Bulkley theory should be used. The critical Reynolds number can then be calculated by:

$$Re_c = 2He_G \times \left(\frac{n}{3n+1}\right)^2 \times \left(\frac{\Psi}{c}\right)^{\frac{2}{n}-1}$$

With He_G the Hedstrom number (Ibarz and Barbosa-Cánovas, 2003):

$$He_G = \frac{D^2 \times \rho}{K} \times \left(\frac{\sigma_0}{K}\right)^{\frac{2}{n}-1}$$

The critical Reynolds number can be obtained graphically, however, in this work the Herschel-Bulkley fluids are only used in the laminar region, which is realistic due to the high viscosity and elasticity of these fluids.

Fanning friction factor

Laminar flow

Since the Herschel – Bulkley equation is the general form of the three previous equations, this will be taken as a starting point, where the friction factor can be calculated as:

$$f = \frac{16}{\Psi \times Re_G}$$

With

$$\Psi = (3n+1)^n \times (1-c)^{1+n} \times \left[\frac{(1-c)^2}{3n+1} + \frac{2c \times (1-c)}{(2n+1)} + \frac{c^2}{n+1}\right]^n$$

For power law and Newtonian fluids c=0, making Ψ=1 and thus the friction factor can be simplified to:

$$f = \frac{16}{Re_G}$$

For turbulent flow, it is thus assumed that the fluids are obeying Newton or Power law equations.

Turbulent flow in smooth pipes:

For Power Law fluids the Dodge and Metzner (1959) equations give good results for (n = 0.4 to 1):

$$\frac{1}{\sqrt{f}} = \left(\frac{4}{n^{0.75}}\right) \times log\left(Re_G \times f^{\left(1-\frac{n}{2}\right)}\right) - (\frac{0.4}{n^{1.2}})$$

This equation is simplified to the Von Karman equation for Newtonian fluids (n=1) (Chhabra and Richardson, 1999):

$$\frac{1}{\sqrt{f}} = 4 \times log\left(Re_G \times \sqrt{f}\right) - 0.4$$

For turbulent flow in rough pipes, the roughness of the pipe has an influence. However, for non Newtonian flows, these relationships are not well studied. The Torrance equation is used for fluids with n<1 (Liu, 2003).

$$\frac{1}{\sqrt{f}} = 2.035 \times log\left(\frac{D}{2\varepsilon}\right) + 3.0 - \frac{1.325}{n}$$

D represents the inner diameter and ε the absolute roughness which depends on the material used. Default values can be found in DATABUO (Table A.15) (Van Der Meeren, 2004). For other fluids it is stated that the equations valid for Newtonian fluids can be used as an approximation, since the turbulence becomes more important (Abulnaga, 2002). A popular equation for Newtonian fluids is given by the Colebrook-White equation (Perry & Green, 1999):

$$\frac{1}{\sqrt{f}} = -4 \times log\left[\frac{1.256}{Re_G \times \left(\sqrt{f}\right)} + \frac{\varepsilon}{3.7 \times D}\right]$$

Table A.15: Default roughness factors of different piping material

Type	Absolute roughness ε in m
PVC, plastic, glass	0
Drawn tubing	0.0000015
Commercial steel and wrought iron	0.000045
Asphalted cast iron	0.00012
Galvanized iron	0.00015
Cast iron	0.00026
Wood stave	0.00018-0.00092
Concrete	0.00030-0.0030
Riveted steel	0.00092-0.0092

Supplementary losses

The second term in friction factor accounts for supplementary losses. In general these factors are determined experimentally for Newtonian fluids and due to insufficient data they are also used for non-Newtonian fluids (Perry & Green, 1999; Chhabra and Richardson, 1999). In general two options exist. For elbows, gates, valves, equivalent lengths are used:

$$h_w = \frac{2f \times u^2 \times L}{D}$$

With equivalent lengths (in m) taken from Table A.16 (Brannan, 2002):

Table A.16: Equivalent lengths for different piping parts

Nominal pipe diameter cm	Globe valve or ball check valve	Angle valve	Swing check valve	Plug cock	Gate or bal valve	45° ellbow Welded	45° ellbow Threaded	Short radius elbow Welded	Short radius elbow Threaded	Long radius elbow Welded	Long radius elbow Threaded	Hard T Welded	Hard T Threaded	Soft T Welded	Soft T Threaded	90 miter bends 2 miter	90 miter bends 3 miter	90 miter bends 4 miter
3.81	16.76	7.92	3.96	2.13	0.30	0.30	0.61	0.91	1.52	0.61	0.91	2.44	2.74	0.61	0.91			
5.08	21.34	10.06	5.18	4.27	0.61	0.61	0.91	1.22	1.52	0.91	1.22	3.05	3.35	0.91	1.22			
6.35	24.38	12.19	6.10	3.35	0.61	0.61	-	1.52	-	0.91	-	3.66		0.91	-			
7.62	30.48	15.24	7.62	5.18	0.61	0.61		1.83		1.22		4.27		1.22				
10.16	39.62	19.81	9.75	9.14	0.91	0.91		2.13		1.52		5.79		1.52				
15.24	60.96	30.48	14.63	21.34	1.22	1.22		3.35		2.44		8.53		2.44				
20.32	79.25	38.10	19.51	36.58	1.83	1.83		4.57		2.74		11.28		2.74				
25.4	100.58	48.77	24.38	51.82	2.13	2.13		5.49		3.66		14.33		3.66				
30.48	121.92	57.91	28.96	51.82	2.74	2.74		6.71		4.27		16.76		4.27		8.53	6.40	6.10
35.56	137.16	64.01	32.00	24.38	3.05	3.05		7.92		4.88		18.90		4.88		9.75	7.32	6.71
40.64	152.40	73.15	36.58	44.20	3.35	3.35		8.84		5.49		21.95		5.49		11.58	8.23	7.32
45.72	167.64	85.34	42.67	48.77	3.66	3.66		10.06		6.10		24.99		6.10		12.80	9.14	8.53
50.8	198.12	91.44	47.24	64.01	4.27	4.27		10.97		7.01		27.43		7.01		14.02	10.06	9.75
55.88	209.70	102.11	51.82	68.58	4.57	4.57		12.19		7.62		30.48		7.62		15.85	10.97	10.36
60.96	228.60	112.78	56.39	77.42	4.88	4.88		13.41		8.23		33.53		8.23		17.07	11.89	10.97
76.2				95.10	6.40	6.40		16.76		12.19		42.67		12.19		21.34	15.54	13.41
91.44					7.62	7.62		20.12		14.33		51.82		14.33		25.60	18.29	15.85
106.68					9.14	9.14		23.47		16.76		60.96		16.76		29.87	21.03	19.51
121.92					10.67	10.67		26.82		19.81		67.06		19.81		34.14	24.69	21.95
137.16					12.19	12.19		30.18		21.34		76.20		21.34		38.40	27.43	24.38
152.4					13.72	13.72		33.53		24.38		79.25		24.38		57.91	30.18	28.04

For enlargements and narrowings, a dimensionless coefficient is used:

$$h_w = k_f \times \frac{u^2}{2 \times g \times \alpha}$$

With k_f a dimensionless loss coefficient, which depends on several parameters for different occasions (Van Der Meeren, 2004):

From pipe to reservoir

Kinetic energy gets lost → k_f = 1 independent of geometry

From reservoir to pipe

Well rounded inlet $k_f = 0.04$

Chamfered inlet $k_f = 0.25$

Square edge inlet $k_f = 0.5$

Inward projecting pipe $k_f = 1$

For abrupt pipe enlargement ($d_1 < d_2$)

$$k_f = \left(1 - \left(\frac{d_1}{d_2}\right)^2\right)^2$$

For gradual pipe enlargements values from Table A.17 can be chosen.

Table A.17: Dimensionless loss coefficient for gradual pipe enlargements

D_2/D_1	Angle of cone °											
	2	6	10	15	20	25	30	35	40	45	50	60
1.1	0.01	0.01	0.03	0.05	0.10	0.13	0.16	0.18	0.19	0.20	0.21	0.23
1.2	0.02	0.02	0.04	0.09	0.16	0.21	0.25	0.29	0.31	0.33	0.35	0.37
1.4	0.02	0.03	0.06	0.12	0.23	0.30	0.36	0.41	0.44	0.47	0.50	0.53
1.6	0.03	0.04	0.07	0.14	0.26	0.35	0.42	0.47	0.51	0.54	0.57	0.61
1.8	0.03	0.04	0.07	0.15	0.28	0.37	0.44	0.50	0.54	0.58	0.61	0.65
2.0	0.03	0.04	0.07	0.16	0.29	0.38	0.46	0.52	0.56	0.60	0.63	0.68
2.5	0.03	0.04	0.08	0.16	0.30	0.39	0.48	0.54	0.58	0.62	0.65	0.70
3.0	0.03	0.04	0.08	0.16	0.31	0.40	0.48	0.55	0.59	0.63	0.66	0.71
∞	0.03	0.05	0.08	0.16	0.31	0.40	0.49	0.56	0.6	064	0.67	0.72

Abrupt pipe narrowing ($d_1 > d_2$)

$$k_f = 0.75 \times \left(1.00 - \left(\frac{d_{i2}}{d_{i1}}\right)^2\right) \quad for \left(\frac{d_{i2}}{d_{i1}}\right)^2 > 0.715$$

$$k_f = 0.40 \times \left(1.25 - \left(\frac{d_{i2}}{d_{i1}}\right)^2\right) \quad for \left(\frac{d_{i2}}{d_{i1}}\right)^2 < 0.715$$

For non cylindrical pipes

$D = D_e$ with

$$D_e = 4 \times \frac{wet\ pipe\ cross\ area}{wet\ pipe\ circumference}$$

Efficiency

The pump efficiency (Eff.) can be calculated by (Brannan, 2002):

$$Eff. = 80 - 0.2855F + 3.78 \times 10^{-4}FG - 2.38 \times 10^{-7}FG^2 + 5.39 \times 10^{-4}F^2 - 6.39 \times 10^{-7}F^2G + 4 \times 10^{-10}F^2G^2$$

With F the developed head (in ft) and G the flow (in GPM). To convert to SI units (head H in meters and flow rate Q in m³/s):

$$F = H \times 0.3048$$

$$G = Q \times 4.403$$

The equation is valid for F=50-300ft and G=100 – 1000GPM

If this is not the case, default values from DATABUO can be used (Table A.18) (www.cheresources.com):

Table A.18: Default pump efficiencies for pumping incompressible fluids

Pump type	flow m³/s	Efficiency
	0.0063	45%
Centrifugal pump	0.0315	70%
	0.63	80%
Axial pump	all	75%
Rotary pump	all	65%
	Power (kW)	
	7.46	70%
Reciprocating pump	37.3	85%
	373	90%

A summary of this BUO can be found in Table A.19

Table A.19: A summary of the BUO pumping incompressible fluids

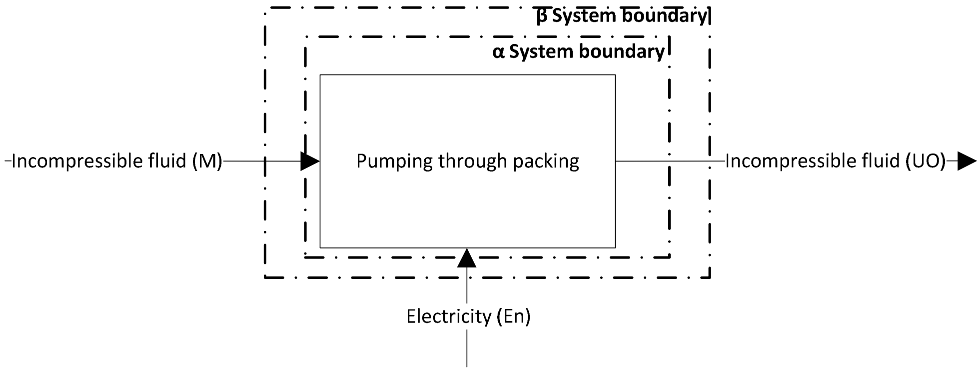
Input values required	DATABUO	DATAPHYSCHEM	Output
Mass (flow rate) and type of fluid Starting and end temperature and pressure Type pipe material, distance of straight pipes, height difference between starting and end point, number and type of turns, valves, enlargements and narrowings	Friction coefficients and roughness factors Efficiencies	Fluid characterisation factors	Electricity use

3.3. Pumping incompressible fluids through packing

This module includes the pumping of incompressible fluids through packings, beds or filters. It can thus be used for pumping operations such as adsorption, filtration, catalytic beds, etc. However, only the electricity use is modelled of the pumping operation. No interactions between the fluid and the bed is included.

System boundary description

The calculations in this module can be widely applied, for several unit operations where beds and packings are involved. However, the equations are only valid if the characteristics of the bed remain constant and if no fluidization occurs. Especially the porosity should be constant (Van Der Meeren, 2004). For example clogging filters are out of the range of this work. The module can be coupled to the pumping operations since they only include the pumping through the bed. The same pumps and pump efficiencies are included as for regular pumping.



Calculation algorithm

The approach is similar to pumping incompressible fluids. However, on top of the regular friction term, an additional head loss is caused by the packing material. To account for this, the approach from Chhabra and Richardson (1999) can be used where the bed head loss is added to the modified Bernoulli equation:

$$H = \Delta z + h_{f.bed}$$

Which can be used in:

$$P_n = \frac{H \times Q \times \rho \times g}{eff.}$$

The head loss of the bed (in m) can be calculated from the pressure drop:

$$h_{f.bed} = \frac{-\Delta p_{f.bed}}{\rho \times g}$$

With:

$$-\Delta p_{f.bed} = \frac{f_{bed} \times \rho \times u^2}{d_p} \times L \times \left(\frac{1-\varepsilon}{\varepsilon^3}\right) \times C_f$$

With ε the pore volume/bed volume, u the superficial velocity (m/s), L the length of the bed (m), ρ the density of the fluid (kg/m³), d_p is the sphere diameter (m). The latter depends strongly on the particle shape:

$$d_p = \Gamma \times d_r$$

With Γ the sphericity of the particles and d_r the equal volume sphere diameter (Table A.20) (Ibarz and Barbosa-Cánovas, 2003; McCabe et al., 2004)

Table A.20: Sphericity of different packing particles

Shape of the particle	Sphericity (Γ)
Sphere	1
Cube	0.81
Cylinders	
h=d	0.87
h=5d	0.70
h=10d	0.58
Discs	
h=d/3	0.76
h=d/6	0.60
h=d/10	0.47
Beach sand	As high as 0.86
River sand	As low as 0.53
Other types of sand	0.75
Triturated solids	0.5-0.7
Granulated particles	0.7-0.8
Wheat	0.85
Raschig rings	0.26-0.53
Berl saddles	0.3-0.37
Coal dust	0.73
Mica flakes	0.28
Crushed glass	0.65

C_f is a correction factor to account for the fact that the packing material is more dense in the center of the column and less dense near the wall. It can be calculated for cylindrical vessels:

$$C_f = \left(1 + \frac{d_p}{3D}\right)^2$$

With D the vessel diameter

f_{bed} is the friction factor of the bed, which can be obtained from the Ergun equation:

$$f_{bed} = \frac{150}{Re^*} + 1.75$$

With the Reynolds number for Power law fluids:

$$Re^* = \frac{d_p^n \times u^{2-n} \times \rho}{K \times (1-\varepsilon)^n} \times \left(\frac{4n}{1+3n}\right)^n \times \left(\frac{15\sqrt{2}}{\varepsilon^2}\right)^{1-n}$$

It is stated that this equation is a good approximation for $\varepsilon \leq 0.41$ and $Re^* < 100$.

For $\varepsilon > 0.41$ and $Re^* > 100$

$$f_{bed} = \frac{150}{Re'} + 1.75$$

With

$$Re' = \frac{d_p^n \times u \times \rho}{K \times (1-\varepsilon)^n} \times \left(\frac{4n}{1+3n}\right)^n \times \left(\frac{\varepsilon^2}{12 \times u \times (1-\varepsilon)}\right)^{n-1}$$

Table A.21: A summary of the BUO pumping incompressible fluids through packing

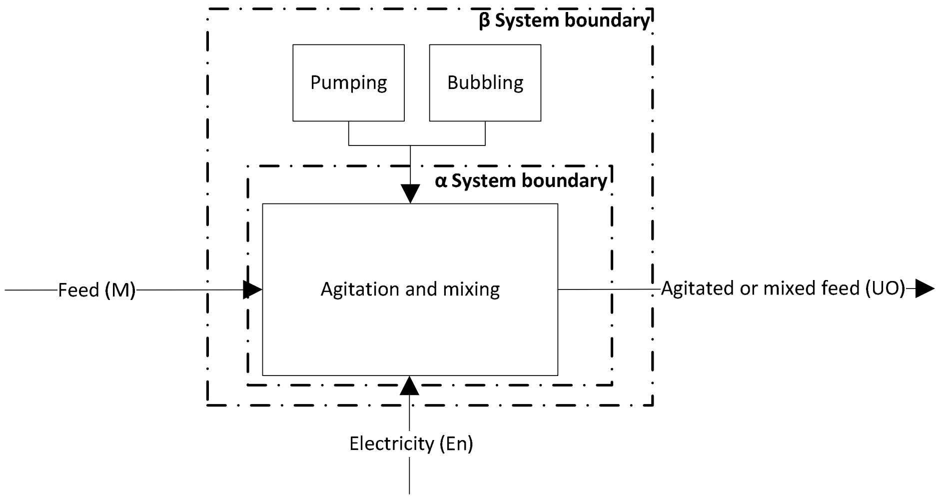
Input values required	DATABUO	DATAPHYSCHEM	Output
Mass (flow rate) and type of fluid Type and size of packing material Pore volume/bed volume (should remain constant)	Sphericity Pump efficiency	Fluid characterisation factors	Electricity use

3.4. Agitation and mixing of liquids and suspensions

Agitation and mixing are operations often needed in process industry and relying on a certain amount of mechanical energy which depends on many different parameters. This module includes mixing two or more liquids or suspensions and agitation of one or more liquids or suspensions. Whilst these two operations might not exactly have the same purpose, their power consumption can be modelled with the same equations.

System boundary description

The mixing and homogenization of liquids operation includes the electricity use necessary for the impeller. Several types of propellers and turbines are included, plus a paddle with 2 blades, an anchor and a helical impeller. Equations are available for Newtonian and Power Law fluids, the latter thus also including pseudoplastic and dilatants suspensions. Furthermore, the effect of gas bubbling can be included. However, the potential power for bubbling the gas and other pumping operations are SUO and thus in the β system boundary.



Calculation algorithm

One of the most important factor for the power requirement is the Reynolds number. Similarly to pumping fluids, a difference can be made between Newtonian and Non-Newtonian fluids. In the latter case the main complication is related to the shear rate (γ). The calculation in the two situations is very similar, starting from the Reynolds number (McCabe et al., 2004):

$$N_{Re} = \frac{\rho \times N \times D_a^2}{\mu_a}$$

With N the rotational speed (rps), D_A the impeller diameter (m), μ_a the apparent viscosity (Pa.s) and ρ the density of the fluid (kg/m³).

Newtonian fluids

For Newtonian fluids: $\mu_a = \mu$

The standard equation for the total power needed for mixing and homogenization (P in W) is calculated by:

$$P = N_P \times \rho \times N^3 \times D_a^5$$

With N_p the power number and N the rotational speed.

This is valid in for intermediate Reynolds numbers between $100<N_{Re}<10000$, whilst for the turbulent region, $N_{Re}>10000$, the modified version is used:

$$P = K_T \times \rho \times N^3 \times D_a^5$$

In the laminar region the viscosity and shear become more important, thus the formula is converted to:

$$P = K_L \times \mu \times N^2 \times D_a^3$$

Power numbers for different flow regimes and impellers can be found in Table A.22.

TableA. 2: Power numbers for Newtonian fluids in the laminar (K_L), intermediate (N_p) and turbulent region (K_T) for different types of impellers (McCabe et al., 2004)

Typical viscosity (cp)	Type	KL	N_p	KT
<2000	Average small propeller (3 blades)	41.00	0.75	0.32
<2000	Average small propeller with pitch of 2 (3 blades)	43.50	0.75	1.00
<2000	Average large propeller (3 blades)	41.00	0.75	0.32
<2000	Average large propeller with pitch of 2 (3 blades)	43.50	0.75	1.00
<20000	Turbine 6 flat blades	71.00	5.00	6.30
<20000	Turbine 6 curved blades	70.00	5.00	4.80
<20000	Fan turbine 6 blades	70.00	5.00	1.65
<80000	Paddle (2 blades)	36.50	2.60	1.70
<100000	Anchor	300.00	10.00	0.35
<1000000	Helical impeller	300.00	10.00	0.35
>1000000	Extruders. roll mill. etc			

Non Newtonian fluids

For non Newtonian fluids, the apparent viscosity should be used in the Reynolds number (Heldman and Lund, 2007):

$$\mu_a = K \times \gamma^{n-1}$$

For dilatants liquids (Perry & Green, 1999)

$$\gamma = 13 \times N \times \left(\frac{D_a}{D_t}\right)^{0.5}$$

For pseudoplastic and Bingham fluids

$$\gamma = 10 \times N$$

For turbines 10 can be replaced by 11.5.

Based on the Reynolds number, the Power Number can then be found in Heldman and Lund (2007) for different types of impellers

Vessel design

The diameter of the impeller is estimated from the volume of the cylindrical tank, on its turn calculated from the flow (Q in m³/s), and the residence time (t in s):

$$Q \times t = V$$

A certain excess volume is added (Ex. in %) to add a buffer volume:

$$V' = V + Ex \times V$$

Standard this excess volume is set on 10%.

A cylindrical vessel is assumed with H = D_t with H the height of the tank and D_t the diameter of the tank:

$$D_t = \sqrt[3]{\frac{4 \times V'}{\pi}}$$

Furthermore, we assume that the diameter of the impeller is 1/3rd of the tank diameter:

$$D_a = \frac{1}{3} D_t$$

Rotational speed and mixing time

For mixing operations, the residence time and impeller speed are 2 interlinked parameters which therefore cannot be fixed by default values. According to Herbert et al. 1994, a dimensionless mixing parameter Θ links the mixing time (t) with the impeller speed for baffled agitated vessels with a centrally located impeller:

$$\Theta = N \times t = 6.7 \times (\frac{D_a}{D_t})^{-\frac{5}{3}} \times N_P{}^{-\frac{1}{3}}$$

With N_P the power number. Typical N values for the different impellers are presented in Table A.23 and typical power numbers can be found in Table A.22 for laminar, turbulent and intermediate region.

Table A.23: typical rotational speeds for different impellers in mixing vessels (McCabe et al., 2004)

Type	Typical N ranges for mixing
Average small propeller (3 blades)	1150-1750
Average small propeller with pitch of 2 (3 blades)	1150-1751
Average large propeller (3 blades)	400-800
Average large propeller with pitch of 2 (3 blades)	400-801
Turbine 6 flat blades	200-400
Turbine 6 curved blades	200-400
Fan turbine 6 blades	200-400
Paddle (2 blades)	20-150
Anchor	50-350
Helical impeller	5-20

The rotational speed of disc turbine blades applied in Newtonian fluids can be estimated by using a scale of agitation S_A based on the pumping number (N_Q) which can be found in Table A.24 (Chhabra and Richardson, 1999):

$$N = \frac{S_A \times \left(\frac{\pi}{4} D_t\right)^2}{32.8 \times N_Q \times D_a^3}$$

The scale of agitation ranges from 1, which is mildly mixed, to 10, which can be taken for intense mixing.

Table A.24: Default pumping numbers for types of impellers

Type	Pumping number (NQ)
Average small propeller (3 blades)	0.5
Average small propeller with pitch of 2 (3 blades)	0.5
Average large propeller (3 blades)	0.5
Average large propeller with pitch of 2 (3 blades)	0.5
Turbine 6 flat blades	0.7
Turbine 6 curved blades	0.8
Fan turbine 6 blades	0.8
Paddle (2 blades)	0.6
Anchor	0.5
Helical impeller	0.5

For gassed liquids, the power (P_g) for mixing and homogenization can be calculated by:

$$P_g = P \times 0.497 \times N_Q^{-0.38} \times (\frac{N^2 \times D_a^3 \times \rho}{\sigma})^{-0.18}$$

With σ the surface tension (N/m) of the liquid and N_Q the pumping number.

Alternatively an adjusted power number ($N_{p.g}$) can be calculated:

$$N_{p.g} = 0.72 \times \left(\frac{N_p \times N \times D_a^3}{Q_t^{0.56}}\right)^{0.45}$$

With Q_t the volumetric gas flow rate (kg/s).

A summary of the BUO agitation and mixing of liquids and suspensions can be found in Table A.25.

Table A.25: A summary of the BUOaAgitation and mixing of liquids and suspensions

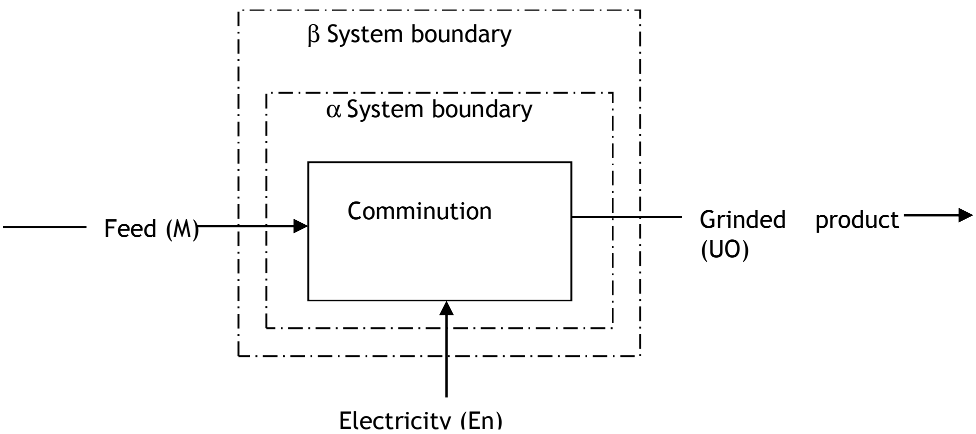
Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow and type of feed(s) Type of impeller Impeller speed and residence time	Tank volume Power number and pumping number Impeller speed and residence time information	Physicochemical properties of mixture	Electricity use Tank volume Residence time

3.5. Comminution

Comminution is a process which is applied to reduce the size of solids and is widely used in industry (e.g. in food processing, minerals processing, ceramic industry and so on). The purposes of comminution are to liberate certain compounds for concentration processes, to reduce the size or to increase the surface area. More recent technologies result in the need to modify the surface of solids, prepare composite materials and to recycle the useful components of industrial waste. The energy efficiency of comminution is very low and the energy required for comminution increases with a decrease in feed or produced particle size. In design, operation and control of comminution processes, it is necessary to correctly evaluate the comminution energy of solid materials (Kanda and Kotake, 2007). In this basic engineering module, the energy for comminution is determined.

System boundary description

The α system boundary of this BUO includes the comminution of a feed in to a grinded product. Electricity is required for this process. No additional processes are assumed in the β system boundary.



Calculation algorithm

Several theories have been developed to estimate the energy requirement of size reduction processes. They are in fact all based on the basic assumption that the energy required to produce a change dL in a particle of typical size dimension L is a simple power function of L:

$$dE / dL = K \cdot L^n$$

Where dE is the differential energy required, dL is the change in a typical dimension, L is the magnitude of a typical length dimension and K and n are constants.

The most widely applied are the theories from Kick, Rittinger and Bond. We will now discuss each of them (Earle and Earle, 2004).

Kick's law

Kick assumed that the energy required to reduce a material in size is related to the change in particle diameter, i.e. to the ratio of the diameter of the particles before and after comminution. In this case 'n' in the above equation is -1. The following formula is known as 'Kick's law':

$$E = K_K \cdot f_c \cdot \ln\left(\frac{L_1}{L_2}\right)$$

In which:

E = Energy for size reduction (J/kg)

K_K = Kick's constant (m^3/kg)

f_c = Compressive strength of the material (N/m^3)

L_1 = Diameter of the feed particles (m)

L_2 = Diameter of the product particles (m)

Kick's law is mainly used for comminution of coarse particles.

Rittinger's law

Rittinger, on the other hand, assumed that the energy for size reduction is directly proportional to the change in surface area and not to the change in length dimensions. This means that 'n' in the above equation is -2, resulting in 'Rittinger's law':

$$E = K_R f_c \left(\frac{1}{L_2} - \frac{1}{L_1} \right)$$

In which:

K_R = Rittinger's constant (m^4/kg)

Rittinger's law is mainly used for comminution of fine particles.

Bond's law

Bond has suggested an intermediate course, in which he postulates that 'n' is -3/2. This leads to:

$$E = E_i \sqrt{\frac{100}{L_2}} \cdot \left\{ 1 - \frac{1}{\sqrt{q}} \right\}$$

and

$$q = \frac{L_1}{L_2}$$

In which:

E = Energy for size reduction (kWh/tonne)

E_i = Work index (kWh/tonne)

L_1 = Feed particle size (□m)

L_2 = Product particle size (□m)

Bond defines work index E_i as the amount of energy required to reduce a unit of mass of the material from an infinitely large particle size down to a particle size of 80% passing 100 µm (Note that therefore L_1 and L_2 have to be expressed in µm as well!). Table A.26 gives an overview of typical values for the work index for various materials (Perry & Green, 1999).

Table A.26: Work Index for various materials in kWh/tonne (Perry & Green, 1999)

Material	No. of tests	Specific gravity	Work index†	Material	No. of tests	Specific gravity	Work index†
All materials tested	2088	—	13.81	Taconite	66	3.52	14.87
Andesite	6	2.84	22.13	Kyanite	4	3.23	18.87
Barite	11	4.28	6.24	Lead ore	22	3.44	11.40
Basalt	10	2.89	20.41	Lead-zinc ore	27	3.37	11.35
Bauxite	11	2.38	9.45	Limestone	119	2.69	11.61
Cement clinker	60	3.09	13.49	Limestone for cement	62	2.68	10.18
Cement raw material	87	2.67	10.57	Manganese ore	15	3.74	12.46
Chrome ore	4	4.06	9.60	Magnesite, dead burned	1	5.22	16.80
Clay	9	2.23	7.10	Mica	2	2.89	134.50
Clay, calcined	7	2.32	1.43	Molybdenum	6	2.70	12.97
Coal	10	1.63	11.37	Nickel ore	11	3.32	11.88
Coke	12	1.51	20.70	Oil shale	9	1.76	18.10
Coke, fluid petroleum	2	1.63	38.60	Phosphate fertilizer	3	2.65	13.03
Coke, petroleum	2	1.78	73.80	Phosphate rock	27	2.66	10.13
Copper ore	308	3.02	13.13	Potash ore	8	2.37	8.88
Coral	5	2.70	10.16	Potash salt	3	2.18	8.23
Diorite	6	2.78	19.40	Pumice	4	1.96	11.93
Dolomite	18	2.82	11.31	Pyrite ore	4	3.48	8.90
Emery	4	3.48	58.18	Pyrrhotite ore	3	4.04	9.57
Feldspar	8	2.59	11.67	Quartzite	16	2.71	12.18
Ferrochrome	18	6.75	8.87	Quartz	17	2.64	12.77
Ferromanganese	10	5.91	7.77	Rutile ore	5	2.84	12.12
Ferrosilicon	15	4.91	12.83	Sandstone	8	2.68	11.53
Flint	5	2.65	26.16	Shale	13	2.58	16.40
Fluorspar	8	2.98	9.76	Silica	7	2.71	13.53
Gabbro	4	2.83	18.45	Silica sand	17	2.65	16.46
Galena	7	5.39	10.19	Silicon carbide	7	2.73	26.17
Garnet	3	3.30	12.37	Silver ore	6	2.72	17.30
Glass	5	2.58	3.08	Sinter	9	3.00	8.77
Gneiss	3	2.71	20.13	Slag	12	2.93	15.76
Gold ore	209	2.86	14.83	Slag, iron blast furnace	6	2.39	12.16
Granite	74	2.68	14.39	Slate	5	2.48	13.83
Graphite	6	1.75	45.03	Sodium silicate	3	2.10	13.00
Gravel	42	2.70	25.17	Spodumene ore	7	2.75	13.70
Gypsum rock	5	2.69	8.16	Syenite	3	2.73	14.90
Ilmenite	7	4.27	13.11	Tile	3	2.59	15.53
Iron ore	8	3.96	15.44	Tin ore	9	3.94	10.81
Hematite	79	3.76	12.68	Titanium ore	16	4.23	11.88
Hematite—specular	74	3.29	15.40	Trap rock	49	2.86	21.10
Oolitic	6	3.32	11.33	Uranium ore	20	2.70	17.93
Limanite	2	2.53	8.45	Zinc ore	10	3.68	12.42
Magnetite	83	3.88	10.21				

*Allis-Chalmers Corporation.

†Caution should be used in applying the average work index values listed here to specific installations since individual variations between materials in any classification may be quite large.

In literature, data for Bond's work index are readily available, while this is not the case for Rittinger's and Kick's constants. Since Bond's law is known to be a general law that is intermediate to Rittinger's and Kick's law, we propose to use Bond's law in comminution calculations.

A summary of the BUO comminution can be found in Table A.27.

Table A.27: A summary of the BUO comminution

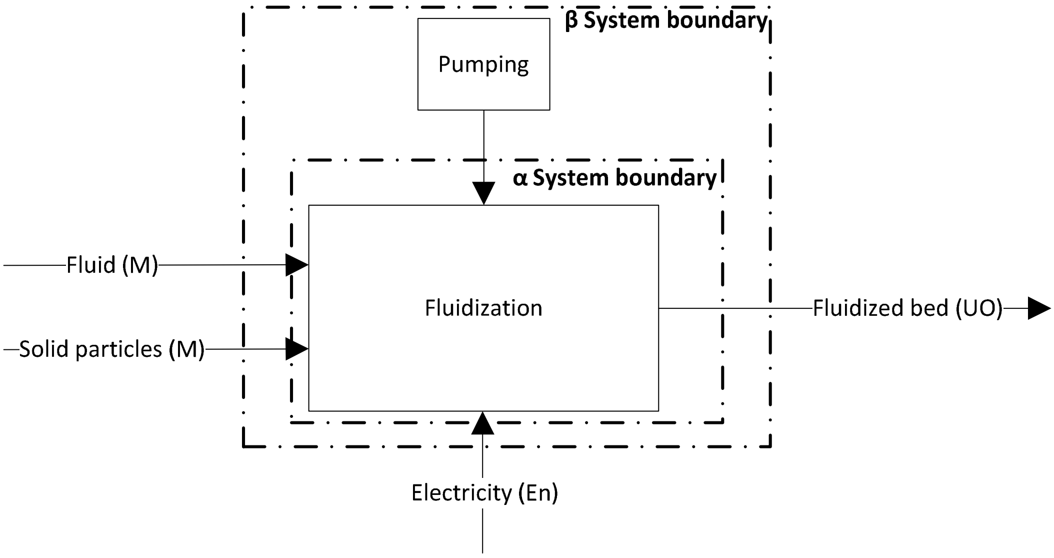
Input values required	DATAPHYSCHEM	Output
Feed particle size Product particle size	Compressive strength of the material Rittinger's constant of the material Kick's constant of the material Work index of the material	Energy use

3.6. Fluidization

Fluidization occurs when a bed of granular material is converted from solid to a fluid or suspended state through the velocity of a gas or liquid. It thus occurs at a certain velocity, where a minimum fluidization velocity is necessary to achieve the fluidized state, higher velocities will result in the transport of the particles, and thus in (pneumatic in the case of a gas) conveying. Fluidization is often used in the process industries during cracking, toasting, roasting(pyrite. lime. coffee), drying (grains, sugars), freezing, heating with sand baths, encapsulation and agglomeration of particles, etc. (Van Der Meeren, 2004).

System boundary description

This BUO includes the mechanical energy (electricity) to obtain a fluidized state. The relationship is based on the pressure drop in the bed and is thus valid for fluidization and conveying the solids. However, it only accounts for obtaining a static fluidized state. To really lift and move the solids, as is the case in conveying, additional energy is required which is supplied by the fluid. This additional demand should be calculated with the SUO 'pumping'.



Calculation algorithm

The basic equation to estimate pump power for fluidization and pneumatic conveying is (Van Der Meeren, 2004):

$$P_n = -\Delta p_{f.fluidization} \times Q$$

With P_n = pump power output in W, Q the capacity in m³/s.

The pressure drop (Pa) over the bed can be calculated by (Richardson, Harker, & Backhurst and Harker, 2002):

$$-\Delta p_{f.fluidization} = L \times (1 - \varepsilon) \times (\rho_s - \rho_f) \times g$$

ρ_s is the density of the particles and ρ_f is the density of the fluid (kg/m³). L is the length of the bed (m), g is the gravity constant (9.81m/s²), whilst the value of ε represents the porosity. If this value is not known, the user can calculate the minimum porosity for fluidization where $\varepsilon = \varepsilon_{mf}$ (Ibarz and Barbosa-Cánovas, 2003):

$$\varepsilon_{mf} = 1 - 0.356 \times (log\ d_p - 1)$$

With d_p the diameter of the particles in μm. This equation is valid for particle sizes going from 50 to 500μm.

A summary of the BUO fluidization can be found in Table A.28.

Table A.3: A summary of the BUO fluidization

Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow and type of feed(s) Diameter of particles	-	Densities	Electricity use

3.7. Conveying solids

Conveying is a frequently used application to transport solids.

System boundary description

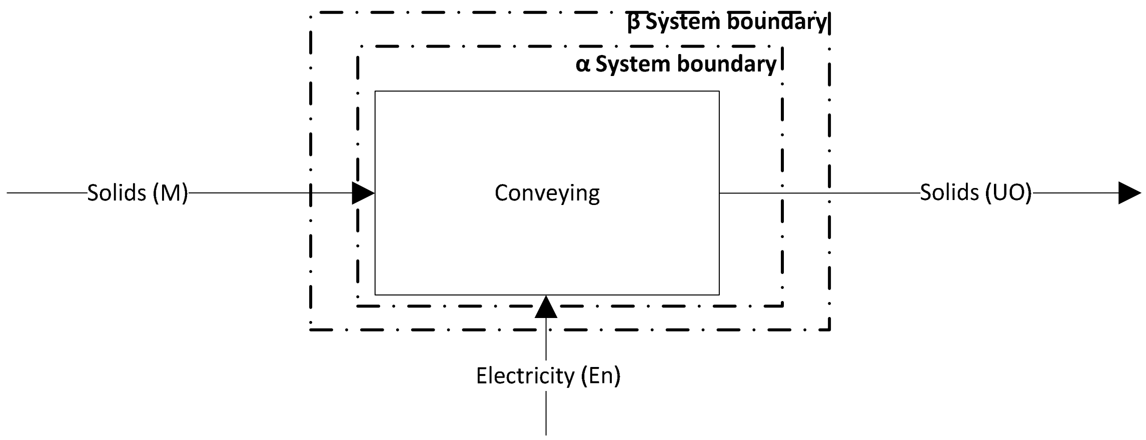
This BUO includes the electricity to move solids over a certain distance with 4 types of conveyors:

Screw conveyors

Belt conveyors

Centrifugal-discharge buckets on belt

Continuous buckets on a chain



Calculation algorithm

Conveying solids requires a certain amount of power which can be found in the Tables 21.6-21.9 (Perry & Green, 1999) for different types of conveyors for certain capacity flow rates.

TABLE 21-6 Screw-Conveyor Data for 50-lb/ft³ Material and Pipe-Mounted Sectional Spiral Flights*

Capacity†		Diam. of flights, in	Diam. of pipe, in‡	Diam. of shafts, in	Hanger centers, ft	Max. size of lumps			Speed, r/min	Max. torque capacity, in·lb	Feed section diam., in	hp at motor§					Max. hp capacity at speed listed
Tons/h	ft³/h					All lumps	Lumps 20 to 25%	Lumps 10% or less				15-ft. max. length	30-ft max. length	45-ft max. length	60-ft max. length	75-ft max. length	
5	200	9	2½	2	10	¾	1½	2¼	40	7,600	6	0.43	0.85	1.27	1.69	2.11	4.8
10	400	10	2½	2	10	¾	1½	2½	55	7,600	9	0.85	1.69	2.25	3.00	3.75	6.6
15	600	10 12 12	2½ 2½ 3½	2 2 3	10 12	¾ 1	1½ 2	2½ 3	80 45	7,600 7,600 16,400	9 10	1.27 1.27 1.27	2.25 2.25 2.25	3.38 3.38 3.38	3.94 3.94 3.94	4.93 4.93 4.93	9.6 5.4 11.7
20	800	12	2½ 3½	2 3	12	1	2	3	60	7,600 16,400	10	1.69 1.69	3.00 3.00	3.94 3.94	4.87 4.87	5.63 5.63	7.2 15.6
25	1000	12 14	2½ 3½ 3½	2 3 3	12	1 1¼	2 2½	3 3½	75 45	7,600 16,400 16,400	10 12	2.12 2.12 2.12	3.75 3.75 3.75	4.93 4.93 4.93	5.63 5.63 5.63	6.55 6.55 6.55	9.0 9.0 11.7
30	1200	14	3½	3	12	1¼	2½	3½	55	16,400	12	2.25	3.94	5.05	6.75	7.50	14.3
35	1400	14	3½	3	12	1¼	2½	3½	65	16,400	12	2.62	4.58	5.90	7.00	8.75	16.9
40	1600	16	3½	3	12	1½	3	4	50	16,400	14	3.00	4.50	6.75	8.00	10.00	13.0

*Fairfield Engineering Co. data in U.S. customary system. To convert cubic feet per hour to cubic meters per hour, multiply by 0.02832; to convert tons per hour to metric tons per hour, multiply by 0.9078; and to convert screw size in inches to the nearest screw size in centimeters, multiply by 2.5.

†Capacities are based on screws carrying 31 percent of their cross section and, in the case of feed sections with half-pitch flights, based on 100 percent of their cross section.

‡Pipe sizes given are for ¼-in (6.35-mm) flights.

§Horsepowers listed are calculated for average conditions and are of the proper motor size with factors for length of conveyor, momentary overloads, etc., taken into consideration.

TABLE 21-7 Belt-Conveyor Data for Troughed Antifriction Idlers*

Belt width	Cross-sectional area of load	Belt speed, ft/min (m/min)		Belt plies		Maximum lump size, in (mm)			Capacity and hp for 100-lb/ft³ material			
in (cm)	ft² (m²)	Normal	Maximum	Minimum	Maximum	Sized material, 80% under	Unsized material, not over 20%	Belt speed, ft/min (m/min)	Capacity tons/h (metric tons/h)	hp/10-ft (3.05-m) lift	hp/100-ft (30.48-m) centers	Add for tripper hp†
14 (35)	0.11 (.010)	200 (61)	300 (91)	3	5	2.0 (51)	3.0 (76)	100 (30.5)	32 (29)	0.34	0.44	
								200 (61.0)	64 (58)	0.68	0.68	2.0
								300 (91.5)	96 (87)	1.04	1.32	
16 (40)	0.14 (.013)	200 (61)	300 (91)	3	5	2.5 (64)	4.0 (102)	100 (30.5)	44 (40)	0.46	0.56	
								200 (61.0)	88 (80)	0.90	1.12	2.5
								300 (91.5)	132 (120)	1.36	1.68	
18 (45)	0.18 (.017)	250 (76)	350 (107)	4	6	3.0 (76)	5.0 (127)	100 (30.5)	54 (49)	0.58	0.70	
								250 (76.2)	134 (122)	1.42	1.76	3.0
								350 (106.7)	190 (172)	2.00	2.42	
20 (50)	0.22 (.020)	250 (76)	350 (107)	4	6	3.5 (89)	6.0 (152)	100 (30.5)	66 (60)	0.70	0.84	3.20
								250 (76.2)	164 (148)	1.72	2.06	
								350 (106.7)	230 (209)	2.44	2.90	
24 (60)	0.33 (.030)	300 (91)	400 (122)	4	7	4.5 (114)	8.0 (203)	100 (30.5)	98 (89)	1.02	1.02	
								300 (91.5)	294 (267)	3.06	3.04	3.5
								400 (121.9)	392 (356)	4.08	4.04	
30 (75)	0.53 (.049)	300 (91)	450 (137)	4	8	7.0 (178)	12.0 (305)	100 (30.5)	158 (143)	1.60	1.50	
								300 (91.5)	474 (430)	4.80	4.50	5.0
								450 (137.2)	710 (645)	7.20	6.74	
36 (90)	0.78 (.072)	400 (122)	600 (183)	4	9	8.0 (203)	15.0 (381)	100 (30.5)	230 (209)	2.44	1.59	
								400 (121.9)	920 (835)	9.74	6.36	7.0
								600 (182.9)	1380 (1253)	14.60	9.52	
42 (105)	1.09 (.101)	400 (122)	600 (183)	4	10	10.0 (254)	18.0 (457)	100 (30.5)	330 (300)	3.50	2.28	
								400 (121.9)	1320 (1198)	14.00	9.12	9.5
								600 (182.9)	1980 (1797)	23.20	13.68	
48 (120)	1.46 (.136)	400 (122)	600 (183)	4	12	12.0 (305)	21.0 (533)	100 (30.5)	440 (399)	4.66	3.04	
								400 (121.9)	1760 (1598)	18.70	12.14	12.8
								600 (182.9)	2640 (2397)	28.00	18.20	
54 (135)	1.90 (.177)	450 (137)	600 (183)	6	14	14.0 (356)	24.0 (610)	100 (30.5)	570 (517)	6.04	3.94	
								450 (137.2)	2564 (2328)	27.20	17.70	20.0
								600 (182.9)	3420 (3105)	36.20	23.60	
60 (150)	2.40 (.223)	450 (137)	600 (183)	6	16	16.0 (406)	28.0 (711)	100 (30.5)	720 (654)	7.64	4.98	
								450 (137.2)	3240 (2941)	34.40	22.40	23
								600 (182.9)	4320 (3921)	45.80	29.90	

*Fairfield Engineering Co. data in U.S. customary system. Metric conversion is rounded off. For inclined conveyors, add lift horsepower to center horsepower for total horsepower. For terminals multiply horsepower by the following factors: 0–50 ft (15.2 m), 1.20; 51–100 ft (30.5 m), 1.10; 101–150 ft (45.7 m), 1.05. For countershaft drives, multiply horsepower by 1.05 for each reduction (cut gears).

†Tripper horsepower is based on material bulk density of 100 lb/ft³ (1602 kg/m³) and a belt speed of 300 ft/min (91.4 m/min).

TABLE 21-8 Bucket-Elevator Specifications for Centrifugal-Discharge Buckets on Belt, Malleable-Iron, or Steel Buckets*

Size of bucket, in (mm), and bucket spacing, in (mm)†	Elevator centers, ft‡	Capacity, tons/h (metric tons/h)§	Size of lumps handled, in (mm)¶	Bucket Bucket speed, ft/min (m/min)	r/min, head shaft	hp required at head shaft	Additional hp/ft for intermediate lengths	Head	Tail	Head	Tail	Belt width, in
6 × 4 × 4¼ – 12	25	14 (12.7)	¾ (19.0)	225 (68.6)	43	1.0	0.02	1 15/16	1 11/16	20	14	7
	50	14 (12.7)	¾ (19.0)	225 (68.6)	43	1.6	0.02	1 15/16	1 11/16	20	14	7
(152 × 102 × 108) – (305)	75	14 (12.7)	¾ (19.0)	225 (68.6)	43	2.1	0.02	1 15/16	1 11/16	20	14	7
8 × 5 × 5½ – 14	25	27 (24.5)	1 (25.4)	225 (68.6)	43	1.6	0.04	1 15/16	1 11/16	20	14	9
	50	30 (27.2)	1 (25.4)	260 (79.2)	41	3.5	0.05	1 15/16	1 11/16	24	14	9
(203 × 127 × 140) – (356)	75	30 (27.2)	1 (25.4)	260 (79.2)	41	4.8	0.05	2 7/16	1 11/16	24	14	9
10 × 6 × 6¼ – 16	25	45 (40.8)	1¼ (32.0)	225 (68.6)	43	3.0	0.063	1 15/16	1 15/16	20	16	11
	50	52 (47.2)	1¼ (32.0)	260 (79.2)	41	5.2	0.07	2 7/16	1 15/16	24	16	11
(254 × 152 × 159) – (406)	75	52 (47.2)	1¼ (32.0)	260 (79.2)	41	7.2	0.07	2 15/16	1 15/16	24	16	11
12 × 7 × 7¼ – 18	25	75 (68.1)	1½ (38.1)	260 (79.2)	41	4.7	0.1	2 7/16	1 15/16	24	18	13
	50	84 (76.3)	1½ (38.1)	300 (91.4)	38	8.9	0.115	2 15/16	1 15/16	30	18	13
(305 × 178 × 184) – (457)	75	84 (76.3)	1½ (38.1)	300 (91.4)	38	11.7	0.115	3 7/16	2 7/16	30	18	13
14 × 7 × 7¼ – 18	25	100 (90.8)	1¾ (44.5)	300 (91.4)	38	7.3	0.14	2 15/16	2 7/16	30	18	15
	50	100 (90.8)	1¾ (44.5)	300 (91.4)	38	11.0	0.14	3 7/16	2 7/16	30	18	15
(355 × 179 × 184) – (457)	75	100 (90.8)	1¾ (44.5)	300 (91.4)	38	14.3	0.14	3 7/16	2 7/16	30	18	15
16 × 8 × 8½ – 18	25	150 (136.2)	2 (50.8)	300 (91.4)	38	8.5	0.165	2 15/16	2 7/16	30	20	18
	50	150 (136.2)	2 (50.8)	300 (91.4)	38	12.6	0.165	3 7/16	2 7/16	30	20	18
(406 × 203 × 216) – (457)	75	150 (136.2)	2 (50.8)	400 (121.9)	38	16.7	0.165	3 15/16	2 7/16	30	20	18

*From Stephens-Adamson Division, Allis-Chalmers Corporation.
†Bucket size given: width × projection × depth. Assumed bucket linear speed is 150 ft/min (45.7 m/min).
‡Elevator centers to nearest SI equivalent are 25 ft 8 m, 50 ft 15 m, and 75 ft 23 m.
§Capacities and horsepowers are given for materials having bulk densities of 100 lb/ft^3 (1602 kg/m^3). For other densities these will vary in direct proportion: a 50-lb/ft^3 material will reduce the capacity and horsepower required by 50 percent.
¶If the amount of lump product is less than 15 percent of the total, lump size may be twice that given.

TABLE 21-9 Bucket-Elevator Specifications for Continuous Buckets on Chain*

Size of bucket and bucket spacing, in (mm)†	Elevator centers, ft‡	Capacity, tons/h (metric tons/h)§	Size of lumps handled, in (mm)¶	r/min, head shaft	hp required at head shaft	Additional hp/ft for intermediate lengths	Head	Tail	Head	Tail
8 × 5½ × 7¾ – 8	25	35 (31.7)	1 (25.4)	28	1.8	0.06	1 15/16	1 11/16	20½	14
(203 × 140 × 197) – (203)	50	35 (31.7)	1 (25.4)	28	3.4	0.06	2 7/16	1 11/16	20½	14
	75	35 (31.7)	1 (25.4)	28	5.0	0.06	2 15/16	1 11/16	20½	14
10 × 7 × 11¾ – 12	25	60 (54.5)	1½ (38.1)	23	3.0	0.10	2 7/16	1 15/16	25	17½
(254 × 178 × 298 – (305)	50	60 (54.5)	1½ (38.1)	23	5.5	0.10	2 7/16	1 15/16	25	17½
	75	60 (54.5)	1½ (38.1)	23	8.0	0.10	2 15/16	1 15/16	25	17½
12 × 7 × 11¾ – 12	25	70 (63.5)	1½ (38.1)	23	3.5	0.12	2 7/16	1 15/16	25	17½
(305 × 178 × 298) – (305)	50	70 (63.5)	1½ (38.1)	23	6.5	0.12	2 15/16	1 15/16	25	17½
	75	70 (63.5)	1½ (38.1)	23	9.5	0.12	3 7/16	2 7/16	25	17½
14 × 7 × 11¾ – 12	25	80 (72.6)	1¾ (44.5)	23	4.0	0.14	2 7/16	2 7/16	25	17½
(356 × 178 × 298) – (305)	50	80 (72.6)	1¾ (44.5)	20	7.5	0.14	2 15/16	2 7/16	29	17½
	75	80 (72.6)	1¾ (44.5)	20	11	0.14	3 7/16	2 7/16	29	17½
14 × 8 × 11¾ – 12	25	100 (90.8)	2 (50.8)	20	5.0	0.17	2 15/16	2 7/16	29	17½
(356 × 203 × 298) – (305)	50	100 (90.8)	2 (50.8)	20	9.3	0.17	3 7/16	2 7/16	29	17½
	75	100 (90.8)	2 (50.8)	20	13.3	0.17	3 15/16	2 7/16	29	17½
16 × 8 × 11¾ – 12	25	115 (104.4)	2 (50.8)	20	6.0	0.20	2 15/16	2 7/16	29	17½
(406 × 203 × 298) – (305)	50	115 (104.4)	2 (50.8)	20	11	0.20	3 15/16	2 7/16	29	17½
	75	115 (104.4)	2 (50.8)	20	16	0.20	4 7/16	2 7/16	29	17½
18 × 8 × 11¾ – 12	25	130 (118.0)	2 (50.8)	20	7	0.22	2 15/16	2 7/16	29	17½
(406 × 203 × 298) – (305)	50	130 (118.0)	2 (50.8)	20	13	0.22	3 15/16	2 7/16	29	17½
	75	130 (118.0)	2 (50.8)	20	20	0.22	4 7/16	2 7/16	29	17½

*From Stephens-Adamson Division, Allis-Chalmers Corporation.
†Bucket size given: width × projection × depth. Assumed bucket linear speed is 150 ft/min (45.7 m/min).
‡Elevator centers to nearest SI equivalent are 25 ft 8 m, 50 ft 15 m, and 75 ft 23 m.
§Capacities and horsepowers are given for materials having bulk densities of 100 lb/ft^3 (1602 kg/m^3). For other densities these will vary in direct proportion: a 50-lb/ft^3 material will reduce the capacity and horsepower required by 50 percent.
¶If the total amount of lump product is less than 15 percent of the total, lump size may be twice that given.

A summary of the BUO conveying can be found in Table A.29.

Table A.29: A summary of the BUO conveying

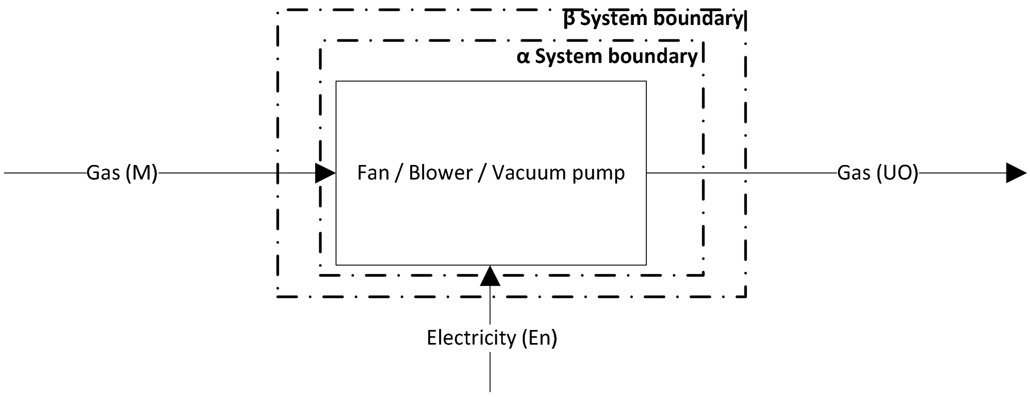
Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow Type of conveyor	Power of equipment	-	Electricity use

3.8. Fans, Blowers & vacuum pumps

Fans and blowers are used to create a driving force to supply a gas, usually air. Examples of applications are ventilation and air blowing in a combustion chamber. A vacuum pump works oppositely, by lowering the pressure.

System boundary description

This BUO includes the electricity use of a fan or blower used to increase the pressure of the gas or the electricity of a vacuum pump, to remove a gas from a certain space.



Calculation algorithm

The power (P in W) needed can be calculated by (Perry & Green, 1999):

$$P = \frac{Q \times \Delta P}{eff}$$

Where Q is the flow rate (m³/s), ΔP is the pressure difference in Pa, and eff is the efficiency of the device.

Typical pressure differences for vacuum pumps, fans and blowers can be found in Table A.30 (Perry & Green, 1999; Brannan, 2002; Silla, 2003), whilst typical efficiencies can be found in Table A.31 (Bureau of Energy Efficiency India).

Table A.30: Typical pressure differences covered in vacuum pumps, fans and blowers

Type of device	Typical pressure differences (Pa)
Vacuum pump	100000
Fans	7500
Blowers	50000

Table 4: Default efficiencies of fans and blowers

Type of fan	Efficiency
Centrifugal fan/blower	
Airfoil, backward curved/inclined	81
Modified radial	75
Radial	72
Pressure blower	63
Forward curved	62
Axial fan	
Vane axial	81
Tube axial	69
Propeller	47
Other	
Other	80

A summary of the BUO bans, blowers & vacuum pumps can be found in Table A.32

Table A.32: A summary of the BUO bans, blowers & vacuum pumps

Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow Type of device	Typical pressure differences Efficiencies	-	Electricity use

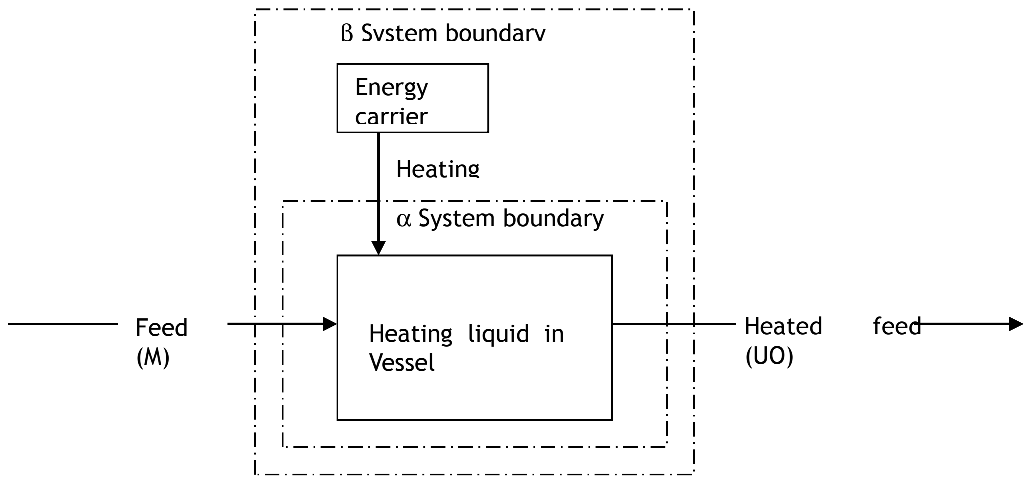
4. Utilities

4.1. Heating

In many industrial processes, liquid substances are heated to a certain temperature and kept at that temperature for a given amount of time. These liquids can be pure chemicals, mixtures, solutions or suspensions. Energy is needed to heat the liquid to the required temperature but also to compensate for heat losses through the wall of the vessel in which it is heated. The latter is specifically relevant when a certain temperature has to be retained for a longer period. In this basic engineering module, we will estimate the energy required for heating a liquid in a vessel for a given amount of time.

System boundary description

The α system boundary for this process includes heating the liquid in a vessel. If, pumping or mixing are required, the energy use can be estimated with the algorithms of those processes as defined in the respective basic engineering modules for agitation or pumping. The β system boundary includes the production of the energy carrier that is needed to heat the liquid. This could for example be steam or natural gas.



Calculation algorithm

For this process, energy is needed for heating the liquid up to a required temperature and maintaining this temperature for a certain amount of time. The energy needed for heating to a certain temperature depends on the specific heat of the liquid and can be calculated with:

$$Q_h = c_p \cdot m \cdot (T_e - T_0)$$

In which:

Q_h = Energy needed for heating (J)

c_p = Specific heat of the liquid (J $kg^{-1}K^{-1}$)

m = mass of the liquid (kg)

T_0 = Initial temperature of the liquid

T_e = End temperature of the liquid

Vessels will have walls that are insulated with isolation material (e.g. polyurethane) to prevent the loss of heat through the walls. However, insulation will never be 100% and some heat is lost resulting in a decrease of the temperature of the liquid. Extra heating is required to compensate for this heat loss. The required heat is determined by (Blok, 2007):

$$Q_r = \frac{\lambda \cdot \Delta T \cdot A \cdot t}{d}$$

In which:

Q_r = Energy required for remaining the temperature at T_e (J)

λ = Thermal conductivity of vessel wall material (W $m^{-1}K^{-1}$)

ΔT = Temperature difference across the wall (K)

A = Surface area of the vessel wall (m^2)

t = Period of remaining temperature at T_e (s)

d = Thickness of the vessel wall (m)

The heat required for the two processes just described is the theoretical minimum amount of energy needed. There will be an efficiency loss from burning a fuel to transmission of heat. In order to calculate the total amount of energy needed (Q_t), we have to account for the heating efficiency (η) :

$$Q_t = \frac{Q_h + Q_r}{\eta}$$

A summary of the BUO heating can be found in Table A.33.

Table A.33: A summary of the BUO heating

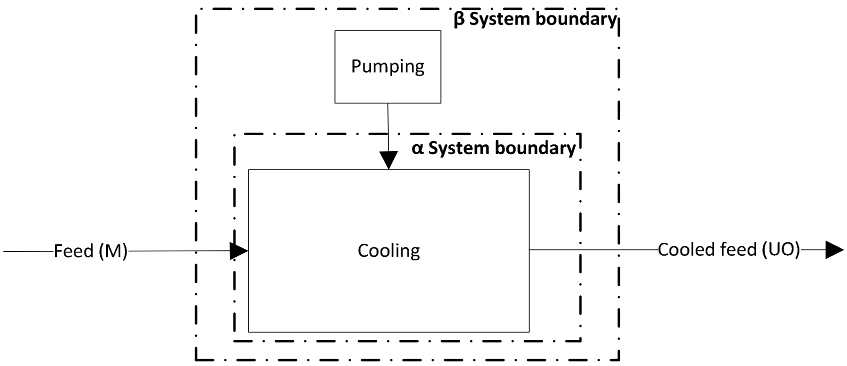
Input values required from user	DATAPHYSCHEM	DATABUO	Output
Mass of the liquid End temperature of the liquid Initial temperature of the liquid Surface area of the vessel wall Thickness of the vessel wall Period of remaining T_e Temperature difference across the vessel wall	Specific heat of the liquid Thermal conductivity of vessel wall material	Heating efficiency	Heating energy required

4.2. Cooling

Cooling is a process often used in process industry to lower temperature of gasses, liquids or solids.

System boundary description

Cooling calculates the amount of cooling medium required to cool/condensate a certain feed stream. The electricity use for pumping the cooling medium should be added with the SUO ‘pumping’. This is not a separation process, thus in the case of a mixture, all components are assumed to end in the same phase at the same temperature and pressure.



Calculation algorithm

The cooling energy (q) needed can be calculated with:

$$q = m_f \times c_{p,g} \times (T_f - T_b) + m_f \times \lambda_f + m_f \times c_{p,l} \times (T_b - T_e)$$

With λ the latent heat of the condensed feed stream, c_p the mean heat capacity of the feed in gas (g) and liquid (l) phase , T_b the boiling temperature of the mixture, T_f the temperature of the feed, and T_e the end temperature.

The amount of cooling medium can then be calculated by:

$$m = \frac{q}{c_p \times \Delta T}$$

With c_p the heat capacity of the cooling medium and ΔT the temperature difference of the cooling medium before and after use.

A summary of the BUO cooling can be found in Table A.34.

Table A.34: A summary of the BUO cooling

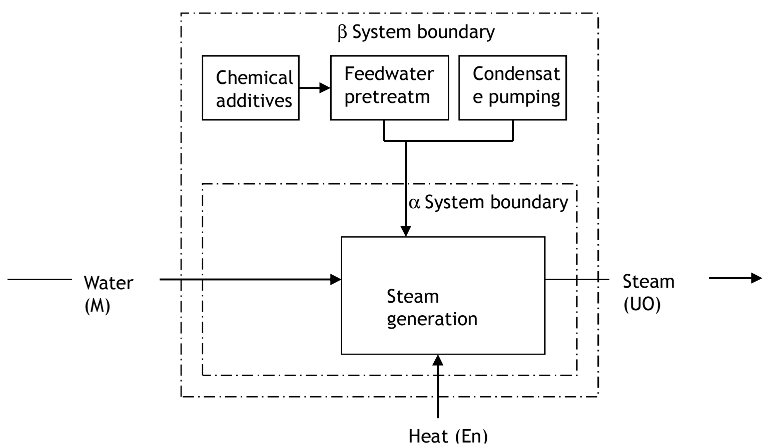
Input values required	DATABUO	DATAPHYSCHEM	Output
Mass flow In and output temperature	-	Boiling temperature Heat capacities and latent heats	Mass flow of cooling medium required

4.3. Steam generation

Steam is used in many chemical processes as a heat source. To produce steam, water is evaporated with heat coming from the incineration of a fuel such as natural gas. In this basic engineering module we will determine the heat requirements for the production of steam and the energy that can be obtained when using steam as heat medium.

System boundary description

The α system boundary of this BUO includes the evaporation of water by means of an externally supplied heat source. The water is pre-treated with chemicals in order to remove impurities and hence avoid foaming and scaling, resulting in lower boiler efficiency, more maintenance, lower boiler life and other problems (Spirax-Sarco Limited, 2001). The required chemicals have not been taken into account in the α system boundary but are part of the β system boundary. This also holds for the pumping requirements for returning condensate.



Calculation algorithm

The energy for heating water to its evaporation temperature, for evaporation of water as well as the energy required to further heat steam depends on the pressure of the liquid and the steam. The pressure at which a liquid at a certain temperature evaporates is called the 'saturated pressure'. In this basic engineering module, we will assume 'saturated steam (i.e. at the boiling temperature at saturated pressure)' as a default.

Steam used for industrial purposes will mostly be applied in closed systems. Figure A.4 is a schematic representation of such a system; water is evaporated to steam in a boiler at a certain pressure and temperature, the steam is transported to the process in which it is needed, it condenses back to water transferring heat to the process and the condensate is returned to the boiler where it is again evaporated to steam.

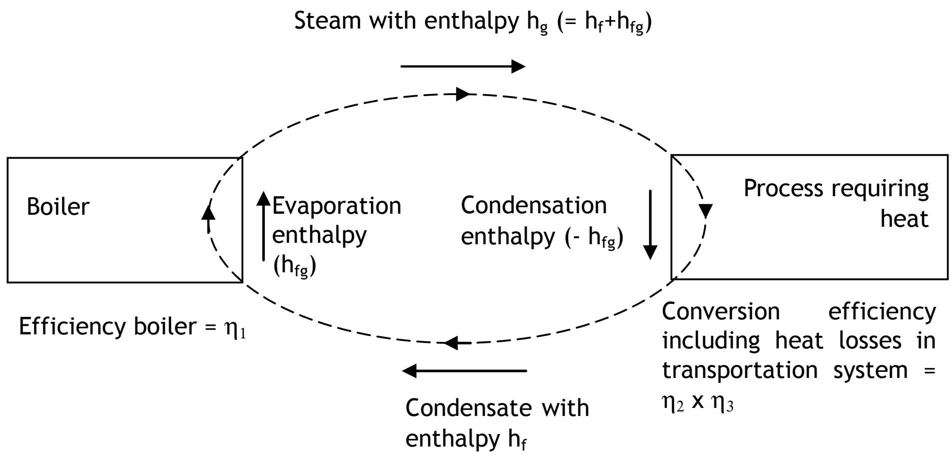


Figure A.4: Closed steam system

In such a system, the water that is evaporated to steam comes from the returned condensate that has a heat content of h_f in case no heat losses are assumed. With heat losses, however, the enthalpy of the water arriving at the boiler is referred to as h0 (see algorithms below). In the boiler it is evaporated to steam with a heat content of h_g. The energy needed for generating and delivering a kilogram of steam (useful heat, i.e. 100% of the heat directly used in a process) is the enthalpy of evaporation (h_{fg}) at a certain temperature and saturated pressure, corrected for the efficiency of the boiler (η_1) and the efficiency of steam distribution and heat transfer (η_2). The amount of energy that can be obtained from the steam is equal to the condensation enthalpy (which is identical with the evaporation enthalpy):

$$E_g = \frac{m \times h_{fg}}{\eta_1 \times \eta_2}$$

In which:

E_g = Energy required for steam generation (kJ)

m = Mass of the steam (kg)

h_{fg} = Enthalpy of evaporation (kJ/kg)

η_1 = Boiler efficiency (dimensionless, generally around 0.9)

η_2 = Efficiency of steam distribution and heat transfer (dimensionless, generally around 0.9)

The values for h_{fg}, h_f and h_g are obtained from steam tables, published by thermodynamic handbooks. Table A.35 gives an overview of enthalpies at different temperature- and saturated pressure levels.

In case no closed system is assumed and water has to be heated from room temperature to the evaporation temperature or in case heat losses in the returned condensate are taken into account, the algorithm is as follows:

$$E_f = \frac{m \times (h_f - h_0)}{\eta_1}$$

In which:

E_f = Energy needed for heating the water (kJ)

m = Mass of the water (kg)

h_f = Enthalpy of the saturated water (kJ/kg)

h_0 = Enthalpy of the water arriving at boiler (kJ/kg)

The value of h_0 depends on the pressure and temperature of the water as it arrives at the boiler. It can be determined with the help of a steam calculator. See for example: http://www.steamtablesonline.com/steam97web.aspx

For water at atmospheric pressure and a temperature of 20 ^{o}C, the specific enthalpy (h_0) is 84.01 kJ/kg. In some cases, returned condensate is expanded to lower pressure to generate flash steam. This flash steam can then be used to recover part of the heat of the initial condensate. After use of flash steam the condensed water has to be reheated to its initial saturated pressure and temperature for regeneration to high(er) pressure steam. As a result, the energy balance of the total system is equal with or without the use of flash steam (assuming no extra heat losses). As a rule of thumb, returned condensate after the use of flash steam has a temperature of 80 ^{o}C. (US Department of Energy, 2006) At atmospheric pressure, h_0 then is 335 kJ/kg.

Table A.35: Steam tables

		Enthalpy, kJ/kg		
Temp, T °C	Sat press, P_{sat} kPa	Sat liquid, h_f	Evap., h_{fg}	Sat vapor, h_g
0.01	0.6117	0.001	2500.9	2500.9
5	0.8725	21.02	2489.1	2510.1
10	1.2281	42.022	2477.2	2519.2
15	1.7057	62.982	2465.4	2528.4
20	2.3392	83.915	2453.5	2537.4
25	3.1698	104.83	2441.7	2546.5
30	4.2469	125.74	2429.8	2555.5
35	5.6291	146.64	2417.9	2564.5
40	7.3851	167.53	2406.0	2573.5
45	9.5953	188.44	2394.0	2582.4
50	12.352	209.34	2382.0	2591.3
55	15.763	230.26	2369.8	2600.1
60	19.947	251.18	2357.7	2608.9
65	25.043	272.12	2345.4	2617.5
70	31.202	293.07	2333.0	2626.1
75	38.597	314.03	2320.6	2634.6
80	47.416	335.02	2308.0	2643.0
85	57.868	356.02	2295.3	2651.3
90	70.183	377.04	2282.5	2659.5
95	84.609	398.09	2269.6	2667.7
100	101.42	419.17	2256.4	2675.6
105	120.9	440.28	2243.1	2683.4
110	143.38	461.42	2229.7	2691.1
115	169.18	482.59	2216.0	2698.6
120	198.67	503.81	2202.1	2705.9
125	232.23	525.07	2188.1	2713.2
130	270.28	546.38	2173.7	2720.1
135	313.22	567.75	2159.1	2726.9
140	361.53	589.16	2144.3	2733.5
145	415.68	610.64	2129.2	2739.8
150	476.16	632.18	2113.8	2746.0
155	543.49	653.79	2098.0	2751.8
160	618.23	675.47	2082.0	2757.5
165	700.93	697.24	2065.6	2762.8
170	792.18	719.08	2048.8	2767.9
175	892.60	741.02	2031.7	2772.7
180	1002.8	763.05	2014.2	2777.3
185	1123.5	785.19	1996.2	2781.4
190	1255.2	807.43	1977.9	2785.3
195	1398.8	829.78	1959.0	2788.8
200	1554.9	852.26	1939.8	2792.1
205	1724.3	874.87	1920.0	2794.9
210	1907.7	897.61	1899.7	2797.3
215	2105.9	920.50	1878.8	2799.3
220	2319.6	943.55	1857.4	2801.0
225	2549.7	966.76	1835.4	2802.2
230	2797.1	990.14	1812.8	2802.9
235	3062.6	1013.7	1789.5	2803.2
240	3347.0	1037.5	1765.5	2803.0
245	3651.2	1061.5	1740.8	2802.3
250	3976.2	1085.7	1715.3	2801.0
255	4322.9	1110.1	1689.0	2799.1
260	4692.3	1134.8	1661.8	2796.6
265	5085.3	1159.8	1633.7	2793.5
270	5503.0	1185.1	1604.6	2789.7
275	5946.4	1210.7	1574.5	2785.2
280	6416.6	1236.7	1543.2	2779.9
285	6914.6	1263.1	1510.7	2773.8
290	7441.8	1289.8	1476.9	2766.7
295	7999.0	1317.1	1441.6	2758.7
300	8587.9	1344.8	1404.8	2749.6
305	9209.4	1373.1	1366.3	2739.4
310	9865.0	1402.0	1325.9	2727.9
315	10556	1431.6	1283.4	2715.0
320	11284	1462.0	1238.5	2700.5
325	12051	1493.4	1191.0	2684.4
330	12858	1525.8	1140.3	2666.1
335	13707	1559.4	1086.0	2645.4
340	14601	1594.6	1027.4	2622.0
345	15541	1631.7	963.4	2595.1
350	16529	1671.2	892.7	2563.9
355	17570	1714.0	812.9	2526.9
360	18666	1761.5	720.1	2481.6
365	19822	1817.2	605.5	2422.7
370	21044	1891.2	443.1	2334.3
373.95	22064	2084.3	0.0	2084.3

A summary of the BUO steam generation can be found in Table A.36.

Table A.36: A summary of the BUO steam generation

Input values required from user	DATAPHYSCHEM	DATABUO	Output
Amount of steam Temperature and saturated pressure of the steam Temperature and pressure of water arriving at the boiler	Enthalpy of evaporation Enthalpy of saturated water Enthalpy of water arriving at boiler	Boiler efficiency Distribution and heat transfer efficiency	Required amount of fuel energy

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