A METHODOLOGY FOR THE GENERATION AND EVALUATION OF BIOREFINERY PROCESS CHAINS, IN ORDER TO IDENTIFY THE MOST PROMISING BIOREFINERIES FOR THE EU

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Thesis summary

The topic of bioenergy, biofuels and bioproducts remains at the top of the current political and research agenda. Identification of the optimum processing routes for biomass, in terms of efficiency, cost, environment and socio-economics is vital as concern grows over the remaining fossil fuel resources, climate change and energy security. It is known that the only renewable way of producing conventional hydrocarbon fuels and organic chemicals is from biomass, but the problem remains of identifying the best product mix and the most efficient way of processing biomass to products. The aim is to move Europe towards a bio-based economy and it is widely accepted that biorefineries are key to this development.

A methodology was required for the generation and evaluation of biorefinery process chains for converting biomass into one or more valuable products that properly considers performance, cost, environment, socio-economics and other factors that influence the commercial viability of a process. In this thesis a methodology to achieve this objective is described. The completed methodology includes process chain generation, process modelling and subsequent analysis and comparison of results in order to evaluate alternative process routes. A modular structure was chosen to allow greater flexibility and allowing the user to generate a large number of different biorefinery configurations

The significance of the approach is that the methodology is defined and is thus rigorous and consistent and may be readily re-examined if circumstances change. There was the requirement for consistency in structure and use, particularly for multiple analyses. It was important that analyses could be quickly and easily carried out to consider, for example, different scales, configurations and product portfolios and so that previous outcomes could be readily reconsidered. The result of the completed methodology is the identification of the most promising biorefinery chains from those considered as part of the European Biosynergy Project.

Key words: biomass, biorefinery, process synthesis, MCDA, process modelling

DEDICATION

This thesis is dedicated to my family, friends and Rich. I could not have done this without your never-ending patience and love.

ACKNOWLEDGEMENTS

Firstly I would like to thank Professor Tony Bridgwater for his encouragement, advice and support during the course of this research.

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Thanks to all partners involved in the Biosynergy project, particularly Hans Reith for his constant encouragement and support.

I would like to gratefully acknowledge the work of Joanneum and the Joint Research Centre for the generation of the environmental model and results used in the biorefinery evaluations. Further thanks to Patricia Thornley for the creation of the socio-economic model which was integrated into the final methodology.

Finally endless thanks to my family and friends who have fed me numerous cups of tea and managed to keep me relatively sane during this process.

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ABBREVIATIONS

ABNT	Abengoa Bioenergía Nuevas Tecnologías, S.A.
ABE	Acetone, butanol, ethanol
AI	Artificial Intelligence
ARD	Agro Industrie Recherches et Developments
Aston	Aston University
ASU	Air separation unit
A&F	WUR Agrotechnology and Food Innovations B.V.
Bioref	Biorefinery.de GmbH
BFIT	Biorefinery and Farm Integrated Tool
BTG	Biomass Technology Group
BtL	Biomass to liquids
BCyL	ABNT's demonstration lignocellulosic ethanol plant, located in Salamanca
CBA	Cost benefit analysis in MCDA analysis or Conflict Based Approach in process synthesis
CEA	Cost effectiveness analysis
CEPCI	Chemical Engineering Plant Cost Index
CFB	Circulating fluidised bed
CHP	Combined heat and power
Cepsa	Compania Espanola de Petrolos, S.A.
Chimar	Chimar Hellas S.A.
COD	Chemical Oxygen Demand
CRES	Centre for Renewable Energy Sources
C5	5 Carbon sugars (e.g. xylose)
C6	6 Carbon sugars (e.g. glucose)
DME	Dimethyl ether
DOW	Dow Benelux B.V.
ECN	Energy research Centre of the Netherlands
ELECTRE	Elimination and choice translating reality
EC	European Commission
EU	European Union
FCI	Fixed capital investment
FDCA	2,5-Furandicarboxylic acid
FT	Fischer-Tropsch

GDP	Gross domestic product
GHG	Green house gas
GIG	Glowny Instytut Gornictwa
GP	Goal programming
HMF	Hydroxymethylfurfural
HP	High pressure (steam)
IAB	Industrial Advisory Board
IBsE	Industrial Biosystems Engineering
IEA	International Energy Agency
IFP	Institut Francais du Pétrole
LCF	Lignocellulosic feedstock
LHV	Lower heating value, MJ/kg
LP	Low pressure (steam)
JR	Joanneum Research Forschungsgesellschaft m.b.H.
JRC	Joint Research Centre
MADM	Multi-attribute decision making
MAVT	Multi-attribute value theory
MCDA	Multi-criteria decision analysis
MCDM	Multi-criteria decision making
MINLP	Mixed Integer Non Linear Programming
MODM	Multi-objective decision making
NNFCC	National Non Food Crop Centre
NREL	American National Renewable Energy Laboratory
OpEx	Operational cost
PROMETHEE	Preference ranking organisation method for enrichment evaluation
RSH	Feedstock reception, storage and handling
SMR	Steam methane reforming
TFCI	Total Fixed Capital Investment
TOPSIS	Technique for order preference by similarity to ideal solution
TUD	Delft University of Technology
VTT	VTT Technical Research Centre of Finland
WP	Work package
WSM	Weighted sum method
WT %	Weight %

1 INTRODUCTION

This thesis is based on the work carried out for the EC funded Biosynergy project (1,2) in particular Work Package 6. Work Package 6 (WP6) is the "Integral biomass-to-products chain design, analysis and optimisation".

The aim of this thesis and WP6 was to create a methodology to identify the most promising biorefinery chains – from mass and energy efficiency, environmental, socio-economic and cost point of view – for the European Union, and for some specific market sectors. The methodology will enable the generation and analysis of the potential for integrated biorefinery concepts within a future bio-based economy. Wheat straw and softwood feedstocks were to be analysed in a variety of integrated biorefinery schemes, including the second generation bioethanol process and an integration possibility in a conventional oil refinery. The final output from the complete methodology was to be the identification of the promising biorefinery process chains that have been ranked and optimised according to the objectives set by the user.

The topic of bioenergy, biofuels and bioproducts remains at the top of the current political and research agenda. Identification of the optimum processing routes for biomass, in terms of efficiency, cost, environment and socio-economics is vital as concern grows over the remaining fossil fuel resources, climate change and energy security. The aim is to move Europe towards a bio-based economy and it is widely accepted that biorefineries are key to this development. Activity in this research field will only gain momentum in the coming years, leading to many interesting and exciting developments.

As government's interest in biofuels grows they have offered monetary incentives to producers and blenders (45) which have also encouraged growth and interest in the sector of renewables. The policies such as the EU's biofuel directive (3) have set targets for the use of bioenergy and these targets are only achieved though the development of biomass based industries and biorefineries.

The concept of a biorefinery has only recently received recognition and prominence, and identifying the most promising process chains is one of the major difficulties. A biorefinery is the concept of complete integration of a biomass processing complex, in an analogous approach to an oil refinery and petrochemical complex, which will maximise the cost effectiveness of utilisation of biomass for energy and bio-products by optimally utilising all products, by-products and residues for the most economical, environmental, technological, and social impact. There are so many feedstock options and process routes

that a methodology needs to be established to identify those that are most promising. This forms the core objective of this thesis.

A methodology designed to identify the most promising biorefinery chains is needed for a number of reasons. These include the need to direct further research and development and to review and assess all biorefinery options for bioenergy and bioproducts (not just focussing on biofuels). There is a need for the identification of the optimum products mixes, depending on the biorefinery design criteria. These design criteria may be to find the most profitable, the most efficient, the most environmentally friendly, the most socioeconomically attractive biorefinery or a combination of these. There is a need to make biofuels and bioproducts more cost competitive to encourage a bio-based economy. One way of doing this is to process the by-products and wastes of biofuel production, into value added products as part of a biorefinery complex. It is generally accepted that the creation of biorefineries producing a wide portfolio of products is the future for the processing of biomass but the greatest challenge is identifying which products to produce, using which technologies. There is currently little published research on this particular area, which makes this project challenging and exciting.

Interpretation of most promising or "best" biorefinery can be considered in many ways such as: most efficient, lowest capital cost, lowest product cost, most environmentally acceptable, most cost effective or most socially acceptable. The "best" biorefinery concept for decision makers is often that which is most financially attractive i.e. which option is likely to bring the most profit, but now other factors must be considered such as the impact on the environment and the local area (socio-economics). The most promising biorefinery is often dependent on the objectives of the person carrying out the analysis, different people may have very different interests, for example the views of a scientist versus industry versus policy makers. The methodology created for this thesis will enable all of these different groups to carry out their own analysis according to their own particular interest or objectives. It will allow the user to carry out virtual experiments, by the creation and analysis of numerous biorefinery process chains.

As well as the usual techno-economic data there includes the quantification of the environmental and socio-economic effects of biomass production, biomass transportation and its conversion in integrated biorefinery processes to different products, based on life-cycle considerations. Examples of the environmental effects to be considered are: global warming potential, acidification, eutrophication, ozone depletion and cumulated primary energy and material demand. (Please note the work on the environmental and socio-

economic profiles was carried out by other partners within the Biosynergy project. The results will then be integrated into the overall process model to enable the biorefinery evaluation.

For this thesis the focus of the evaluation was on technologies contained within the scope of the Biosynergy project, but the methodology created may be applied to other processes and technologies in the future. The aim was to create a methodology that was highly flexible, so that it may be revisited and expanded in the future. Biomass based research is moving so quickly that the methodology had to be able to cope with this ever changing field. A useful tool was created for investigating the impact of these changes such as fluctuations in feedstock price, product prices, location etc.

There has been a significant amount of work carried out on biomass related technologies, and a number of good techno economic studies (see Section 8.2), but as yet there is no defined methodology for the creation, analysis and comparison of all the possible options. This work leads on from the targeted optimisation research underway, to give a broader overview of the technologies and processes available for transforming biomass into useful products. It was important that it become possible for decision and policy makers to view all the available options, and to view all criteria to form a valuable assessment tool.

With regards to contribution to knowledge, this research demonstrates the original application of flexible decision support methodologies, process synthesis, modelling and evaluation techniques combined in a single methodology to the area of biorefineries. The results are important to inform markets and industry about the possibilities available from biorefineries, to help inform policy makers about the potential of biorefineries in the future bio-based economy and to prevent research time and effort being spent in the wrong direction. The methodology and results will help the development of a bio-based economy for the European Union.

1.1 BIOSYNERGY PROJECT

The work for this thesis formed part of the Biosynergy Project. The Biosynergy project was a Framework 6 project partially funded by the European Commission. The existence of this project signifies the level of interest in this topic and this interest will only increase as concern grows over the remaining fossil resources, climate change and energy security.

The full description and definition of the IP Biosynergy project is “The IP BIOSYNERGY aims to use *BIO*mass for *SYN*thesis processes (transportation fuels, platform chemicals) and en*ERGY* production (power, CHP) by application of innovative fully integrated,

synergetic biorefinery concepts, using advanced fractionation and conversion processes, and combining biochemical and thermochemical pathways."

The research within this project was focussed on the development of advanced and innovative fractionation and conversion processes combining both biochemical and thermo-chemical pathways, and process development from lab-scale to validation at pilot-scale.

The aim of Biosynergy was to achieve sound techno-economic process development of the integrated production of chemicals, transportation fuels and energy, from lab-scale to pilot plant. The four main general scientific and technological project objectives of the Biosynergy project were:

- To develop the best thermochemical/biochemical conversion and fractionation technologies for major side-streams of an ethanol fermentation plant, but also applicable for other wet and dry feedstocks.
- To define the potential of platform chemicals for both (fine) chemical and petrochemical industries.
- To come from lab-scale to pilot-scale processes using techno-economic assessments and clear exploitation guidelines.
- Making the production of biofuels more cost competitive

Many projects have been funded over the last 20 years on a range of biomass growing and production systems as well as different biomass conversion technologies for the production of conventional and second generation bio-transportation fuels, heat and power; with only a few projects on biomass conversion processes for higher added value bio-based products (chemicals/materials). Few studies have examined the complete chain where biomass production is integrated with the conversion to give an energy product, and none has examined the important benefits to be derived from a comprehensive integration of all components of an integrated biorefinery system for co-production of both bio-based products and secondary energy carriers.

Expected achievements of the Biosynergy Project

The most important results, i.e. those with great relevance towards meeting the EU programme goals were:

- Technical, socio-economic and environmental EU-perspective of integrated refinery processes for the co-production of chemicals, transportation fuels and energy from

biomass by performing integral biomass-to-products chain design, analysis and optimisation.

- Lab-scale development and pilot-scale demonstration of biorefinery-based composing sub-processes, i.e. physical/chemical fractionation processes, thermo-chemical conversion processes, biochemical conversion processes, and chemical conversion and synthesis processes.
- Basic design of an innovative cellulose ethanol based biorefinery process in which the residues are upgraded to added-value products (chemicals, power, CHP).
- Proper trained persons in relevant industries, research institutes and universities.
- Knowledge dissemination (website, workshops, lectures)

There were 17 partners involved in the Biosynergy project from across the EU and across different market sectors. The full list of partners may be found in Table 1.1 .

Table 1.1 – Biosynergy partners

Participant name	Participant short name
Energy research Centre of the Netherlands	ECN
Abengoa Bioenergía Nuevas Tecnologías, S.A.(ABNT)	ABNT
Compania Espanola de Petrolos, S.A.	Cepsa
Dow Benelux B.V.	DOW
VTT Technical Research Centre of Finland	VTT
Aston University	Aston
WUR Agrotechnology and Food Innovations B.V.	A&F
Agro Industrie Recherches et Developments	ARD
Institut Francais du Pétrole	IFP
Centre for Renewable Energy Sources	CRES
Biomass Technology Group	BTG
Joanneum Research Forschungsgesellschaft m.b.H.	JR
Biorefinery.de GmbH	Bioref
Glowny Instytut Gornictwa	GIG
Joint Research Centre	JRC
Chimar Hellas S.A.	Chimar
Delft University of Technology	TUD

The project consisted of 8 different work packages (WPs), each studying different components of a biorefinery process. This thesis was based on the work carried out for Work Package 6 (WP6). WP6 brings together the work from across the project for use in the construction and evaluation of complete integrated biorefinery plants. The full list of work packages with short description of the tasks is shown in Table 1.2.

Table 1.2 – Biosynergy work packages

Management	**WP 0 – Management activities**
Research & Technology Development (RTD)	**WP 1 Advanced physical/chemical fractionation** Lab-scale experimental development of advanced technologies for the physical/ chemical fractionation of biomass in separate C5-sugar, C6-sugar and lignin fractions. C6 sugars -> bioethanol; C5 sugars -> added-value products; Lignin -> added-value products
	WP 2 – Innovative thermo-chemical conversion Lab-scale experimental development of (catalytic) staged degasification and pyrolysis processes for the fractionation/conversion of lignin/ biomass into chemical intermediates and/or secondary energy carriers.
	WP 3 – Advanced biochemical conversion Advanced biochemical conversion processes will be developed for the conversion of sugars and lignin into higher alcohols, sugar acids and functional lignin derivates; all products/intermediates with an added financial value.
	WP 4 – Innovative chemical conversion and synthesis Lab-scale experimental development of promising chemical conversion technologies for the valorisation of C5-sugars, lignin and thermo-chemical derived bio-based intermediates. Further, synthesis processes will be analysed and developed for the synthesis of final products from added-value intermediates (furfural, phenol, HMF …) produced. Also the potential integration into a conventional oil-based refinery plant will be analysed.
	WP 5 – Conceptual design Biorefinery pilot-plant ABNT, Salamanca Conceptual design of an innovative biorefinery plant at an existing bioethanol site (Salamanca) owned by ABNT (BCyL) consisting of integrated physical/chemical or thermochemical fractionation processes coupled to advanced biochemical or (thermo-)chemical conversion processes for the co-production of upgraded bio-products (chemicals and/or materials), refined transportation fuels and energy (power and/or heat). Data-input from WPs 1, 2, 3,4,6,7.
	WP 6 – Integral biomass-to- products chain design, analysis and optimisation Technological, socio-economic and environmental assessments and optimisations of full biomass – refinery processes – product chains will be performed to analyze the total potential of integrated Biorefinery concepts within a future European Bio-based Economy. The use of various European representative biomass feedstocks will be analyzed in a variety of integrated biorefinery schemes, including the Biorefinery demo-plant of ABNT (WP5) and integration possibilities in conventional oil refineries
Demonstration	**WP 7 – Demonstration at pilot-scale** Pilot-scale facilities will be used to: – Produce market sound samples of bio-based intermediates for the lab and bench-scale technology developments. This WP includes 10-15 days running of the BCyL bioethanol validation plant (alternative: York plant in Nebraska for sample delivering). – Scale-up of the lab and bench-scale technology developments. Scale-up and pilot-scale demonstration of technologies developed in WPs: 1, 2, 3, and 4.
Training & Knowledge dissemination	**WP 8 – Training of people and knowledge dissemination.**

The partner's involvement in each of the separate work packages is shown in Table 1.3, along with each WP co-ordinator.

Table 1.3 – Partners involvement in each WP

WP #	Contents	Participating partners	WP Co-ordinator
WP 0:	Management activities	ECN, ABNT, A&F, Aston, ARD, IFP, JRC, all other partners	**Hans Reith, ECN (overall co-ordinator)**
WP 1:	Advanced physical/chemical fractionation	ECN, ABNT, A&F, ARD, Bioref, TUD	Rob Bakker, A&F
WP 2:	Innovative thermo-chemical conversion	ECN, Cepsa, Aston, BTG	Paul de Wild, ECN
WP 3:	Advanced biochemical conversion	VTT, A&F, IFP, GIG, Aston, ABNT, ECN (p.m.)	Frédéric Monot, IFP
WP 4:	Innovative chemical conversion and synthesis	ECN, DOW, Aston, A&F, ARD, Bioref, GIG, Chimar, TUD	Boris Estrine, ARD
WP 5:	Conceptual design Biorefinery validation pilot-plant of ABNT Salamanca	ECN, ABNT, Aston	Reyes Capote , ABNT
WP 6:	Integral biomass-to- products chain design, analysis and optimisation.	ECN, Aston, IFP, CRES, JR, Bioref, JRC, Cepsa, ABNT	Tony Bridgwater, Aston University
WP 7:	Demonstration at pilot-scale	ECN, ABNT, A&F, ARD, BTG, Bioref,	René van Ree, A&F
WP 8:	Training activities and knowledge dissemination	ECN, ABNT, Cepsa, DOW, VTT, Aston, A&F, ARD, IFP, CRES, BTG, JR, Bioref, GIG, JRC, Chimar	Boyan Kavalov, JRC-IE

1.1.1 WORK PACKAGE 6

This thesis was based on the work carried out to meet the objectives of WP6. The full title of WP6 is "Integral biomass to products chain design, analysis and optimisation". There were two main objectives detailed in the project Description of Work (DOW) for WP6. These were:

- Identification of the most promising biorefinery chains – both from energy efficiency, environmental performance and cost point of view – for the European Union and some specific market sectors.
- Based on life-cycle considerations the environmental effects of biomass production, biomass transportation and its conversion in integrated biorefinery processes to different products are quantified.

The first of these two objectives was also the objective for this thesis. A comprehensive, thorough and methodological approach to consideration of the full range of process and product opportunities would allow both their short term and long term evaluation and allow the identification of the most promising biorefinery concepts. This would provide some clear directions for research and policies in the short, medium and long term as well as identifying the most interesting opportunities for industry to enable the development of a robust bio-based industrial sector.

WP6 utilised the results from the other experimental work packages. The other work packages focussed on specific components of a biorefinery, for example WP1 research focussed on pre-treatment processes. The aim of WP6 was to evaluate these processes as part of a complete biorefinery process concept. In this way the experimental results can be scaled up and tested for validity in a full production process. It may be the case that something that looks appealing in the laboratory at the gram scale, does not transfer to an industrial sized plant processing thousands of tonnes.

Since a biorefinery would be expected to have multiple products, the key objectives include:

- Maximisation of efficiency in useful products.
- Minimisation of capital cost.
- Minimisation of product cost.
- Minimisation of environmental effect.

The first phase (1-18m) of the project involved the creation and validation of the process synthesis methodology and modelling tool (see Figure 1.1).

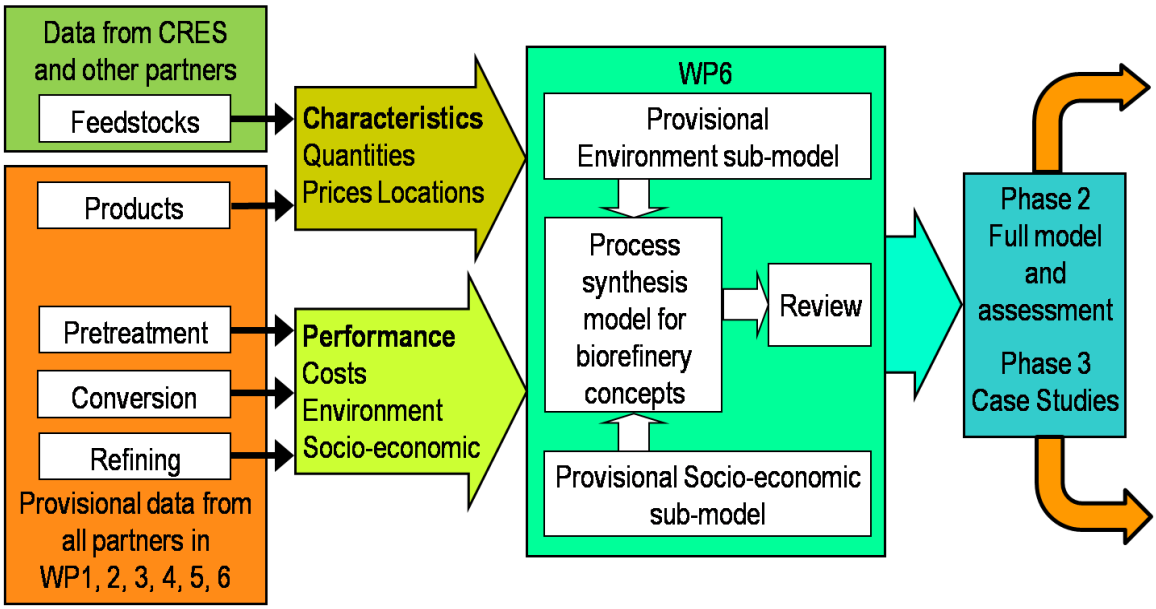

Figure 1.1 – Phase 1 workflow

During the first phase of the project, provisional data was collected from work packages 1-5 on feedstocks, pretreatment methods, conversion and refining methods and products. This data was used to research and build the first versions of the modelling methodologies. The methodologies had to be proven, there had to be confidence that the chosen methods could produce valuable results.

The first phase of the project integrated the provisional information into a process chain generation model based on logical and coherent relationships between the feed material, the various processes and the product. All inputs and outputs were considered to predict process performance and capital and production cost.

The basic approach used in the initial phases of the project to design and evaluate biorefinery concepts was process chain synthesis. This can be considered as a methodology for the generation of processes for converting a raw material into one or more valuable products that properly considers performance, cost, environment, socio-economics and all other factors that influence the commercial viability of a new process. The significance of the approach is that the methodology is defined and is thus rigorous and consistent and may be readily re-examined if circumstances change. Evaluation of the processes created can be carried out within the process synthesis model or additionally through mechanisms such as decision support systems, which also relies on a defined methodology so that previous outcomes can be readily re-considered.

One of the advantages of this approach to process definition and evaluation is that it is based on a set of defined rules or relationships. These are transparent and can be readily changed by the project team to reflect changing scenarios such as feedstock or product prices, crude oil prices, new technology developments, new processes etc. This will enable the final model to be updated and can be maintained as a valuable procedure for evaluation of new opportunities.

The other work packages within the project; WP1, WP2, WP3, WP4 and WP5 provided the information about the feedstocks, products and technologies in the form of a datasheet. Each datasheet had to include sufficient information to enable a complete process to be constructed or synthesised and include data on performance, costs, products, by-products and wastes in a consistent format so that they can be linked together into a coherent process. As well as bioenergy processes, suitable orthodox separation and reaction steps and waste disposal processes were included so that complete and feasible processes were produced.

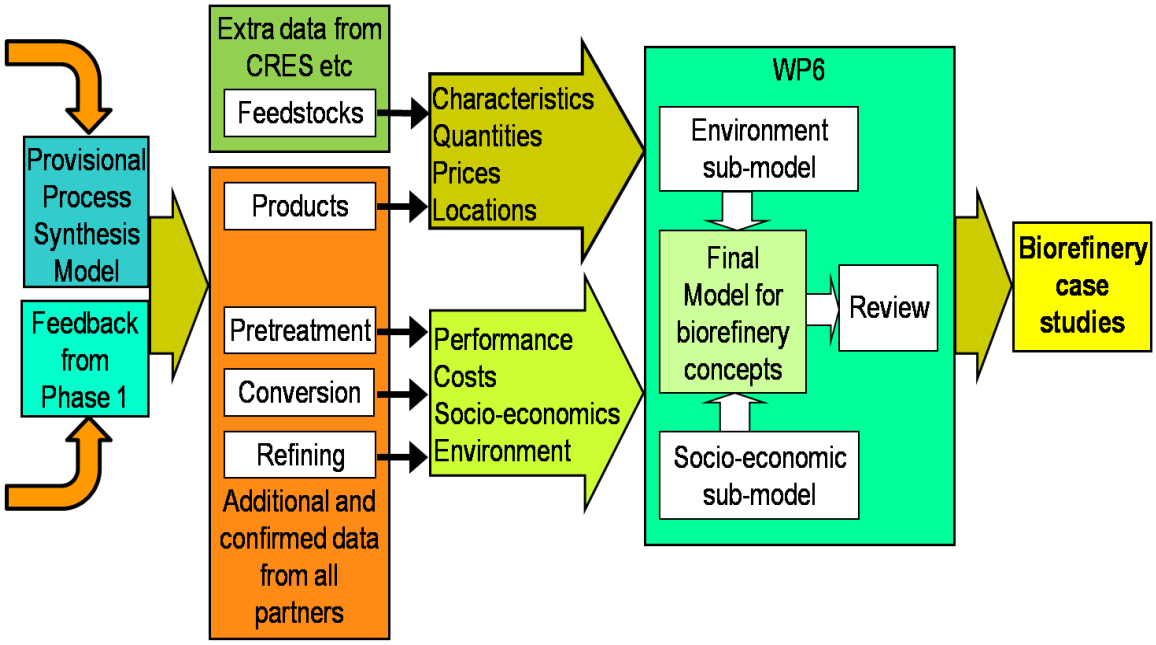

Figure 1.2 – Phase 2 workflow

In the second phase the models and data were finalised (see Figure 1.2). Once tested the initial provisional models were expanded to include many more processes and products from within the Biosynergy Project. This was an ongoing process where the models and methodologies were continually improved, and information from partners validated and finalised. The environmental and socio-economic model results were finalised, and integrated into the process models where possible in an attempt to create a fully integrated system. The tool could then be used to identify the most promising biorefinery concepts from the technologies and concepts considered within the Biosynergy Project.

A user interface was created so that the model can be used externally to the project. The user interface allows users to specify feed and product, key variables such as biomass feed rate and preferred technology combinations. The final output of the project was to provide biorefinery process chains ranked by performance, cost, environmental performance or socio-economic performance. Consideration was given to unifying these outputs so that comparative pictures of different products, process chains and scenarios could be produced.

Environment and socio-economic sub models

In order to provide an environmental and socio-economic assessment of each process chain, independent sub-models were created for both aspects, so that attempts could be made to integrate them into the final model.

These models were not created as part of this thesis submission, but were created by other work package partners. The results were combined with those from the process modelling and used in the evaluation.

For the environmental assessment of different process chains, a methodology was developed by JR and JRC to establish an environmental profile for the performance of the considered biorefinery process concepts based on a life-cycle perspective. The environmental profile provided a set of parameters for the impact assessment and gave an instrument for comparing different aspects of the biorefinery process chains on complex environmental situations. This environmental profile allows a compact summary of advantages and disadvantages of different process chains within the production system and products generated through these processes. Based on this a comparison to conventional products – e.g. raw oil based products that will be substituted – was be made to identify possible benefits and impacts of integrated biorefinery processes (163,164).

For the socio-economic assessment a flexible modelling methodology was developed by Patricia Thornley. The model focussed on employment, agricultural land use and a trade assessment for the countries under consideration. The model gave a generalised view of the impact of a biorefinery plant on a particular country (88,161).

1.2 THESIS OBJECTIVES AND STRUCTURE

1.2.1 OBJECTIVES

There were two main objectives for the work carried out for this thesis. These were:

- Creation of a methodology for the generation, analysis and comparison of full biomass to product chains.
- The identification of the most promising biorefineries for the European Union.

1.2.2 STRUCTURE

Chapter 2 provides an introduction to biomass and biorefineries detailing the reasons for the interest in biomass as a source of energy, fuels and chemicals. The difference between first and second generation feedstocks are described and the obstacles for the utilisation of biomass discussed (Section 2.1.2.). The term biorefinery is defined in Section 2.2 followed by a review of biorefineries in the literature in Section 2.2.2. Finally a discussion of the main challenges facing the implementation of biorefineries is described in Section 2.2.3.

Chapter 3 describes the steps involved in creating the methodology beginning in Section 3.1 by defining the requirements for the methodology are specified followed by a short description of each of the steps included in the methodology.

The first step in the methodology, process synthesis is described in Chapter 4. The term process synthesis is defined in Section 4.1 followed by a review of the key process synthesis methods available in Section 4.2. The application of process synthesis to biorefinery evaluation is described in Section 4.3 followed by a definition of the method applied to this thesis in Section 4.4.

The second step in the methodology is process modelling, described in Chapters 5 and 6. Chapter 5 begins with an outline of the modular modelling approach taken followed by a review of process modelling techniques available and the choice of technique for this thesis. In Section 5.4 the 27 biorefinery concepts chosen within the Biosynergy project are introduced and the data collection and validation techniques described in Section 5.5. In Chapter 6 the process modelling step is described further with individual descriptions of each of the process modules. Each module is described with a block diagram, process description and main assumptions, plus validation data if this is available.

Chapter 7 described the second element of the process synthesis step. In this chapter the user interface and the methodology for linking of process modules is described. The logic rules and possible connections for each of the modules defined.

Chapter 8 describes the final step in the methodology; process evaluation. This chapter begins with a specification of the required characteristics for evaluation methodology. In Section 8.2 methods for biorefinery evaluation found in the literature are reviewed, with discussion of suitability for application to this project.

Chapter 9 introduces process evaluation by multi-criteria decision analysis (MCDA) with a description and review of the main multi-criteria techniques. In Section 9.3 there is a description of the application of MCDA to this project including the choice of criteria, use of modelling results and the weighting choice is explained.

In Chapter 10 the modelling and MCDA results are described and discussed. In Section 10.1.1 the likely uncertainty contained within the results is described and estimated. The process modelling results are given in Section 10.2.1 followed by a sensitivity analysis in Section 10.3.. The MCDA results are given in Section 10.4 for the evaluation and ranking of the 27 biorefinery concepts.

In Chapter 11 the conclusions for this thesis are given. A summary of the results are discussed as well as the significance of the results and how this work may be used beyond the scope of this project.

Finally in Chapter 12 are the recommendations for further improvements to the work or for future research.

2 BIOMASS AND BIOREFINERIES

The interest in biomass and biorefineries has grown exponentially in recent years, due to increasing concern over the remaining fossil resources, climate change and energy security. Biomass and biorefineries are seen to offer a solution to these concerns, but much work still needs to be completed in order to move from a fossil based to a bio-based economy.

This chapter will provide the reader with background information on the topic of biomass and biorefineries. In Section 2.1 the benefits of biomass as a feedstock and why biomass is so important for a sustainable future is described along with the main challenges of biomass utilisation.

In Section 2.2 the term biorefinery is defined with a description of the various biorefineries under consideration in the literature. Details of how biorefineries offer solutions to many of the current challenges are given. The challenges in the implementation of biorefineries are explained and the core problem to be overcome by the methodology created in this thesis is described.

2.1 BIOMASS

There is agreement across the literature as to the main reasons for the development of renewable energy, the use of biomass and the interest in biorefineries (4, 5, 6, 7, 9, 62).

These are:

- Energy security
- Climate change
- Rural development
- Continued population growth creating a greater demand for energy and products (29, 9).

Biomass is seen to provide a partial solution to these problems as it offers the only renewable means of producing fuels and chemicals. Biomass is the oldest source of energy used by humans (4) and can be used as a fuel itself or converted into liquid, solid or gaseous products in a biorefinery complex.

Currently 80% of energy consumed in the world originates from 3 fossil sources; petroleum, natural gas and coal (8). As well as energy, most chemical products originate from fossil sources (9, 10). There is concern that fossil resources may begin to dwindle

(15, 76) and become prohibitively expensive over the coming years which has led to an increased interest in renewables. Biomass is viewed as part of the solution to overcome the world's dependence on fossil resources. It is possible to generate heat and electricity from other renewable sources; such as solar, wind and geothermal (10, 9, 11, 19), but there are only limited options for renewable sources of fuels and chemicals (76). Biomass is an abundant and low cost feedstock. It is the only sustainable source of carbon rich material (9, 12, 13) that may be processed into fuels, energy and chemical products (145, 14) as an alternative to fossil based products.

As well as concern over the availability of fossil resources there is an uneven distribution of these resources throughout the world. The remaining resources are controlled by only a small number of countries, giving the potential for political instability (4, 15, 16) and fears over the security of energy and fuel supply. Biomass overcomes this problem as it can be found in almost all locations throughout the world. Biomass resources are often available domestically, so no imports are needed which gives a country increased energy security (17). Furthermore, the move towards a bio-based economy gives the oil controlling countries less ability to influence world events (4).

In addition to the availability and location of fossil resources, there is concern about climate change and green house gas (GHG) emissions leading to an increase in the Earth's temperature. This is a large factor influencing the use of biomass as it can be used to help mitigate these emissions. Biomass fixes CO_2 from the atmosphere by photosynthesis (33) storing solar energy within the plant as chemical energy through photosynthesis (8, 33, 4). The carbon stored is then exhausted when a bio-based product is used but is recycled with new plant growth (17).

A major benefit of the use of biomass is rural development. The cultivation and transport of biomass feedstocks will provide a boost to regional and national agricultural sectors in the form of job creation and regional development (6). For developing countries the production of biomass feedstocks could provide useful economic opportunities (18).

Governments around the world have realised the importance of moving towards more sustainable energy, fuels and products, and have implemented minimum targets for the utilisation of bio-based products for the future (11). The European targets are shown in Table 2.1 and illustrates how seriously governments are taking the move towards a more sustainable future.

Table 2.1 - Targets for EU (19)

	2001	2005	2010	2020 - 2050
Bioenergy share of wind power, photo voltaic, biomass and geothermal electricity and heat demand in utilities and industry	7.5%	~	12.5%	26% (2030) 58% (2050)
Biofuels Biomass share of demand in transportation fuels (petrol and diesel)	1.4%	2.8%	5.75%	20% (2020)
Bio-based products Share of the target chemicals that are bio-based	8%	~	~	~

2.1.1 BIOMASS FEEDSTOCKS

Biomass is defined as any non-fossilized, biodegradable organic material originating from plants and micro-organisms (4). The composition of biomass is dependent on the species and type, for example, hardwoods have a lower proportion of lignin than softwoods (4). An advantage of these composition variations is that a wide range of products can be produced allowing greater opportunities for biorefinery configuration (20). The molecule derivatives from biomass represent one of the most important potentials for producing chemical intermediates (29) and as mentioned previously, biomass is the only renewable source of carbon.

The main difference between fossil feedstocks and biomass is the oxygen content (33, 21). Biomass feedstocks often contain 40-60wt% oxygen whereas conventional fossil fuels typically only contain very small amounts <1wt% (4). One of the tasks in biomass processing is to remove the oxygen to result in products comparable with those derived from fossil sources.

Biomass utilised in biorefineries are generally categorised as first generation or second generation feedstocks. The two categories are described in the following sections.

2.1.1.1 FIRST GENERATION FEEDSTOCKS

The majority of commercial biofuel plants are fed with first generation feedstocks (sugar, starch, oil crops) (11). For example, Brazil and the USA are the two largest commercial bioethanol producers utilising the first generation feedstocks of sugar cane and corn (150, 22). Other examples of first generation feedstocks are shown in Table 2.2.

Table 2.2 – First generation biomass feedstocks (8)

Sugar crops	Starch crops	Oil crops
Sugar cane	Corn	Soybean
Sugar beet	Potato	Canola
Sweet sorghum		Palm

The reason for the use of these feedstocks is the relative ease of conversion of sugar, starch and oil crops to biofuels (11). These crops are also used for food production, hence the

food versus fuel debate. The use of these crops for biofuels has lead to fear of food shortages and price increases where these commercial plants are built (23).There are socio-economic concerns regarding the effects of the potential increase in food prices, such as the impact on public health and the economies of developing countries (11). The continued use of food crops for bio-products may cause conflict as the world's population grows (23). This has led to a negative image of biofuels amongst some consumers (28) and it has been argued that the sugar or starch in first generation crops has a greater value as food in food applications (15).

2.1.1.2 SECOND GENERATION FEEDSTOCKS

To overcome the food versus fuel issue, research has moved towards second generation feedstocks. Examples of second generation feedstocks are shown in Table 2.3 and include energy crops, agricultural and forestry residues and waste. These crops do not compete directly with food crops, removing the negative associations and fear amongst consumers. It has been stated that lignocellulosic feedstocks can help reduce GHG emissions (9, 24) and give a better economic performance than first generation feedstocks (76).

Table 2.3 – Second generation feedstocks (19, 145, 24)

Energy crops	Agricultural food and feed crop residues	Aquatic plants	Wood and wood residues	Waste materials
Switchgrass	Corn stover	Macro-algae (seaweed)	Hardwood (e.g. Aspen, Poplar)	Pulp and paper waste residues
Hybrid poplar	Wheat straw	Micro-algae	Softwood (e.g. pine)	Organic municipal fraction
Salix	Rice straw			
Miscanthus	Bagasse			

In the long term, energy crops and residues offer the best potential for the production of bio-based products because of high yields and the lack of competition with food crops (25). Fast growing energy crops do not have to be cultivated on high quality agricultural land (8) and there is still potential for improvement in the production of these feedstocks (24) in terms of yields, fertiliser requirement and composition (28).

Future biorefinery plants will focus on the use of lignocellulosic feedstocks, as these make use of the readily available low cost residues or energy crops (24). Within Europe straw is the major agricultural residue available for processing (25). Lignocellulosic feedstocks were chosen by the Biosynergy Project as the feed for the biorefinery plants evaluated.

Lignocellulosic biomass structure

Lignocellulosic biomass consists of 3 components in varying proportions. These are cellulose, hemicellulose and lignin. The proportion of these three constituents varies according to the type of biomass; some examples are given in Table 2.4. The key to exploiting lignocellulosic feedstocks is depolymerising the structure and accessing the component parts (11) and this forms one of the challenges for biorefinery operation.

Table 2.4 – Various lignocellulosic biomass compositions (24)

Component	Aspen	Hybrid poplar	Switchgrass	Corn stover
	Wt% dry basis	Wt% dry basis	Wt% dry basis	Wt% dry basis
Cellulose	53.0	43.7	33.8	37.4
Xylan	19.1	15.6	22.1	21.1
Arabinan	4.2	0.7	2.8	2.9
Mannan	2.1	2.3	0.2	1.6
Galactan	1.6	0.9	0.9	2.0
Lignin	19.1	27.2	16.8	18.0
Ash	0.9	1.4	6.0	5.2
Extractives	0	3.4	15.5	4.7
Acetate	0	0	0	2.9
Protein	0	0	0	3.1
Soluble solids	0	4.8	1.9	1.1

Cellulose - $(C_6H_{10}O_6)_n$ - Has a strong chain structure made up of glucose molecules. It is more difficult to hydrolyse than starch (9, 11) and is the most common bio-polymer. Cellulose can be converted into six-carbon sugars (C6) and fermented to ethanol or processed to other value added products (14).

Hemicellulose - $(C_5H_{10}O_2(OCH_3))_n$ - Has an amorphous structure and is easier to break down than cellulose. When broken down hemicellulose produces a mixture of mostly five carbon (C5) and a smaller quantity of six carbon (C6) sugars (9). Hemicellulose has a lower degree of polymerisation than cellulose and hence is easier to hydrolyse (11). The sugars can be processed into a large variety of products.

Lignin - $(C_9H_{10}O_2(OCH_3))_n$ - Is the glue that provides the overall rigidity and acts as the scaffold in the biomass structure (30). Lignin is a complex material with a high molecular weight (4). It is made up of phenolic polymers and cannot be fermented (9). It currently has limited uses (34) but is a potential source of aromatics (34).

2.1.2 OBSTACLES FOR THE UTILISATION OF BIOMASS

There are still a number of challenges to overcome in the use of biomass as a feedstock. Although biomass feedstocks are relatively cheap, the cost of the feedstock greatly influences the profitability of the biorefinery process as the cost of the feedstock typically

accounts for 30-40% of the production costs. In order for industry to recover the cost of the feedstock, they must make the biorefinery as efficient as possible, obtaining the most financial, environmental and social benefits.

A disadvantage of biomass as a feedstock is the cost of transportation due to its bulk and low density (26). It is likely that biomass supply will be from various locations, rather than from a single oil well or pipeline as for petrochemical refineries. The scale of operation will be dependent on the transportation cost of the biomass (26). This means that the ultimate limit to the potential of a biorefinery in a particular location will be the feedstock availability (62). This must be considered carefully when deciding on the location and scale of a biorefinery plant.

To ensure maximum environmental benefits from biomass it has to be produced and utilised in a sustainable way, with consideration of factors such as the use of the land so as not to deplete soil organic material or to cause soil erosion (27, 9). Second generation feedstocks can be grown on non-agricultural land, although displacement of land use may still be an issue (28) as will the use of fertilisers and other resources in order to grow the crops. The impact of the resources required to supply the biorefinery as well as the biorefinery itself must provide optimal environmental benefits.

One of the main challenges in the utilisation of biomass is making the valuable component parts of the biomass accessible for further processing. Biomass has a complex structure which must first be broken down with some kind of pretreatment process before valuable products can be extracted or synthesised. The composition of the biomass feed affects the processing efficiency and the overall economics (24). In order to obtain valuable fuels, chemical and energy from biomass, with optimum benefits it must be processed in a highly efficient processing scheme known as a biorefinery. A number of processing options for biomass conversion are relatively immature and have not yet been commercialised. Research is still needed to make them commercially viable and attractive to industrial stakeholders.

2.2 BIOREFINERIES

In this section the term biorefinery is carefully described and defined. Section 2.2.2 describes biorefinery plants followed by a discussion of the main challenges in Section 2.2.3. The focus for this thesis is second generation biorefineries i.e. those utilising second generation feedstocks.

2.2.1 DEFINITION

Products such as liquid biofuels and other chemicals can be made from biomass through a number of different conversion routes (28) in an integrated processing plant called a biorefinery. The aim of a biorefinery is to convert the energy contained in biomass into a more useful and usable form maximising valuable products whilst minimising waste (34) and environmental impact.

Biorefineries are analogous to oil refineries, as similar to crude oil, biomass has a complex structure and composition (29, 30) and there needs to be a number of processing steps applied to release and separate the useful fractions from the feed. Fuels are the main product for petrochemical refineries, and it is very likely that this will also be true for biorefineries (4); although chemicals (and materials) are of particular commercial interest because of their higher value.

There are a number of definitions for the term biorefinery in the literature. A selection of these is detailed below.

The definition of a biorefinery from the members of IEA Bioenergy Task 42 "Biorefinery is the sustainable processing of biomass into a spectrum of marketable products (food, feed, materials, chemicals) and energy (fuels, power, heat)." (31). Similarly Demirbas (8) defines a biorefinery as "a facility that integrates biomass conversion processes and equipment to produce fuels, power and value added chemicals from biomass."

The American National Renewable Energy Laboratory (NREL) defines a biorefinery as "a facility that integrates biomass conversion processes and equipment to produce fuels, power and chemicals from biomass. The biorefinery concept is analogous to today's petroleum refineries, which produce multiple fuels and products from petroleum, industrial biorefineries have been identified as the most promising route to the creation of a new domestic bio-based industry." (32)

There are a number of different definitions but the aim of the biorefinery is always the same; to gain the optimum "value" from the biomass feedstock. Where this "value" can be defined in economic terms, or according to other criteria such as environmental or socio-economic impact.

For this thesis, a biorefinery is defined as a fully integrated process to produce a variety of products (energy and chemicals) fully utilising all fractions of the biomass feedstock, resulting only in value added products or benign waste streams.

2.2.2 BIOREFINERIES IN THE LITERATURE

Biorefineries have been described in the literature with labels attached to those processing certain feedstocks or containing certain processes, such as "green", "forest", "aquatic", algae", "sugar platform" and "syngas platform".

Some examples of the second generation biorefineries described in the literature are:

- Syngas based (33) – Focuses on thermochemical conversion of biomass to syngas, and subsequent synthesis.
- Pyrolysis based (33) – Focuses on the pyrolysis of biomass to bio-oil.
- Hydrothermal based (33) – Biomass is treated by high temperatures and water.
- Fermentation or sugar based (33, 34)) – Focuses on the biochemical conversions for the fermentation of sugars (19, 34).
- Green biorefinery (33, 35) – Utilises "green" crops such as clover, lucerne and grass (19). These naturally wet feedstocks are available in large quantities (34).
- Whole crop (1^{st} and 2^{nd} generation) (34, 35) – Utilises the grain (e.g. wheat, rye) and also the straw. Crops are used such as wheat, rye, triticale, maize.
- Lignocellulosic biorefinery – Uses a variety of non-food crops such as straw, wood, agricultural and forestry residues.

Each of these biorefinery types has their own advantages and disadvantages. The thermochemical routes offer the advantage of being able to cope with variation in the feedstock, as no complex pretreatment or fractionation is required, the whole biomass is fed to the reactor. With biochemical routes, the feedstock composition effects downstream processing, so biochemical biorefineries cannot cope with large fluctuations in feedstock type or composition. The choice of enzyme, for example, is often tailored to a particular feedstock to obtain high efficiency. But conversely biochemical plants are capable of producing a wider spectrum of products than the thermochemical routes.

It may not be useful to sort biorefineries into such categories as in reality the most promising plants may contain a combination of processes and feedstocks. It is more constructive to use the general term biorefinery to describe any combination of configurations that process biomass into value-added fuels, energy and chemicals. A fully integrated biorefinery combining several technologies may improve overall efficiency, reduce costs and offer greater flexibility in the product mix (34). Ideally the biorefinery will also provide its own heat and power by utilising process residues and/or additional

feedstock to further reduce demand on fossil resources and improve environmental impact. A generalised biorefinery block scheme is shown in Figure 2.1.

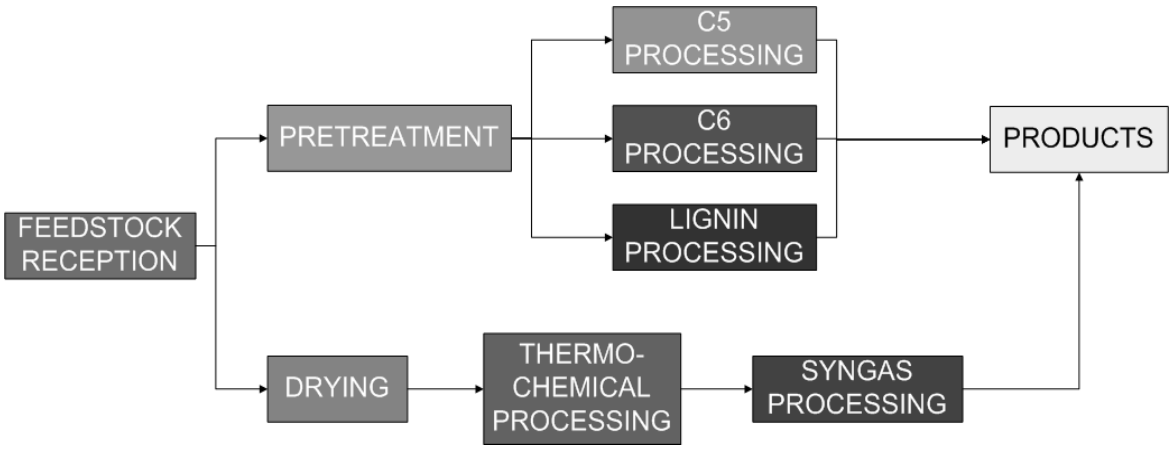

Figure 2.1- Generalised biorefinery diagram

Much has been written about biorefineries and the books by Kamm and Kamm (36, 37) and the book by Demirbas (4) provide an extensive overview of biorefineries and the topics surrounding this research area. They include chapters on the background to biorefineries, the possibilities of biorefinery systems, the production of biomass, more detailed information on biomass conversion and the potential of bio-based products from a market perspective. From these books the scope of the subject and large potential for biorefinery based systems can be realised. The implementation of biorefineries brings together and integrates knowledge from various subject areas; agriculture (for feedstock production), biotechnology (for enzymes and other chemicals), process engineering, environmental analysis and socio-economic impact assessments.

There has been significant work on specific topics or processing areas within a biorefinery, such as the identification of the most promising products from biomass. Extensive reviews of this subject have been produced by Holladay (38), Werpy (39), Huber (40) and Corma (41). These reviews contain information about potential process routes, but also help identify those bio-based products likely to be of most promise for industry and from a market perspective. These pieces of work illustrate the vast number of possible products from biomass and therefore the potential for wide product portfolios in biorefinery processing plants.

The focus of much biorefinery research has been on cellulosic bioethanol (42, 75, 111, 145, 150). This is demonstrated in Table 2.5 which lists the current (2010) biorefinery demonstration plants in operation, planned or under construction. The reason for the interest in ethanol is that transportation represents about 27% of the world's secondary

energy consumption and is almost exclusively fuelled from fossil sources (76). Bioethanol may be used as an alternative to fossil fuels and it currently accounts for 94% of global biofuel production (43). It is mainly used as an oxygenated fuel additive displacing a proportion of the fossil based fuel and has the potential to reduce particulate emissions (43, 44). The potential demand for bioethanol as a fuel, calculated on the basis of the EU directive 2003/30/EC is estimated to be 12.7billion litres in 2010 (43). The global ethanol industry has grown rapidly in recent times, mainly due to monetary incentives offered by local and national governments (45). This has made ethanol production significantly more attractive to ethanol producers and investors.

Table 2.5 – Biorefinery demonstration plants (18).

Name	Location	Product and annual capacity (million gallons)
Iogen	Idaho, Canada	18 cellulosic ethanol (250 in future plants)
BlueFire Ethanol	California, USA	32 cellulosic ethanol
Poet	Ohio, USA	65 corn ethanol
Ecofin, LLC	Kentucky, USA	1.3 corncob ethanol
ICM Incorporated	Missouri, USA	1.5 lignocellulosic ethanol
Lignol Innovations	Colorado, USA	2.5 cellulosic ethanol
Royal Nedalco	Rotterdam, Netherlands	60 cellulosic ethanol
Mascoma	New York, USA	0.5 cellulosic ethanol
Pacific Ethanol	Oregon, USA	2.7 lignocellulosic ethanol
Abengoa Bioenergy	Kansas, USA	25 lignocellulosic ethanol
Verenium	Louisiana, USA	1.5 cellulosic ethanol
RSE Pulp	Maine, USA	2.3 cellulosic ethanol
Flambeau	Wisconsin, USA	14.2 lignocellulosic ethanol
NewPage	Wisconsin, USA	12.8 biofuels, FT liquids
Choren	Freiberg, Germany	1.5 biofuels, FT liquids
Alico	Florida, USA	7.5 ethanol, electricity, ammonia, hydrogen
Range Fuels	Colorado, USA	1.2 biofuels, FT liquids
Flambeau River	Louisiana, USA	6.5 biofuels, FT liquids

The development of biorefineries is so challenging and interesting because of the potential for a wide portfolio of products from the biomass feedstock making it difficult to choose the configuration offering the most benefits. As well as fuel and energy there is the potential to produce high value specialty chemicals and other bio-based products. The diversity of products possible may give some protection from seasonal demand cycles and market downturns (4). The economies of scale provided by the biorefinery plant can help lower the cost of producing low volume high value products also giving process integration benefits (4). Another advantage of biorefinery complexes is the potential to create new markets and tax incentives are likely to promote investors (4). Incentives are offered by governments keen to meet their renewable targets and to improve their country or regions “green” credentials.

Biorefineries offer the potential for integration into conventional petrochemical refineries (72) or other processing facilities as described in the paper by Huber and Corma (13). This is possible because a biorefinery is capable of producing chemical intermediates which may then be processed in existing plants. Huber and Corma (13) describe a number of options for integrating bio-products into the refinery such as the application of fluid catalytic cracking, hydrotreating-hydrocracking of bio-liquids or the utilization of bio-derived syngas for hydrogen production. In this way the biorefinery can utilise existing infrastructure, reduce costs and the risks associated with new plants. Another potential pathway for integration is for a biorefinery to provide heat and power to the existing refinery plant, reducing overall primary fossil energy demand and giving environmental benefits.

Among the potential large-scale industrial biorefineries the lignocellulose feedstock (LCF) biorefinery will most probably be pushed through with highest success. The raw material situation is optimal (straw, reed, grass, wood, paper-waste etc.) and there is the potential for production of a variety of products, tailored to fit a particular feedstock, location or market situation. Lignocellulosic based biorefineries allow the use of non-food crops that are more environmentally efficient to produce and generate less greenhouse gases than first generation based facilities (14).

2.2.3 MAIN CHALLENGES

Although the processing of biomass in a biorefinery complex offers many benefits there are still some major challenges to overcome. There are still a number of technical barriers to the creation of second generation biorefineries and more research, development and demonstration is needed to ensure efficiency and sustainability (4).

A disadvantage of a biorefinery compared to a petrochemical refinery is the range of processing technology required (20). To process biomass often involves numerous and complex processing steps, frequently using technology that has not been proven at large scale. The technologies involved in biomass processing are often immature so are risky for stakeholders to develop and build. Continued research is needed to improve the efficiency and cost effectiveness of these technologies to make them more competitive and more attractive to investors.

A barrier to the implementation of biorefineries is the negative image of biofuels and biorefineries resulting from the food vs. fuel debate. Robust research and excellent knowledge dissemination is essential for the future development of these plants.

It should not be assumed that because the products are manufactured from biomass that biorefineries are environmentally attractive and sustainable, and do not add to the problems of climate change. There will still be GHG emissions from a biorefinery, directly and indirectly. Fuels, such as ethanol, do have a positive impact on reducing GHG emissions but there are still some unavoidable direct and indirect emissions such as the use of fertilisers in feedstock cultivation and from transport of feed and products, as these will generally rely on fossil fuels (45). When considering the biorefinery as a whole, taking into account all inputs and emissions, it must prove itself to be of no detriment to the environment.

One of the major challenges facing the implementation of biorefinery plants is the efficient production, harvesting and storage of the feedstocks. Many of the feedstocks are only available on a seasonal basis, requiring careful management to allow continuous supply to the plant and to prevent spoilage from long term storage. This in addition to availability and transport cost mean that an improved infrastructure is required for collection and storage of crops and residues (18).

The demand of the biorefinery for feedstock requires careful consideration as this will limit the potential size of biorefinery plants. Biomass cannot be transported by pipeline and there is an economic limit as to how far the biomass can be transported. As biorefinery development increases, so will the demand for feedstock and it is likely that the price for lignocellulosic feedstocks will increase as more biorefinery plants are brought on stream. To try and mitigate this, there should be increased efforts made to develop feedstock cultivation such as dedicated energy crops on set aside land, which will not compete with food crops. There needs to be careful management of Europe's natural resources as even though biomass is a renewable resource, its use should not be wasteful.

The problem of finding the "best" arrangement of technologies within a biorefinery still needs to be answered (19). There is the need for a comprehensive, thorough and methodological approach to consideration of the full range of process and product opportunities. This will allow both their short term and long term evaluation and will provide some clear directions for research and development policies in the short, medium and long term as well as identifying the most interesting opportunities for industry to develop. This problem is open ended and there may be more than one solution that is attractive or near optimal (56). Bio-products (chemicals and/or materials) are of greater commercial interest because of their much higher value, but competition from traditional fossil fuel based industries keeps market prices sufficiently low that biomass derived

products have difficulty competing. Sometimes there is not a clearly defined market for the bio-products that can be recovered, for example, lignin.

The paper by Alvarado-Morales (46) recognises the key challenge facing the development of a bio-based economy. That is “which products to produce and how to produce these to make the biorefinery most profitable”. They identify the need for a methodology to achieve this and make the point that a methodology can help to reduce man-power and resources. An advantage of a defined methodology for the generation and analysis of biorefinery process chains is that users always follow the same procedure as without the methodology no two users would solve the problem in the same way (56).

The key issue remains, what is the best product mix and what is the most efficient way of processing biomass into value added products? The biomass should be utilised in the most efficient way, to gain the most “value” in terms of cost, efficiency, environmental and other benefits. Finding the best biorefinery configuration will become crucial as competition for feedstock increases. The biorefinery should process every fraction of the biomass to products, analogous to the petrochemical refinery that uses every fraction of the crude oil. Finding the optimum is an iterative process; many different combinations may need to be tested before finding the optimum and the process may have to be repeated as new research breakthroughs are made. A system is needed to enable the user to quickly build and analyse biorefineries in a repeatable fashion. It is hoped that the methodology created for this thesis will help to solve this problem.

3 METHODOLOGY

One of the key objectives of this thesis was to establish and implement a methodology to generate, model and evaluate biorefinery process chains. This chapter describes the steps taken in order to establish methodologies to meet this objective. The steps taken are illustrated in Figure 3.1:

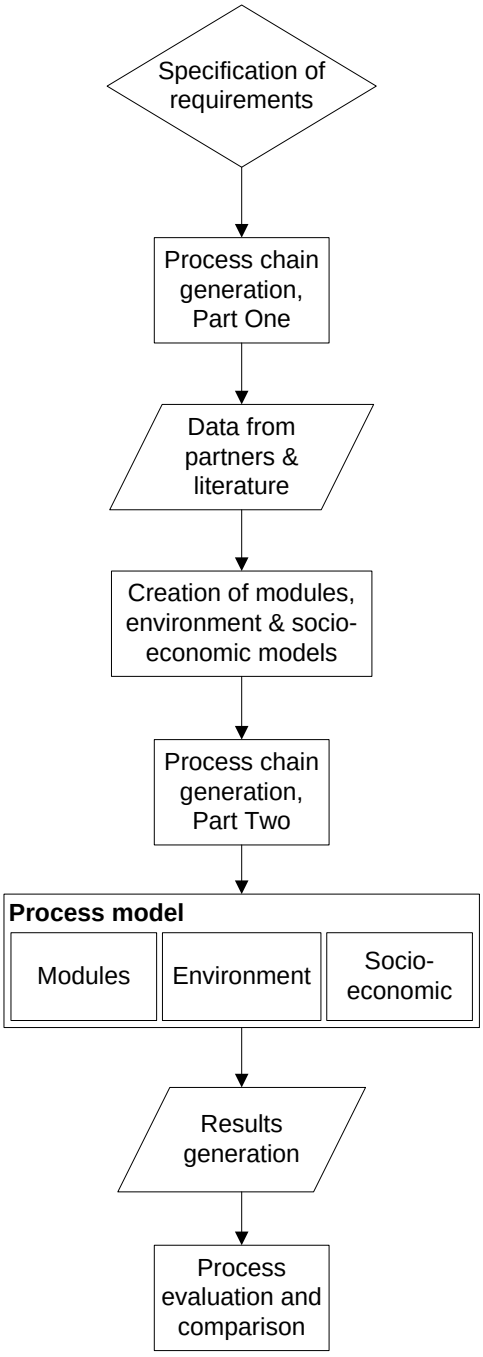

Figure 3.1 – Methodology to generate and evaluate biorefineries

1. Specification of requirements
2. Process synthesis, Part One (Chapter 4)
3. Data acquisition, modules and process modelling (Chapters 5 and 6)
4. Process synthesis, Part Two (linking of the process modules) (Chapter 7)
5. Results generation (Chapter 10)
6. Process evaluation and comparison (Chapter 10)

3.1 SPECIFICATION OF REQUIREMENTS

The Biosynergy project objective stated that a comprehensive, thorough and methodological approach was required to consider the full range of process and product possibilities that would allow evaluation and identification of the most promising biorefinery options. A highly flexible and reproducible methodology was therefore required. The systems needed to be capable of accepting additions and changes to the feedstocks, processes and products. The methodologies chosen had to be flexible enough to be reapplied as the project progressed, as new developments were made and new information derived.

The methodology needed to be user friendly and accessible so that project partners could utilise the finished system without training beyond a user manual. The results needed to be presented in a clear and understandable fashion that satisfied the requirements of project partners and other users. There was the requirement for consistency in structure and use, particularly for multiple analyses. It was important that analyses could be quickly and easily carried out to consider for example different scales, configurations and product portfolios.

3.2 PROCESS SYNTHESIS, PART ONE

The first step was to identify a method for generating biorefinery process chains from biomass through to the finished product/s as a fully integrated process. Chains should only be created that are technically feasible, for example, it should not be possible to create a process where the biomass undergoes saccharification followed by thermal gasification. The methodology needed to be constructed with in-built logic to prevent incompatible processes being chosen, therefore a set of rules defining compatibility of sequences of operations was necessary. The user needs to generate the biorefinery one step at a time from feedstock through to finished products and should receive a clear and concise summary of their chosen biorefinery concept. The user interface needed to be clear and easy to follow, as potential users would not necessarily be engineers or scientists. The method chosen had to be compatible with the subsequent steps in the overall methodology.

More details of process synthesis methods and the method chosen for this thesis can be found in Chapter 4.

3.3 DATA ACQUISITION, MODULES AND PROCESS MODELLING

The second step was to model the processes from data on performance, cost, environmental and socio-economic impacts. This was acquired from the partners in the project or literature when data was not available. The decision had to be taken as to the level of detail required for the process models and how the models should be created and the software system employed. Based on the level of information available and the status of the technologies to be modelled, simple models and relationships were constructed to describe the processes in Microsoft Excel.

Any processing plant can be broken down into a series of connected processing steps or modules. An early decision was taken to model each process step as a discrete module containing technical and economic performance. The modules could then be linked together, based on inbuilt logic and feasibility rules, to form complete biorefinery concepts using process synthesis operations. The modular structure allowed greater flexibility because the configurations were easily manipulated, and additional modules could be added without re-working the entire process model. The background to process modelling and the method chosen for this project is discussed in more detail in Chapters 5 with a description of the process modules in Chapter 6.

Each module model needed to include the following information to enable evaluation of the biorefineries and the identification of the most promising.

- Mass balances – All material flows.
- Energy balances – Heating, cooling and power requirements.
- Economic analysis – Capital and operational costs.

The process model was constructed from a combination of the modules and also produced results on:

- Production cost – Calculated from the capital and operational costs.
- Profit/loss
- Environmental impact - These calculations were carried out by partners Joanneum Research and Joint Research Council at Petten. They provided environmental impact

factors for the complete process chains that were incorporated into the process models to give a more comprehensive evaluation.

- Socio-economic impact - These calculations were carried out by Patricia Thornley at Aston University who provided overall socio-economic models and data that was incorporated into the process models to give a more comprehensive evaluation.

A disadvantage of the modular approach was that the complete biorefinery concepts could not be integrated and optimised (e.g. for heat, water) to the same level as if the complete biorefinery concepts were modelled as a whole. An effort was made to optimise each module separately, such as recycling of water and materials, to try and improve process integration. The aim of the methodology and the models was to carry out a generalised analysis of the biorefinery concepts. It was envisioned that detailed optimisation and design of the most promising concepts would follow on from the results of this project.

3.4 PROCESS SYNTHESIS PART TWO, LINKING OF THE PROCESS MODULES AND RESULTS GENERATION

Once the process modules had been created and modelled, they needed to be linked together to form the complete biorefinery process model, in conjunction with the environmental and socio-economic models. To achieve this, logic and compatibility rules were required within each module to ensure that the biorefineries created were modelled correctly and that only feasible connections between successive modules were made.

In addition there was the requirement for the creation of a user interface to enable flexible process synthesis. This was the page on which the user chose the processes and products to be included in the biorefinery, the scale of the operation, the feedstock and the location of the plant. The outcome on connection of the modules into a viable process by means of the user interface would be detailed results describing the complete process in terms of mass, energy, efficiency, cost, environment and socio-economics.

3.5 PROCESS EVALUATION AND COMPARISON

The final step was to develop a method for evaluating and comparing numerous biorefinery process chains. A technique was required to utilise the results generated by the models to compare biorefinery concepts, on the basis of cost, efficiency, environment, socio-economic and other criteria. The comparison method needed to consider all criteria in a flexible, transparent, repeatable and user friendly way. A method known as Multi Criteria Decision Analysis was employed which is described and justified in Chapter 9. This utilises the detailed information generated by the process model on conversion,

efficiency, costs (capital, operating, production, profit/loss) and also the socio-economic and environmental results in order to rank the biorefinery process chains.

The following chapters will look at each of these steps (shown in Figure 3.1), detailing the available methods, the method chosen for this thesis and how this was applied to achieve the objectives.

4 PROCESS SYNTHESIS

The first step in the methodology for the identification of the most promising biorefineries was biorefinery process synthesis. In Section 4.1 process synthesis is defined followed in Section 4.2 by a literature review of the main process synthesis methods. These are discussed and an assessment made of their suitability for this project as well as their application to similar bio-based design problems (Section 4.3). Finally in Section 4.4 the application of process synthesis to this project is defined. A further description of the application of the process synthesis method is found in Chapter 7 as elements of the process synthesis method, such as the linking of modules and the user interface were created during and after the creation of the module models.

4.1 DEFINITION

Process synthesis is defined as a methodology for the generation or synthesis of processes that thoroughly considers and evaluates all possibilities, according to their cost, performance, environmental impact and any other criteria that are considered important (47, 56, 57, 54). The methodology is based on a set of defined rules or relationships and is rigorous and defined so that previous outcomes can be readily reconsidered

4.2 PROCESS SYNTHESIS REVIEW

Process synthesis is a well established subject in the chemical and process industries and has been studied extensively and applied to many processes (54, 58). Currently process synthesis methodologies are most often applied to specific process areas to improve process integration, intensification and optimisation (47). Examples of this are the optimisation of heat exchanger networks (48, 49), reactor networks (50, 51) and separation trains (52, 53). The scope of process synthesis has widened over recent years to include many more criteria, such as social and environment factors as well as the more traditional economic indicators (54) with a growing interest in its application to the renewable sector.

Process synthesis is an important step in the development of new process designs, as the design of any chemical product begins with the identification and creation of potential production pathways (56). Process synthesis forms the first step in the design process leading to a successful commercial plant and allows the elimination of unsuitable configurations. Throughout the synthesis of production processes, branches are added to the synthesis tree, representing the alternative routes (56). From these branches a flowsheet is constructed and interconnections made between processing activities (55).Hence process synthesis forms the foundation of the movement towards a bio-based economy, since it

deals with the integration of process operations into plants, and plants into existing infrastructures (63).

No two engineers will formulate a process in the same way unless using process synthesis methods, so the defined methodologies given by process synthesis techniques are valuable for groups of people working towards the same objectives (56). The use of a defined methodology ensures consistency and repeatability as the same methodology is applied independently of the operator.

The general tasks in process synthesis were defined by Motard and Westerberg (57) and Li and Krawslawski (54):

- Representation – Is it possible to fully represent the problem to allow all alternatives to be included, but intelligent enough to automatically ignore options that are not feasible?
- Evaluation – Can the different alternatives be effectively assessed against the multi-objective criteria?
- Strategy – Can a strategy be developed to quickly locate the best alternatives?

These tasks form the core objectives for the process synthesis methodology created in order to identify the most promising biorefinery process chains.

4.2.1 KEY METHODS

Process synthesis methods can generally be classified into two groups; optimisation and knowledge based (54). The optimisation approach seeks to find the optimum arrangement for a defined base case superstructure or from a selection of process routes. Knowledge based methods focus on the systematic organisation and representation of the design problem (54, 58). Peters and Timmerhaus (79) illustrate the high level of complexity involved in process synthesis for manufacturing even a single chemical product, by the application of optimisation and knowledge based process synthesis methods to the synthesis of vinyl chloride. In their examples flowsheets are obtained using the hierarchical (knowledge based) and algorithmic (optimisation based) approaches. In comparison, a biorefinery has the potential to produce a large variety of finished products from a variety of potential feedstocks rather than a single product as given in the example. This highlights the complicated problem that biorefinery process synthesis offers.

From the literature numerous process synthesis methodologies were identified (listed in Table 4.1) but these are all a variation on a set of standard methodologies. There are only

perhaps five or six key techniques utilised in process synthesis which are described in the following Sections 4.2.1.1 - 4.2.1.5.

Table 4.1 – Process synthesis methods (56, 59, 61, 64, 68, 72)

Process synthesis methods	
Evolutionary synthesis	Conflict based approach (CBA)
Simulated annealing	Case-base reasoning
Genetic algorithms	Reactor network synthesis
Expert panel	Separation train synthesis
Implicit enumeration	Process network synthesis
Superstructure optimisation	Reaction path synthesis
MINLP Mixed integer nonlinear programming	Graph theoretic superstructure generation
Expert systems	Evolutionary modification
Combinatorial	Means-end analysis
Heuristics	The Onion model
Artificially intelligent (AI) methods	Phenomena-driven design
Hierarchical decomposition	Product driven synthesis
Design rationale	

4.2.1.1 OPTIMISATION BASED APPROACH

Optimisation based methods generally use a mathematical algorithmic approach to describe the problem and find the optimum solution. A common feature of these methods is the formal, mathematical representation of the problem followed by the use of optimisation (54) in order to achieve the objective.

In these methods the development of the optimum design is based on the determination of the objective function to be maximised or minimised (79). The objective function is usually an economic performance measure, for example, maximum profit. The methodology aims to identify the configuration, based on a set of representative equations, which achieves the optimum value for the objective function. This method is purely mathematical and quantitative.

The advantage of optimisation based process synthesis is the systematic framework that is applied to the process synthesis problems which allows rigorous analysis (54). The same framework may be applied to numerous problems in a consistent manner. Optimisation methods are very effective, so long as the objectives and problems are well defined (54).

A disadvantage of this approach is that it is not able to automatically generate flowsheets (54) and it requires substantial computational effort (54). Optimisation based methods have difficulty dealing with under-defined problems and uncertainties that result from multi-objective analyses (54) and in many cases integrated models are too complex to solve directly, and have to be broken down into small subsystems (63). Another problem with

this method is ensuring that the options under consideration are fully representative of all the options in order to achieve the optimum design (58).

4.2.1.2 HEURISTIC APPROACH

Heuristic methods are based on the long term knowledge of researchers and engineers (54). These methods apply heuristics or rules of thumb to reduce the number of possibilities until the final result is obtained. The heuristic approach relies on knowledge, intuition and physical principles (54) to systematically rule out processing options. The flowsheet evolves as the heuristics are applied until the final arrangement is reached. In the past, this was the most common form of process synthesis, but this has changed with the introduction of more quantitative and scientific methods aided by mathematical programming (79). A disadvantage of the purely heuristic approach is that the decisions rely purely on the knowledge and expertise of those present, and will vary according to the opinions of the decision making group. The end results are not reproducible and the level of consistency could also be questioned.

Following on from the purely heuristic approach, is the application of heuristic rules at different design stages to generate the alternatives (54). This method is called the hierarchical heuristic method. A disadvantage of this method is the sequential structure which makes it impossible to view or manage the interactions between different stages in the process design (54). This causes problems in handling design problems with multi-objective outcomes and heuristics are not guaranteed to find the best design (54). An example of the application of heuristics to a process synthesis problem is given by Douglas (60) in which heuristics are applied to the hydrodealkylation of toluene. This example applies a defined list of heuristics to the problem. Hierarchical heuristics are appropriate for well defined problems, but the rules of thumb may not be applicable to under-defined or more innovative processes.

4.2.1.3 MEANS-END ANALYSIS

In this method the beginning and end conditions of the feed and products are known. Means-end analysis begins with the starting chemical state of the feedstock and successively applies transformation operations to produce intermediate states with fewer differences until the final product is achieved (54). The differences between states include the amount, the concentration, temperature, pressure and form (54). Means-end analysis was used as an early systematic approach for flowsheet synthesis (54). The main disadvantages of this approach include the inability to consider all of the property changes

included in a complete flowsheet and some are temporarily ignored (54). This means that important processing steps may be neglected from the calculations. This method is strongly limited as it excludes the influences and effects on other properties and it cannot guarantee a feasible flowsheet (54). It would not be suitable for application to biorefinery process synthesis, as the problem is too complex and all the options could not be considered. In addition the end products of the optimum biorefinery are not yet known, making it near impossible to apply this method to all the possible combinations.

4.2.1.4 CASE BASE REASONING

Case base reasoning imitates human reasoning and aims to solve new problems by applying old solutions to past problems (54). This is a knowledge based approach that reuses results and experience to match the new problem against old solutions (54). If the proposed solution does not meet the requirements then the problem and solutions are adapted until an agreeable solution is met (54). The main disadvantage is the strong influence of the old decisions on the result (54) and due to the fact that this method relies on old solutions, it does not support innovative design (54). The adaptation of problems and solutions also leads to insufficiently accurate results as there are no defined methods for carrying out these adaptations (54). This method would not be suitable for biorefinery process synthesis, as past biorefinery solutions do not yet exist, making it very difficult to carry out effective biorefinery process synthesis.

4.2.1.5 EXPERT SYSTEM

An expert system is a knowledge based form of process synthesis. The creator of an expert system takes knowledge from experts about the processes including procedures, strategies, data and rules of thumb applicable to that field (61). The knowledge is built into a so-called “expert system” that solves the problems in the same manner as a human expert (61). An expert is defined as someone with a high level of expertise in that particular subject area and who is significantly better than novices at problem solving in that field (61).

The knowledge base forms the core of the expert system with the knowledge organised in order to simplify decision making by the use of facts and rules (also known as heuristics) (61). Expert systems are often built using programming languages such as FORTRAN or PASCAL (61). An advantage of an expert system is that they are derived from experts in that particular research area so the solutions are accurate. Expert systems allow consistent, reproducible results through the use of a structured system (61). Expert systems tend to be

flexible and can grow incrementally to meet the needs of the particular user (61). When creating an expert system it is essential that the goals are well defined, in order to create a useful system.

4.3 APPLICATION OF PROCESS SYNTHESIS TO BIOREFINERIES – LITERATURE REVIEW

There has been extensive research in the area of process synthesis, but most has been about well defined chemical problems (54). There has been little published work on the application of process synthesis to the area of biorefineries. The extent and complexity of the biorefinery problem becomes clear when the numerous options for feedstock, processing and products are identified. If those included within the Biosynergy Project alone are considered there are the potential for 3252 different process configurations.

It is only recently that the field of process synthesis for biorefineries has started to receive some attention. The small amount of work identified in the literature on this topic may be due to the relatively poor understanding of biorefineries and the level of complexity involved in solving biorefinery process synthesis problems. It became clear that there was the need for a process synthesis methodology to sensibly generate and analyse biorefinery process chains, in order to identify the optimum configuration. When generating biorefinery process chains the process synthesis tree resembles Figure 4.1, with different possibilities represented by the different branches; beginning at the feedstock there are a number of options for pretreatment, followed by a number of options for processing and so on.

In the literature, it is widely acknowledged that there is a requirement for the application of process synthesis techniques to the identification of optimum biorefinery configurations (72, 46, 68, 47). It is agreed that current process synthesis methods may not be supportive of this innovative application (72) and that new approaches to process synthesis may have to be taken. There has even been the suggestion by Chen (62) of a new branch of engineering to meet the needs of a bio-based economy, which he calls Industrial Biosystems Engineering (IBsE). This proposed subject group is entirely for the design and management of biorefinery systems and highlights the requirement for integration between multiple disciplines to create successful biorefinery plants. For example, improved integration is required between feedstock producers, industry stakeholders and end-product users. The suggestion of a whole new subject group illustrates the importance and scope of biorefinery research for the development of a sustainable future.

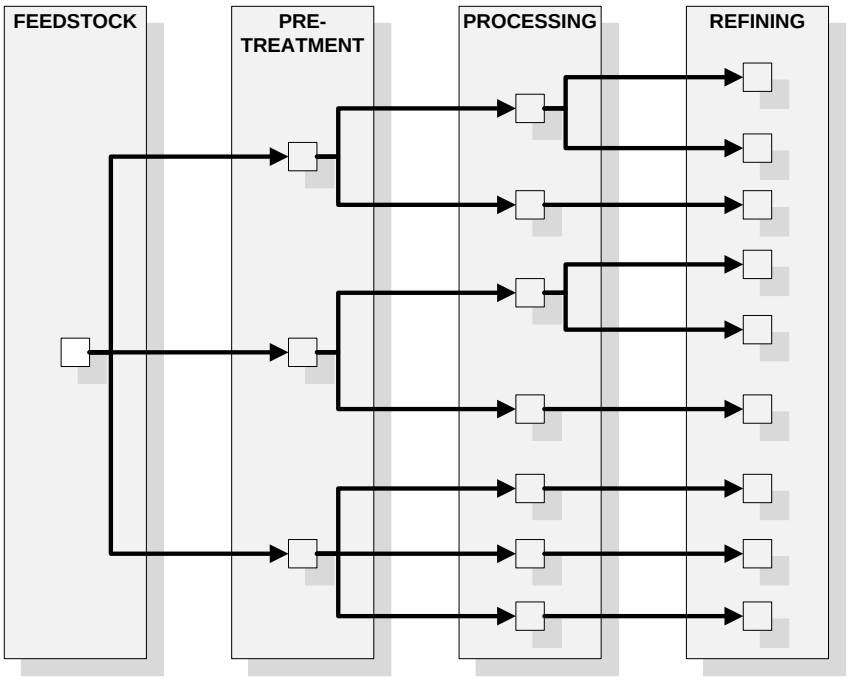

Figure 4.1 – Biorefinery process synthesis tree

In the paper by Kokossis and Yang (72) they identify the need for process synthesis to coordinate a concept based analysis prior to detailed evaluations and flowsheet designs. They state that something is required that will allow users to make a quick assessment before spending valuable time and resources on detailed design studies. A quick assessment will allow users to make rapid judgements and help direct research efforts in an attempt to avoid "dead-ends" (72). The methodology created for this thesis will aim to make this possible.

Most of the applications of process synthesis to renewable or bio-based technologies involve optimisation based methods, as described earlier in Section 4.2.1. These methods use complex algorithms to solve the problem of biorefinery process synthesis and are often targeted to achieve maximum economic performance (64, 65, 69, 71). The research tends to focus on a small number of alternative processing routes for a defined feedstock (64, 68, 69) or alternative integration options (63, 46, 70, 69) based on a defined feedstock and product portfolio.

Work with similar objectives to this thesis was found in the papers by Sammons et al. (68, 69). Their work illustrates the application of optimisation based process synthesis in the form of a methodology to identify the optimum product portfolio for a given feedstock. The aim of their methodology was to enable decision makers to evaluate different production pathways to maximise profit and minimise environmental impact. The methodology was based on a library of knowledge in the form of process models and

performance metrics. The models were then utilised in a mathematical optimisation methodology to identify the optimum product or mix of products. Sammons' mathematical optimisation methodology used algorithms to describe the processes and make calculations to judge the optimum. Sammons illustrates the method by applying it to find the optimum product or products from chicken litter (68, 69).

An advantage of the method used by Sammons (68, 69) was the consistency of analysis. The same methodology was applied to each of the biorefinery options. A disadvantage of the method was that the complete processing schemes and models had to be added to the library on a case by case basis. This is time consuming and limits the flexibility as even within each case there may be further options for process configurations, such as alternative pretreatment methods. It was not possible for the user to define the biorefinery configurations and the analysis was limited to only those cases defined in the model library. It was not made clear by Sammons whether more possibilities will be included in the finished library so it may not be assured that the optimum route has been included in the analysis. Their method requires a high level of system knowledge in order to understand how the relationships and results were derived using the complex algorithms. When assessing the options only the economic and environmental impacts were considered, whereas for the creation of real biorefineries it is likely that many more criteria would be considered. Sammons method of process synthesis may be more suited for further optimisation of biorefineries that have already been identified as promising using.

Another example of optimisation based process synthesis was found in the work by Ng (64). The objective of the work by Ng (64) was to find the configuration of a biorefinery based on a set of target objectives using an optimisation based automatic targeting procedure. His work had similar attributes as for the methods required for this thesis in that differing objectives could be tested. Ng also supports the idea that a biorefinery that produces the most product or products may not necessarily be the biorefinery that gives the most profit. Ng's method was used in this paper to determine the maximum biofuel production and profit levels in an integrated biorefinery. His automatic targeting procedure used a pinch point type analysis to reach the targets. A number of technologies with assumed conversion rates were included for illustration. The automated targeting approach was then applied to these technologies according to the particular objective. In this paper Ng used the example of identifying the optimum biorefinery to give the maximum production of a single product from a given amount of biomass. The processes were described using algorithms and a mathematical solver is employed to calculate the

optimum. A cascading series of algorithms were solved and the optimum route identified from the results.

An advantage of the pinch point type analysis used by Ng (64) was that is helped identify process bottlenecks. It has potential for expansion to study more process routes and to include other factors and objectives such as environmental results. Disadvantages of this method are that the process routes included were very simplified, with only one main product. Ng's method did not have a high level of flexibility and to include all possibilities would lead to an increasingly complex system. The use of a mathematical solver meant that the method was not particularly user friendly, and any users would require training in order to properly utilise the system and understand the algorithms. Similar to the previous work by Sammons (68, 69) due to the relatively small number of configurations considered, there was no guarantee that the optimum biorefinery had been included.

Other examples of optimisation based process synthesis work can be found in the papers by Rentizelas et al. (65), Alvarado-Morales et al. (46) and Halasz et al. (66). The limitations of these optimisation methods include the lack of transparency. Their work involves highly complex algorithmic relationships, making it difficult for the user to follow the logic without time consuming training. These methods also have limited flexibility as biorefineries must be included on a complete case by case basis.

A different approach to process synthesis and modelling has been taken by Klein-Marcuschamer et al. (67). Klein-Marcuschamer applies a superstructure approach to process synthesis in which the overall process has been defined but will evolve to a more efficient process as new information becomes available or new developments are made. Klein-Marcuschamer constructed a model for the processing of biomass to bioethanol which has been made available to the research community. Their model is claimed to be interactive and dynamic and will be updated as new information is provided by the user community. The aim of their work was to produce a transparent, transferable and flexible tool that allowed users to carry out comparative analyses for themselves by using the model to generate results. The tool was for widespread and repeated use, rather than providing a defined set of results. Their model would allow evolutionary process synthesis to take place as new knowledge is implemented in the base case over time to create the optimum configuration.

It was noted that the integration between different processing routes was uncommon in the literature with most processing paths studied in isolation (72). For example, in most cases

it was not possible to combine thermochemical and biological processing routes, with the utilisation of side streams and residues often omitted altogether. These streams may be crucial for the success of the plant and to improve conversion efficiency. The optimisation methods used in the majority of the literature found on biorefinery process synthesis were more suited for application to a smaller number of configurations. This method may prove useful for optimisation work once biorefineries have been identified as promising in order to improve overall integration and efficiency.

The work found in the literature do not take into account the fact that the base cases chosen may not be optimum; processing of that particular feedstock into that particular product may not be the best route. There is little possibility for flexibility of feedstock or product portfolio based on user interaction, and these analyses are likely to only be relevant to a particular location where that specified feedstock is readily available. To carry out a full analysis of each of the possible configurations using the methodologies found in the literature would be too time consuming and highly complex. In addition there was often no consideration of other factors such as environmental, socio-economic and market performance.

A biorefinery process synthesis method was required to systematically generate and assess the options for biorefinery configuration, beginning at the feedstock and moving through to the finished products. One of the most important factors was to ensure that all possibilities were considered within the system, to ensure that the optimum arrangement was included. It was important for the system to be highly flexible so that it could evolve and easily include more technologies as new developments were made.

4.4 APPLICATION OF PROCESS SYNTHESIS METHODS TO THIS PROJECT

Having investigated the various process synthesis approaches, a method was chosen for this thesis. The key requirements of the methodology are described in the following section, followed by the choice of method (Section 4.4.3) and application to this thesis (Section 4.4.3.2).

4.4.1 REQUIREMENTS

The key requirements of the process synthesis methodology for this thesis were:

- Flexibility – The method chosen had to be capable of evolving over the project lifetime to include new technologies and information as this became available.

- Applicable to the modular approach – A modular approach to the modelling was chosen at an early stage in the project (see Section 3.3) so the process synthesis method had to be compatible with this approach.
- Compatibility with subsequent steps in the overall methodology – The method chosen had to be compatible with the process modelling step and also the process chain evaluation step. In addition, thought had to be given to the potential integration with the socio-economic and environmental models.
- Transparency – The method had to be clear, with the logic behind the system and decisions derived available for audit.
- User interface – It was a requirement of the Biosynergy Project that the system have a user interface, in which the user can generate process chains depending on a particular interest. It was not the aim to produce a static set of results, but to provide a comprehensive and flexible tool that could be implemented by the user to carry out their own investigations.
- User friendly for non-experts – It was a requirement of the Biosynergy project that the system be made available to the project partners. The method chosen had to be user friendly, so that no time consuming or expensive training was required. The overall system was to be utilised by users from different backgrounds who may not be familiar with complex operating systems.
- Transferable –The final system had to be made available to the other partners so needed to be easily transferred and disseminated without the need to purchase expensive software licenses.

4.4.2 DISCUSSION

It became clear from the review of the available techniques and applications in the literature that the most common algorithmic optimisation techniques for process synthesis would not be applicable to this project. The complexity of the optimisation problem would be too great considering the high level of flexibility required within the system. In addition, using the optimisation methods only a relatively small number of technologies could be assessed in the allocated time period for the thesis. The aim of the project was to include as many of the processes as possible from within the Biosynergy Project, and for it to be possible to evaluate as many biorefinery configurations as possible. The methodology had to ensure that no promising configuration be overlooked. These objectives could not be met using optimisation based process synthesis.

Most of the work carried out on process synthesis for biorefineries, examples of which are given in Section 4.3, use complex mathematical algorithms and software, not accessible to the average computer user (68, 69, 70, 71). It was a requirement that the system created for this project be user friendly, transferable and accessible. This was not possible with the algorithmic optimisation approach, without the user receiving training and the purchase of relevant software programs. The complexity of these optimisation systems makes it difficult for a non-expert to use the methodology.

The processes under consideration within Biosynergy were relatively under defined, with many still at the laboratory scale. Current algorithmic based software is not sufficiently developed to allow the creation and analysis of under defined process systems (79). Even in the literature, researchers realise that it is very difficult to achieve a fully integrated solution to the multi criteria biorefinery problem (63, 72) and that there is still significant progress to be made. The algorithmic methods would not be sufficient as they do not support innovation. There was the requirement for a new set of tools to cope with the complexity of this problem (72).

The means end analysis process synthesis method was considered unsuitable because the beginning and end conditions have to be known. For this thesis these were not known and establishing the product portfolio was one of the aims. In addition the elimination of configurations using this method takes place using the physical and chemical properties of the streams only. No consideration is given to other factors such as cost, environmental and socio-economic performance. For this thesis a number of criteria were to be included in the evaluation, eliminating means end analysis as a suitable process synthesis technique.

The case-base process synthesis method was eliminated as it relied on comparison of the new problem to old solutions. These solutions do not exist for biorefinery plants. There was a lack of flexibility and consistency with this method, and the comparisons were time consuming. It was not user friendly, or easily reproducible. For these reasons it was not used for this thesis.

The superstructure method was not suitable for application to this project because there was the requirement to consider many biorefinery configurations, whereas the superstructure method focuses on variations of a single configuration. These approaches to process synthesis could be used to screen the options for a particular part of the biorefinery concept, for example the pretreatment options (72) or for optimisation activities once the

promising biorefineries have been identified but did not meet the requirements of the full biorefinery process synthesis method.

4.4.3 APPROACH TAKEN

4.4.3.1 DESCRIPTION

A hybrid approach to process synthesis was adopted based on the principles of expert systems combined with heuristics, and integrated in a traditional process design approach. In effect a rule-based expert system was created. The hybrid approach taken for this project included the creation of a simple expert system, utilising heuristics or rules for the connection of processing modules. The methodology utilises key aspects of expert systems in conjunction with the creation of process models to describe the processes in more detail. The use of rules or heuristics makes finding a solution much easier and more practical (61) and mean that the system is based on a set of clearly defined assumptions. The approach involved the creation of a process synthesis user interface which takes the user's preferences and presents the options available. The creation of biorefinery process chains involves a series of decisions such as scale and connection of processing units (63). The rules specify how the system reacts to changes made by the user (61) with the steps and decisions taken being transparent.

In order to integrate with the module models and the socio-economic models, the process synthesis elements were created using Microsoft Excel.

An advantage of this approach is the flexibility. As new processes or modules are included new rules and relationships are added; the entire system does not have to be recreated. It is easy to examine the reasoning process and explain the operation with fast system development and de-bugging (61). The use of this method makes it easier for the user to carry out sensitivity analysis by changing the options or situations included. The finished system will allow the user to understand how the variables are related to the finished results (61) as the logic rules and relationships are clearly defined.

This system acts as a "memory" of the Biosynergy project and the status of the technologies included in the project at a particular point in time. It will represent a permanent record of the knowledge of the experts from within the project (61). In addition the method can be updated and developed to provide a long lasting process synthesis tool. The methodologies applied to this problem may also be reapplied to other problems with similar objectives.

4.4.3.2 APPLICATION

A modular structure for the process modelling was chosen, as described in Section 3.3 and in more detail in Section 5.1. The rules and logic built around the processes as part of the process synthesis operations had to fit in with the modular structure. The rules were written into each of the process modules to define the relationships and links, with the connection of the modules controlled through the user interface. The options displayed on the user interface were dependent on the user's choice and were displayed according to the rules applied.

To build the process synthesis aspect of the project, knowledge first had to be obtained from the partners and from literature about the processes to be included. This formed the basis of the creation of the system and from this information the logic and rules could be written. These rules were written based on facts, such as the composition of a particular feedstock, or heuristics (rules of thumb) such as that gasification should not be followed by steam explosion pretreatment. The user interface controls the connection of modules and enables the user to generate process chains based on the knowledge stored within the system (see Figure 4.2).

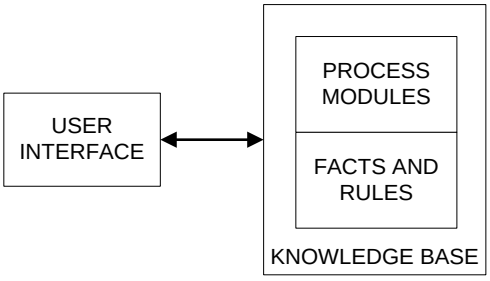

Figure 4.2 – Process synthesis applied to project

The system created was forward chaining, which means that the user begins with the choice of feedstock, and decisions move forward through the process chain until the full process route and products were defined.

The method focused on the use of the IF condition and the THEN action statement within Excel. When the choice made by the user matched the IF part, the action specified by the THEN part was performed. This directed the system as to the calculation or module to include. The elements of an expert system created for this project were relatively basic, in comparison to the sophisticated systems possible (61**)**. Such high levels of sophistication were not required in order to achieve the objectives for this thesis. It is often advantageous not to overcomplicate problems and solutions and an advantage of a simpler system is that it is easier to de-bug and test (61).

The collection and organisation of the knowledge was of great importance in the creation of this methodology. This knowledge base contains the data and rules that are used as the basis for the process chain generation (more details about data collection can be found in Section 5.5).

The application and creation of the process synthesis elements of this project is described further in Chapter 7. In Section 7.1 the creation of the user interface is described, which allows the user to generate complete biorefinery process chains and obtain results describing that particular configuration. In Section 7.2 the inbuilt logic rules and relationships linking the process modules are described in detail.

5 PROCESS MODELLING

This chapter describes the process modelling employed in the overall methodology (see Chapter 3). It begins with a description of the modelling approach and the modular structure chosen for the modelling in Section 5.1. In Section 5.2 a review of process modelling, techniques and software, with the choice for this project detailed and justified. In Section 5.4 the biorefinery concepts chosen for study by the Biosynergy project partners are introduced. In section 5.4.1 the choice of processing for lignin is described based on initial analysis. The collection of data from the project partners and literature is discussed in Section 5.5 including the data validation procedure. The methods for estimating capital, operating, production cost and profitability are found in Section 5.6. In sections 5.7 and 5.8 the environmental and socio-economic models created by Joanneum and Aston are described including a description of the impacts considered.

5.1 MODULAR MODELLING APPROACH

The objective of the process synthesis and modelling methodology was to allow the user to construct a complete and feasible process from feed reception to delivery of end products. The important elements in the creation of the modelling methodology were flexibility and consistency. There was the requirement to allow users of the finished methodology to quickly and easily generate biorefinery concepts and receive results including mass and energy balances, capital and production estimates, socio-economic and environmental impact assessments. These results will allow the user to carry out subsequent analysis and comparison of the biorefinery concepts studied.

Mathematical modelling of processes and plants is a lot less time consuming, less costly and safer than physical modelling (55). It allows the user to carry out virtual experiments looking at the effects of changes to scale, efficiency, costs etc. by adjustment of the variables. The individual process steps were modelled as separate process modules in order to construct a variety of feasible processes by linking of the modules. In order to identify possible modules based on technologies within the Biosynergy project, several biorefineries were broken down into modules with each module representing a unit operation or process step. The module model consists of a mathematical description of the process step which combines experimental information, literature information and assumptions to establish relationships between the process variables and the outputs in terms of performance. The modules were connected together by the process synthesis operations built into the model, based on logic and feasibility rules to create the complete biorefinery process model (see Section 7.2 for more details).

The modelling approach is illustrated in Figure 5.1. The biorefinery concept is constructed from process modules using the user interface. Results are generated by the process modules which form the input for the environmental and socio-economic models. Together the modules, environmental and socioeconomic models form the overall process model. The full results from the process model are then used in the subsequent analysis and comparison step.

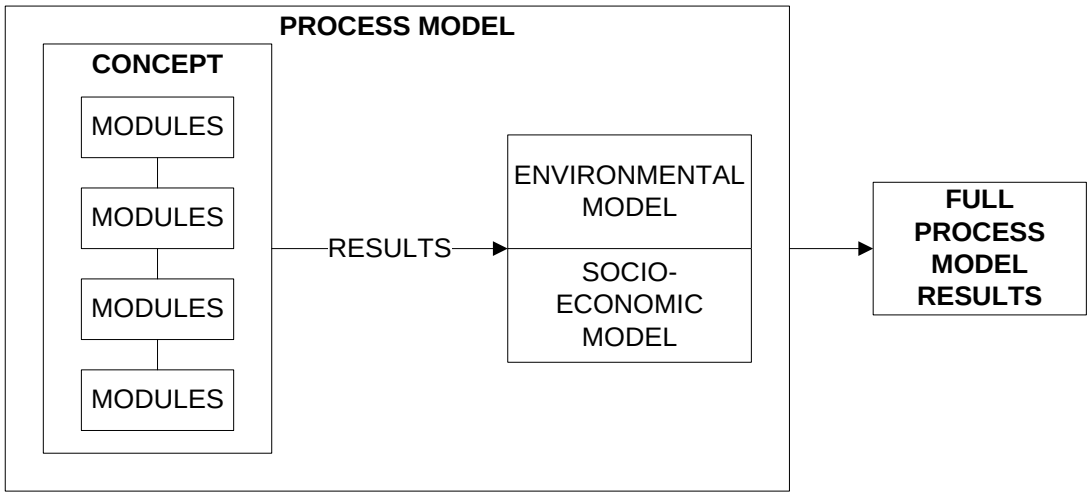

Figure 5.1 – Structure of process model

To model in this way allowed the creation, analysis and comparison of many more options than if each complete biorefinery concept were modelled separately on a case by case basis. It greatly increased the flexibility of the methodology and allowed the possibility of evaluating many more biorefinery concepts in the time available.

Each module only had to be created once, and then used in combination with other modules to create the full concepts. This was beneficial when it came to updates, as only the module had to be changed and not the complete model, which helped minimise the risk of errors. A major advantage of the modular approach was that the methodologies could readily be expanded to include more process modules as the project progressed, by creating a new module and then linking into existing modules using logic rules.

Also included in the modelling were modules for heat and power generation, wastewater treatment and water and residue collection. The heat and power modules may be included to make the biorefinery self-sufficient i.e. all heat and power needs are met using biomass and residues from the plant or to fuel the plant by natural gas and electricity purchased from the grid. The wastewater treatment module was included to estimate the treatment and re-use of process water as high water usage is often a problem associated with biorefinery plants (46). The wastewater plant generates bio-gas which can be used to

provide additional heat and power. The inclusion of these utility modules meant that a complete biorefinery process chain was evaluated. More details of the modules to be found in Chapter 6.

5.2 MODELLING REVIEW

A modular structure was chosen for the process modelling with each processing step modelled as a separate module. Modules were connected using the process synthesis user interface and inbuilt logic rules within the models (see Chapter 7 for more details) to form full biorefinery concepts.

5.2.1 REQUIREMENTS

When choosing the software for creating the module models there were a number of factors to consider:

- The availability of information about the processes to be modelled.
- The level of detail required in the model.
- What results were required once the models were completed and in what format.
- The flexibility required.
- The modular structure chosen.
- The potential to integrate the socio-economic and environmental models with the concept model.
- The requirement for a user interface.

The level of detail included in the model was dictated by the availability of information from partners and literature. It was known that many of the processes under consideration within Biosynergy were innovative and still at the lab scale, so it was likely that the information would not be as extensive as preferred. A compromise had to be made as to the level of detail included in the module models so a simplified approach was taken and in some cases even a black box approach as the exact mechanisms and interactions within the process were still unknown or under investigation. The black box principle is concerned with the main inputs and outputs, and to some extent ignores the interior structure of the process and only focuses on main streams. It was stated in the book by Babu (55) that "A compromise between a rigorous description and getting an answer that is good enough is an engineering compromise carried out when considering process modelling". The models for this thesis were to be simplified, but still provide enough information to enable a sensible analysis to be carried out.

In order to carry out subsequent analysis and comparison, data was needed for each biorefinery concept about:

- Mass balances - All material flows.
- Energy balances - Heating, cooling and power requirements.
- Economic analysis - Capital cost estimation, operational cost, production cost, Profit/loss.
- Environmental impact - Carried out by partners Joanneum Research and Joint Research Council (163, 164).
- Socio-economic impact - Carried out by Patricia Thornley at Aston University (88, 161).

A high level of flexibility was required in order to include as many biorefinery possibilities within the time frame. The technologies and processes to be included were to evolve throughout the project and the model had to evolve at the same time to include the chosen routes, so flexibility was essential. This was one of the reasons for the modular structure and was one of the main factors to be considered when choosing the modelling software. Having a flexible and robust modelling tool meant that the tool could be developed after the project and applied to other processes.

Another consideration when creating the module models was the potential to integrate the socio-economic and environmental models to create one comprehensive system. It was hoped that all the systems would be integrated and therefore compatible software had to be chosen by the partners involved in the modelling.

It was a requirement of the project that the finished system be available to partners and have a user interface to enable users to carry out their own investigations and analyses. This factor had to be taken into account when choosing the software as the finished model had to be accessible, transferable, and user friendly for non-specialists.

5.2.2 PROCESS MODELLING REVIEW

For the creation of the modules and process model there were two broad options when it came to choosing the process modelling software. These were:

- Complex and rigorous models using process simulation software such as Aspen, IPSEpro, HYSYS, CHEMCAD, SUPERPRO DESIGNER.
- Simplified models using standard spreadsheet software such as Microsoft Excel.

These two broad options were investigated and evaluated for suitability. Both options had their advantages and disadvantages and a choice was required before the modelling could begin. The modelling software had to be highly flexible and customisable, as many of the processes to be modelled were new or innovative. It was required that user intervention with the connection of modules and the completed modules themselves be kept to a minimum, to reduce error. Ideally the connection of modules was to be automatic based on the user's choice in a front page user interface.

5.2.2.1 PROCESS SIMULATION SOFTWARE

The first option available for process modelling was to use complex process simulation software such as Aspen or IPSEpro. These are highly powerful and complex tools operated under license from the software developers. The main advantages and disadvantages are shown in Table 5.1. These software programs enable accurate, detailed and rigorous heat and material balances, and in the case of Aspen also provide cost estimations. Due to the level of detail in these models they offer insight into the reaction mechanism and stream behaviour; in effect allowing detailed virtual experiments. These types of software use a combination of process equipment models, physical property estimation models and numerical solvers to create the process models (79).

Table 5.1 – Advantages and disadvantages of simulation software such as Aspen

Simulation software e.g. Aspen	
Advantages	**Disadvantages**
Provides detailed and accurate models in the form of rigorous heat and material balances	Difficult to accurately create models for processes/products not contained in the software model libraries
Gives insight into reaction mechanisms and stream behaviour	Does not easily show how the information is calculated
	Expensive software licence required by user
	Unless already familiar with the software, users would require training in order to use the system

The main features of process simulation software such as Aspen (73, 77, 79):

- Equipment database – This is a library of equipment performance used to simulate basic operating principles to provide material and energy balances.
- Component database – Data bank of physical properties such as reaction kinetics, thermodynamic properties, enthalpy and transport properties.
- Thermodynamic model solver – Used for the calculation of thermodynamic interactions such as vapour-liquid equilibria and stream enthalpies.
- Mathematical solver – Solves the equations that are used to simulate the process operations.

- Main flowsheet program – Controls and keeps track of the flowsheet calculations. This part of the software interacts with the data banks and solvers and controls the order of calculation. This part usually has a graphical user interface.
- Data output generator – Data can usually be exported from the models created in the form of a data table or flowsheet.

Software such as Aspen can provide detailed and accurate models that supply rigorous heat and material balances and in some cases cost estimation. This level of detail is very useful when carrying out a detailed process design, as the exact interactions and behaviour of the process streams is simulated. The models may help highlight and troubleshoot potential problems in the process design.

For this thesis a number of the processes and product streams were new and not included in conventional model libraries, for example aquathermolysis, mechanical/alkaline fractionation or the properties of pre-treated biomass streams. New library data would have to be created about the physical properties of the streams and the processing equipment, which would be difficult considering the uncertainty and developmental stage of these new technologies. For these programs it is imperative that the correct physical property model is chosen; otherwise the results produced by the models are not accurate and cannot be trusted (73, 46) and is often the most influential decision in simulation (73). Assumptions would have to be made which would compromise the accuracy of these models, so in effect they may not be any more accurate than a simple spreadsheet based model. This suggested that a complex simulation software package was of little value when evaluating the biorefinery concepts at this relatively early stage in development. It has been stated that these methods should only be used when they can be applied easily, and when the vigorous models can be justified (56). This was not the case for the Biosynergy project as new model libraries would have to be created and detailed process designs were not required at this early stage in development.

A disadvantage of such a complex simulation model is the transparency and accessibility of the models. It is not easy to look at or understand the inbuilt calculations and assumptions unless the user has undergone extensive training. The calculations are often written in programming code which makes it difficult to quickly assess and troubleshoot whether the correct interactions are being modelled.

There have been a large number of bio-based Aspen models created, especially based around bioethanol production (137, 120, 121, 145, 14, 24). These pieces of work

demonstrate the level of detail that can be achieved and highlight Aspen's usefulness in detailed process design work. They also highlight the disadvantages and demonstrate that custom software often has to be created to deal with the newer and more innovative streams and interactions (137, 74).

One of the objectives of this project was to make the system available to the project partners meaning that it had to be user friendly and easy to operate. This would not be possible with software such as Aspen as most normal computer users do not have access or the training necessary to use such software. Users would lose valuable time learning to use the package (56) and would have to obtain expensive software licenses.

5.2.2.2 SPREADSHEET BASED SOFTWARE

The second option available for process modelling was standard spreadsheet software such as Microsoft Excel or Lotus 123. The main advantages and disadvantages of using a spreadsheet based software program are shown in Table 5.2.

Table 5.2 – Advantages and disadvantages of standard spreadsheet software such as Microsoft Excel

Standard spreadsheet software e.g. Microsoft Excel	
Advantages	**Disadvantages**
Quicker for creation and testing of custom models	Not the same level of detail obtained as for a full simulation model
Simpler model, no detailed thermodynamics or reactions. This is particularly useful for some of the newer innovative processes that are still relatively undefined in terms of thermodynamics.	Model is only as accurate as the data and assumptions made to build it.
Accessible to most computer users	
Not intimidating for users	
No specialist knowledge required	
Easily transferable, can use the models on any computer, not just those with specialist software	
Models are transparent, easier to track and resolve mistakes.	
Excel is a powerful mathematical tool, often underestimated	

One of the major advantages of creating the models in spreadsheet software such as Microsoft Excel was that it is accessible to all and most computer users would feel comfortable when faced with a spreadsheet based interface. Most people are literate in using such software and would not require any time consuming and costly training or software upgrades. Creating the model using Excel means that it is easily transferable; it can be used on any computer and disseminated effortlessly.

It was known that in some cases data availability would not be as extensive as hoped, and a spreadsheet based model would allow for a black box approach to be more easily applied.

It is easier to create custom relationships and simple equations to describe some of the more innovative process steps. All equations and relationships are displayed on the worksheets making the models more transparent and making it easier to track and resolve errors.

A disadvantage of modelling in Excel is the lesser level of detail than from simulation software. Only simple relationships are represented and the complex interactions and thermodynamics of the processing streams are not included to the same level. This could mean that the model may not truly represent the process and the user may miss potential problems. A model in Excel is more than sufficient for a simple techno-economic assessment, but it is recommended that a more sophisticated tool be used for detailed process design work.

5.3 MODELLING SOFTWARE CHOSEN

After consideration of the modular structure chosen, the likely availability of data and the software choices available, modelling using standard spreadsheet software Microsoft Excel was chosen. Microsoft Excel is a very powerful tool, often underestimated by the average user. It was viewed to be more than sufficient for the modelling needs of this project, as a black box principle had to be employed to some extent with complex chemical interactions cut down to simple relationships. The module models were to be relatively simple and include simple mass, energy, efficiency and economic information. Therefore the highly involved and technical modelling software such as Aspen was not suitable. It was stated by Sinnott in Coulson and Richardsons Chemical Engineering Design (77) that "In the early stages full simulation is not justified and simple material balance program more suitable." These simplified calculations and balances enable preliminary flowsheets to be quickly and cheaply produced (77) and during the initial stages of process design simple material balances are viewed to be sufficient (55). It is only at a later stage in development that detailed mass and energy balances and complex interactions and reactions would be required (55). The aim of the project was to give first estimates and guidance, not detailed process designs. It was only at a later stage, once promising technologies have been identified by this methodology that the detailed design work would occur and hence the detailed process simulation work.

In the paper by Hamelinck et al. (75) Excel was used successfully in the techno-economic assessment of different options for the production of ethanol, in particular looking at the performance in the short, middle and long term. Hamelinck et al. (75) used projected

conversions and performances for their medium and long term models. Another example of a spreadsheet based model is given in the work by Nguyen and Saddler (94) where an ethanol production process is modelled to give techno-economic results. They emphasize the point that using such software makes updating and modifying the model relatively simple. In other work by Hamelinck (76) a combination of Aspen and Excel was used to model ethanol based processes. Aspen was used for the thermochemical processes, whereas Excel was used for the biological routes. These papers all demonstrate how spreadsheet based software can be used to successfully model biorefinery processes and provide valuable results for biorefinery evaluation.

Another benefit of modelling in Excel was that the integration of the models created for environmental and socio-economic analysis was simpler. These models would have been more difficult to integrate into a software program such as Aspen and it would be likely that Excel would act as the interface. Modelling in Excel reduces the complexity of the integration.

Each process module was built as a separate worksheet in the Excel workbook named Biosynergy Process Synthesis Model (Appendix 5 on attached CD). The sheets/modules were then connected by the user in the process synthesis user interface worksheet through logic rules and equations built into the module models. Depending on the choices made in the "User interface" work sheet, the front page of the process synthesis aspect, the chosen modules populate and generate the modelling results. The modules are described in Chapter 6 and the logic behind the connection of the modules described in Sections 7.2.

5.4 CONCEPTS CHOSEN FOR BIOSYNERGY

In order to form a starting point for the modelling, to produce some initial results and prove the methodologies, the Biosynergy partners generated complete biorefinery concepts for evaluation. The concepts were generated by the whole group of WP6 partners based on feedback from across the project. They were based on the particular interests of the project and the availability of accurate data to create the models. There was a large focus on cellulosic ethanol to create synergies with other Biosynergy work packages, which focussed on the bioethanol plant of ABNT.

The first 4 complete biorefinery concepts were chosen and agreed by the project partners in July 2008. An additional 6 concepts were chosen in October 2008. These 10 concepts are shown in Table 5.3.

Table 5.3 – The first 10 complete concepts chosen for modelling

Concept	Feed	Pretreatment	C5	C6	Lignin
1	Straw	Steam explosion	Furfural	Ethanol	Fast pyrolysis followed by bio-oil fractionation
2	Softwood	Steam explosion	Furfural	Ethanol	Fast pyrolysis followed by bio-oil fractionation
3	Straw	Gasification	Syngas to ethanol/ mixed alcohols		
4	Straw	AVIDEL	Furfural	Ethanol	Fast pyrolysis followed by bio-oil fractionation
5	Straw	Steam explosion	Ethanol	Ethanol	Gasification to ethanol
6	Straw	AVIDEL	Surfactants	Ethanol	Fast pyrolysis followed by bio-oil fractionation
7	Straw	Organosolv	Ethanol	Ethanol	Fast pyrolysis followed by bio-oil fractionation
8	Softwood	AVIDEL	Furfural	Ethanol	Fast pyrolysis followed by bio-oil fractionation
9	Straw	Steam explosion	Furfural	Ethanol	Lignin pyrolysis to bio-oil (possible integration in conventional refinery)
10	Straw	Steam explosion	ABE	Ethanol	Fast pyrolysis followed by bio-oil fractionation

In March 2009, 16 additional concepts (11-26) were chosen to begin the second phase of the modelling in WP6. The chosen concepts are shown in Table 5.4. Again, these were chosen based on feedback from project partners about the feasibility and information availability. Technologies were chosen based on the knowledge of partners or a particular interest in those particular processes for potential scale-up activities. In July 2009 an additional concept, Concept 0 was added that included the mechanical/alkaline pretreatment process. This concept was added due to specific interest in the mechanical/alkaline pretreatment for scale up (as part of another work package within the Biosynergy project). These concepts formed the basis of the modelling, analysis and comparison work, although the methodologies may be applied to many more configurations.

Table 5.4 – Remaining 16 concepts to be included in WP6

Concept	Feed	Pretreatment	C5	C6	Lignin
0	Straw	Mechanical/alkaline fractionation	Furfural	Ethanol	Fast pyrolysis followed by bio-oil fractionation
11	Straw	Mechanical/alkaline fractionation	ABE fermentation	Ethanol	Lignin dried and sold
12	Straw	Mechanical/alkaline fractionation	ABE fermentation		Lignin dried and sold
13	Straw	Mechanical/alkaline fractionation	Furfural	Ethanol	Lignin dried and sold
14	Straw	Aqua-thermolysis + further processes	Products: furfural, phenolic fraction		
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
16	Straw	Steam explosion	ABE fermentation		Lignin dried and sold
17	Straw	Steam explosion	Xylonic acid	Ethanol	Lignin dried and sold
18	Straw	Organosolv	Surfactants	Ethanol	Lignin dried and sold
19	Straw	Organosolv	Surfactants	FDCA	Lignin dried and sold
20	Straw	AVIDEL	Furfural	FDCA	Lignin dried and sold
21	Straw	Fast pyrolysis	Bio-oil for heat and power in petrochemical refinery		
22	Softwood	Gasification	Fischer-Tropsch synthesis to hydrocarbon fuels		
23	Straw	Fast pyrolysis	Bio-oil gasification --> alcohol synthesis		
24	Straw	Mechanical/alkaline fractionation	Ethanol		Lignin dried and sold
25	Straw	Steam explosion	Ethanol (stillage sold as animal feed)		Lignin dried and combusted
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Lignin dried and sold

5.4.1 LIGNIN

For the second batch of concepts (11-26), the decision about processing of the lignin component was not made immediately. It was important to choose the optimum route for lignin, as it has a large impact on the overall efficiency of the plant, but due to time pressures only processing options from within the Biosynergy project could be considered. It has been stated that using lignin purely for heat and power may not give optimum benefits (38) and the aim of this short study was to evaluate the lignin options within the Biosynergy project. The processing of lignin is one of the most underdeveloped areas within the biorefinery complex and it is recommended that more work be carried out on this area after this project.

In choosing the optimum lignin processing route there were a number of questions that needed to be answered:

- Should fractionation to separate lignin from cellulose be included in the pretreatment step? (see Figure 5.2). Most pretreatment processes offer the option of fractionating the biomass into two streams; a solid cellulose/lignin stream and a liquid C5 rich stream or into three separate fractionated streams; cellulose, lignin and C5. Including the lignin fractionation step is expensive in terms of operating costs and fixed capital investment

so is the increased capital and operating cost outweighed by the benefit of the income from the purer lignin stream or lignin derived products?

- How should the lignin stream be utilised – the best option in terms of performance and cost?

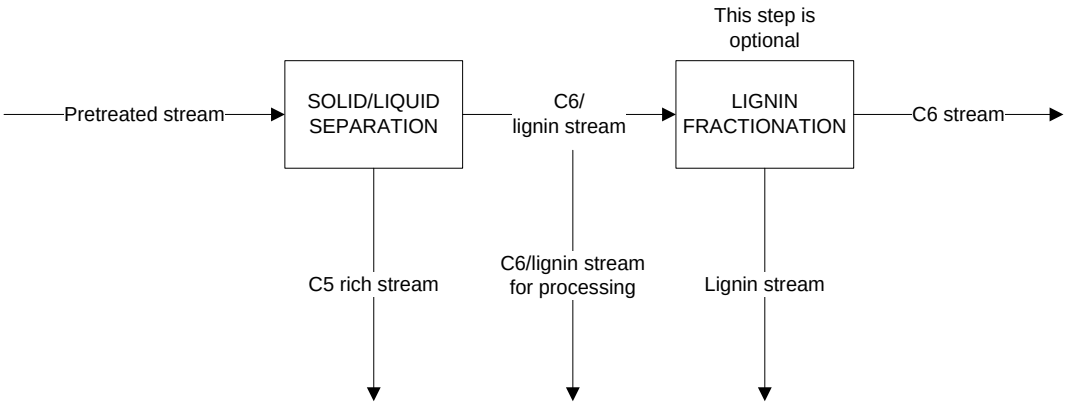

Figure 5.2 – Fractionation of lignin

There were four options investigated for processing lignin. The processing options were based on the technologies included within the Biosynergy project and the time available. These were:

- Biomass pretreatment with fractionation followed by fast pyrolysis of the lignin stream. The bio-oil then fractionated to obtain a phenolic fraction that may be substituted for phenols in phenol-formaldehyde resins.
- Biomass pretreatment with fractionation followed by combustion of the lignin stream for heat and power purposes
- Biomass pretreatment with fractionation followed by drying of the lignin stream. The pure dry lignin then sold as a finished product.
- Biomass pretreatment without fractionation, lignin rich stillage from the fermentation of cellulose/lignin stream to ethanol used for heat and power generation.

In order to identify the optimum route for lignin processing the four lignin options described above were compared, as part of two different biorefinery concepts. The processes were modelled using information available at the time (March 2009) and the results then compared to identify the optimum. Please note the models used for the analysis were at a relatively early stage in development, therefore the results may not match results in the final results section (Chapter 10).

The first analysis was based around Concept 1, shown in Table 5.5 with lignin processed in the four routes described.

Table 5.5 – Lignin options based around Concept 1

	Feedstock	Pretreatment	Lignin fractionation included?	C6	C5	Lignin
1a	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin fast pyrolysis followed by bio-oil fractionation
1b	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin combustion for heat and power
1c	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin dried and sold
1d	Wheat straw	Steam explosion	No fractionation	Ethanol	Furfural	Lignin rich stillage for heat and power

The second analysis was based around Concept 11. The four options are shown in Table 5.6.

Table 5.6 – Lignin options based around Concept 11

	Feedstock	Pretreatment	Fractionation included?	C6	C5	Lignin
11a	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin combustion for heat and power
11b	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin fast pyrolysis followed by bio-oil fractionation
11c	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin dried and sold
11d	Wheat straw	Mechanical/ alkaline fractionation	No fractionation	ABE	Ethanol	Lignin rich stillage for heat and power

The choice of concept used for this analysis was completely arbitrary. Data was generated for these options using the process modules. This data was then used as the input for the decision analysis tool (See Section 9.3) in order to rank the biorefinery process chains (see Appendix 1 for detailed results).

The results indicated that the most promising route for lignin processing from the four options was to include fractionation in the pretreatment step, dry the lignin and then sell it as a dry lignin product. For future work it is recommended that a more thorough analysis be carried out. The analysis for this project was carried out at a relatively early stage, when the models were not finalised. The analyses did not take into account environmental, socio-economic impacts or the markets associated with the finished products. These extra criteria should be included in a more detailed study. Furthermore only four options for processing lignin were considered when there are many other available.

5.5 DATA COLLECTION AND VALIDATION

A large amount of information was required to create the module models and the overall process model. This had to be provided by the project partners or taken from the literature. For each process under consideration enough information was needed to:

- Create mass and energy balances.
- Create a detailed description of the process and the equipment needed.
- Create a cost estimation; capital, operating, production.

The information was provided by project partners where possible. If no information about a process could be provided by the partners, then assumptions were made about the process operation based on information taken from the literature. The data and assumptions were carefully considered as they impose limits on the model and were kept in mind when evaluating results (55).

The flow of information from the project partners/literature through to the generation of the full model results is illustrated in Figure 5.3. This shows how the information was used to construct the process modules and models. This data then feeds into the environmental and socio-economic models to give the full process model results.

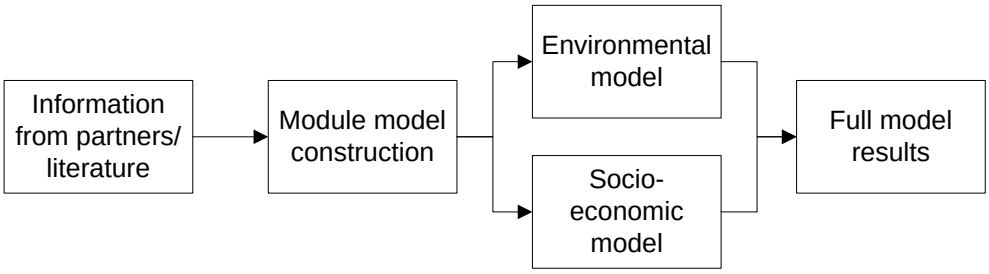

Figure 5.3 – Information flow

To facilitate the collection of data a simple datasheet template was created (Appendix 2). Each datasheet completed by the partner had to include sufficient information to enable a complete process to be constructed or synthesised and included data on performance, costs, products, by-products and wastes in a consistent format. These datasheets were utilised to create the process modules.

The module models created are listed in Table 5.7 as well as the main data source and whether the information used was for current performance or anticipated future performance. The decision was made by the project co-ordinator and the WP6 partners to use anticipated performance where possible. This was due to the fact that many of the processes were still in the developmental stage, and if models were created based on the

experimental results obtained from the project then the finished process would not be representative of the potential commercial process. For this reason partners supplied their anticipated assumptions and data for a process where possible, based on their research experience.

Table 5.7 – Modules and data source

Module	Data source	Current or anticipated data
RSH	Toft (89)	Current
Steam explosion	ABNT, Aden (137)	Anticipated
Fractionation	ABNT, Li (95), Nguyen (94)	Anticipated
AVIDEL	ARD	Anticipated
Organosolv	ECN	Anticipated
Mechanical/alkaline fractionation	A&F	Anticipated
Concentrated HCl	Bioref	Anticipated
Aquathermolysis	ECN	Anticipated
Fluidised bed gasification and gas clean up	ABNT, ECN, Phillips (120, 121), Dutta (122), Boerrigter (114)	Anticipated
Fluidised bed gasification, gas clean up and Fischer-Tropsch synthesis	Kreutz (116), Bechtel (117)	Anticipated
Mixed alcohol synthesis	ABNT, Philips (120, 121)	Anticipated
Mixed alcohol distillation	ABNT	Anticipated
C5 to ethanol	ABNT, IFP, Aden (137)	Anticipated
C5 to ABE	IFP	Anticipated
C5 to furfural	TUD	Anticipated
C5 to surfactants	ARD	Anticipated
C5 to xylonic	VTT	Anticipated
C6 to ethanol	ABNT, Sassner (145), Aden (137)	Anticipated
C6 to ABE	IFP	Anticipated
C6 to FDCA	Bioref	Anticipated
Ethanol distillation	ABNT, IFP	Anticipated
Fast pyrolysis	Aston (AVB), ECN	Current
Lignin drying	Toft (89)	Anticipated
Stillage drying	ABNT	Anticipated
Bio-oil fractionation	BTG	Anticipated
Bio-oil gasification	ECN, Drift (136)	Anticipated
Heat and power from biomass	JR, ABNT, Aden (137)	Anticipated
Heat from biomass	JR, ABNT, Aden (137)	Anticipated
Heat and power from non-renewables	JR, ABNT, Toft (89)	Anticipated
Wastewater treatment	Aden (137)	Anticipated

5.5.1 DATA VALIDATION

To ensure the accuracy of the finished models, validation of the modules and assumptions was essential. Validation was required so that the modelling results could be considered representative of the processes and could be used with confidence. There was still a level of uncertainty associated with the use of the models (see Section 10.1.1) but by validating the models an attempt was made to keep this to a minimum.

To try and ensure that the modules were accurate and representative, upon completion they were sent to the relevant partner for validation. The partner was requested to check over the model and assumptions made, and confirm that they were sensible and in line with

expectations. The vast majority of the processes modelled were being studied within the Biosynergy project, which meant that nearly all of the modules have been checked and validated by partners who are experts in that particular process area.

In addition to validation by the project partners, the modules and module results were compared to literature values (where available). A number of the processes were newly developed, which meant that comparison and validation with literature data was not possible. If a comparison and validation for a module was carried out, this is included in the module descriptions, found in Chapter 6. In this way the accuracy of the modules and models created could be confirmed.

5.6 ECONOMICS

It was important that the economics of the biorefinery concepts were calculated, as this is often the main interest for industrial stakeholders. For each process module the Fixed Capital Investment (FCI) and the Operational Cost (OpEx) was estimated. For a complete biorefinery process concept, the Total Fixed Capital Investment (TFCI) was the sum of the FCI of the individual modules. The TFCI along with the OpEx was then used to calculate the production cost, using a simple equation (see Section 5.6.3). These values, in combination with the income from the biorefinery products could be used to do a simple profit/loss calculation to give an indication of biorefinery profitability. The methods used to calculate each of these costs are detailed in the following sections. All costs were calculated on the basis of Euro (€) value in January 2009.

5.6.1 FIXED CAPITAL INVESTMENT

The fixed capital investment (FCI) is the capital required to supply all equipment and facilities needed to run a process plant. Each module contains its own separate fixed capital investment estimate. To calculate the overall total capital investment (TFCI) for the complete biorefinery concept the cost of each module is added together. Preliminary estimates of fixed capital investment, like those carried out for this thesis, have an accuracy of typically ±30% (77). Garrett states that "these preliminary estimates are for guidance only and high accuracy is neither possible nor necessary. Estimates need to be in the correct range, and if reasonable care is taken this will be the case" (78). It is envisioned that a more detailed economic study would be carried out at a later design stage following on from this thesis to obtain more accurate cost estimations.

The FCI includes the costs for (77):

- Design engineering and construction
- All equipment and installation
- All piping installation and control
- Buildings and structures
- Auxiliary facilities

There are a number of different methods for calculating TFCI. These are often based on the cost of the process equipment required. The chosen method was dependent on the level of detail required and also the amount of information available about the process plant (79). For this thesis a factor method based on the delivered equipment cost was used. This method is commonly used for preliminary estimates (79) and requires the determination of delivered equipment cost for the plant. Other cost items are then estimated as a percentage of the delivered equipment cost.

5.6.1.1 CALCULATING INSTALLED EQUIPMENT COST

The first step was to calculate the installed equipment cost for each module. Where cost data was not available from the partners or from literature, estimates were made from the creation of equipment lists and estimating the installed equipment cost using the estimating charts in the book Chemical Engineering Economics by Garrett (78). For preliminary estimates and where actual equipment costs cannot be taken from quotations these charts provide a good starting point (78). The size and specification of the equipment came from the mass and energy balances and this information along with the required material of construction was enough to make an initial estimate. The module cost (not to be confused with the process modules) was calculated for each piece of equipment (see equation 1). The 'module cost' includes not only the installation cost but the cost of all supporting equipment and connections (78).

Cost of installed module = purchase price * module factor [1]

The 'module factor' was used as the biorefinery plants are likely to be completely new, so all of the supporting equipment and connections would be required. It was assumed that the biorefinery would not be an addition to an existing plant. Where charts were not available for the exact piece of equipment needed, charts for similar equipment were used to give a rough estimation.

5.6.1.2 ADJUSTED MULTIPLICATION FACTORS

The installed equipment cost factors from Peters and Timmerhaus (2003) (79) were adjusted in order to calculate the fixed capital investment for each module. The original factors for a solid-liquid processing plant are shown in Table 5.8 the adjusted factors in Table 5.9.

Table 5.8 – Original capital cost estimation factors (79)

	Fraction of delivered equipment
	Solid-fluid processing plant
Direct costs	
Purchased equipment installation	0.45
Instrumentation and controls (installed)	0.26
Piping (installed)	0.31
Electrical systems (installed)	0.1
Buildings (including services)	0.29
Yard improvements	0.12
Service facilities (installed)	0.55
Indirect costs	
Engineering and supervision	0.32
Construction expenses	0.34
Legal expenses	0.04
contractors fee	0.19
Contingency	0.37
Fixed capital investment	

Table 5.9 – Adjusted capital cost estimation factors

	Fraction of installed equipment
	Solid-fluid processing plant
	Adjusted factor
Direct costs	
Installed equipment	1
Buildings (including services)	0.11
Yard improvements	0.05
Total direct cost	
Indirect costs	
Engineering and supervision	0.12
Construction expenses	0.13
Legal expenses	0.02
contractors fee	0.07
Fixed capital investment	
Additional factors	
Design and resolution of uncertainties	0.20
Permitting (including publicity etc)	0.20
Finance procurement	0.10
Contingency	0.10
Location factor	(dependent on location chosen)
FCI	

The original factors were adjusted to give a fraction of the installed equipment cost, rather than delivered equipment cost. Further factors were added to take into account the additional costs likely to occur due to the development of these new and innovative process plants. These factors were generated in discussion with Prof. Anthony Bridgwater, based on his personal knowledge and experience (80).

The method was adapted slightly on a module to module basis as the information supplied by partners or taken from the literature was not consistent. Information varied from no cost data available to a list of equipment which then had to be used to estimate delivered equipment cost to a complete FCI estimate. The source of the cost estimate and how the TFCI was calculated for each module is shown in Table 5.10.

The cost estimation method is illustrated in Figure 5.4 showing the various stages at which information was supplied. The method was normalised to ensure consistency so that the same factors were applied to generate the estimate for each module.

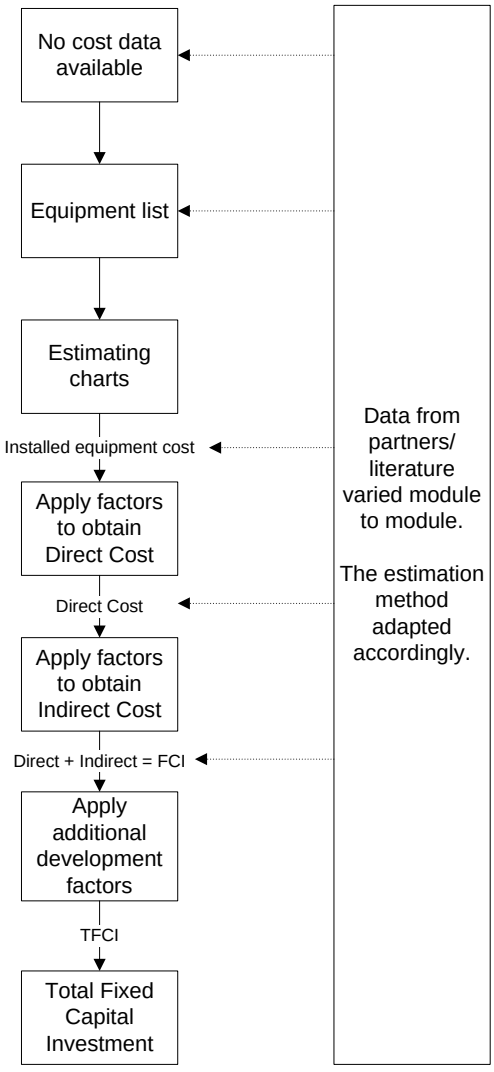

Figure 5.4 – Method for estimating Total Fixed Capital Investment (TFCI)

Table 5.10 – Module FCI estimations

Module	Source of estimate
RSH	Total plant cost based on equations from Toft (89). This gave figures in $k1995. Converted to €Jan 2009 and additional development factors applied.
Steam explosion	FCI given by ABNT. Additional factors applied to obtain FCI.
AVIDEL	By generating equipment list and estimating installed equipment cost. Equipment cost for band extractor provided by ARD. Factors then applied to obtain the total FCI.
Organosolv	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Mechanical/alkaline	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Conc. HCl	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Aquathermolysis	Installed equipment cost provided by ECN. Factors then applied to obtain the total FCI
Fractionation	FCI given by ABNT. Additional factors applied to obtain FCI.
Gasification and gas clean up (prior mixed alcohol synthesis)	FCI given by ABNT. Additional factors applied to obtain FCI.
Gasification and Fischer-Tropsch synthesis	Plant capital cost taken from literature. Converted to € (Jan 2009) Additional development factors applied.
Bio-oil for heat and power	Total plant cost based on equations from Toft (89). This gave figures in $k1995. Converted to €Jan 2009 and additional development factors applied.
Bio-oil entrained flow gasification	Plant capital cost taken from literature (81). Converted to € (Jan 2009) Additional development factors applied.
C5 fermentation to ethanol	Direct cost given by IFP/ABNT. Additional factors applied to obtain FCI.
C5 fermentation to ABE	Direct cost supplied by IFP. Additional factors applied to obtain FCI.
C5 to furfural	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
C5 to surfactants	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
C5 to xylonic acid	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
C6 enzymatic hydrolysis and fermentation to ethanol	Direct cost given by ABNT. Additional factors applied to obtain FCI.
C6 fermentation to ABE	Direct cost given by IFP/ABNT. Additional factors applied to obtain FCI.
C6 to FDCA	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Fast pyrolysis	Equation to calculate FCI supplied by AVB
Lignin drying	Total plant cost based on equations from Toft (89). This gave figures in $k1995. Converted to €Jan 2009 and additional development factors applied.
Stillage drying	Direct cost given by ABNT. Additional factors applied to obtain FCI.
Alcohol synthesis	Direct cost given by ABNT. Additional factors applied to obtain FCI.
Phenolics from bio-oil	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Ethanol distillation	Direct cost given by IFP/ABNT. Additional factors applied to obtain FCI.
Mixed alcohol distillation	Direct cost given by ABNT. Additional factors applied to obtain FCI.
Heat and power	Total plant cost based on equations from Toft (89). This gave figures in $k1995. Converted to €Jan 2009 and additional development factors applied.
Heat only	Total plant cost based on equations from Toft (89). This gave figures in $k1995. Converted to €Jan 2009 and additional development factors applied.
No heat and power	By generating equipment list and estimating installed equipment cost. Factors then applied to obtain the total FCI.
Wastewater treatment	Plant capital cost taken from literature (25). Converted to €(Jan 2009)

5.6.1.3 LOCATION FACTOR

Within the Biosynergy project 5 different countries were chosen for investigation. Cost estimations would vary according to location so an effort was made to estimate the likely differences between the different locations. To do this, different factors were applied to the FCI depending on the country under consideration (chosen by the user in the process

synthesis user interface). These factors were based on expert knowledge from within the project and are shown in Table 5.11.

Table 5.11 – Location factors (80)

Location factors for capital cost	Factor applied to FCI depending on country under consideration
Germany	+10%
Netherlands	+10%
Poland	-10%
Spain	0%
UK	0%

5.6.1.4 PLANT COST INDICES

If information for estimating FCI was taken from the literature, these costs were often given for a different year or currency than the basis taken for this thesis of € January 2009. Cost data is only valid at the time it is created so a cost index was used to adjust to the required date. To adjust the costs between different years the Chemical Engineering Plant Cost Index (CEPCI) was used (82).The CEPCI is an inflation indicator made specifically for the chemical industry to correct the cost of plants (78). The values for CEPCI used are shown in Table 5.12. The equation used to adjust costs between years is shown below in equation 2.

$$\text{Cost in year A} = \text{Cost in year B} \times \frac{\text{CEPCI in year A}}{\text{CEPCI in year B}} \quad [2]$$

Table 5.12 – Chemical Engineering Plant Cost Index (82,83,84,85)

Year	CEPCI	Year	CEPCI
1987	320 (78)	1999	390.6
1988	342.5	2000	394.1
1989	355.4	2001	394.3
1990	357.6	2002	395.6
1991	361.3	2003	402.0
1992	358.2	2004	444.2
1993	359.2	2005	468.2
1994	368.1	2006	499.6
1995	381.1	2007	525.4
1996	381.7	2008	575.4
1997	386.5	Jan 2009	539.7
1998	389.5		

5.6.1.5 SIZE FACTORING EXPONENT

When estimates were required for a scale different from that originally estimated a size factoring exponent of 0.7 was used in the equation shown below in equation 3. This value was chosen based on discussions with industrial partners (IFP, ABNT) within Biosynergy, as this is the factor generally used in industry assessments. This relationship is widely used in making approximations of equipment and plant costs (79).

$$\text{Cost of second size} = \text{known cost of first size} * \left(\frac{\text{size of second}}{\text{size of first}}\right)^{\text{size exponent}} \quad [3]$$

5.6.2 OPERATIONAL COSTS

For each module the operational cost was estimated. The operational cost included anything required to operate the module in terms of feedstock, auxiliary materials and energy. The costs of the auxiliary items are shown in Table 5.13. These costs were supplied by the partners and agreed by the overall project coordinator, as the same values were used across the whole project. These values are based on the Euro value in January 2009.

Table 5.13 – Operational costs

	Cost, €/tonne
Straw	50
Softwood	65
Water	0.08
H_2SO_4 (98%)	72
NaOH (50%)	148
Acetic acid	400
Formic acid	650
Ethanol	700
HCl (35%)	80
Sand	294
C5 yeast	7500
C6 yeast	6580
Toluene	342
Butanol	1000
Growth medium	32
Enzyme (dry basis)	1000
Wastewater treatment chemicals	375
Natural gas €/MWh	24
Electricity €/kWh	0.04
Boiler feedwater chemicals	3045

5.6.3 PRODUCTION COSTS

Based on the operational costs and the TFCI an estimate was made of the production cost. This included the cost of capital repayments, fixed costs and other miscellaneous costs. The annual capital related charges or capital related operating costs are typically between 15-20% of the TFCI (86). This covers repayment of capital and interest over a 10 year plant life and operating costs related to capital investment such as insurance, local taxes and maintenance. While this varies according to location, plant type and time, this is a typical value for Europe. For example it has been calculated that Germany uses 16% for biofuel plants (86), so this was the value assumed for this project. It was also assumed that 90% of the total production cost would be due to the capital operating cost and the plant operational costs, thus 10% would cover labour and utility costs. If the plant is self

sufficient in energy from residue or biomass processing, the utility cost become zero, leaving 5% for labour. Using these factors the equation used to calculate the production cost was:

$$\text{Production cost} = \frac{(\text{OpEx}+0.16\text{FCI})}{0.95} \quad [4]$$

5.6.4 PROFIT/LOSS

Using the potential income from the products and the production cost estimation a simple profit/loss calculation was carried out. The total income minus the production cost gives an indication of the likely profitability of the biorefinery concept. The potential income for the biorefinery was calculated using the European selling price for that particular product (€2009). These prices were supplied by the Biosynergy project partners and are shown in Table 5.14.

Table 5.14 –Product values

Products	Value, €/t
Ethanol	700
Furfural	625
Phenolic fraction	750
ABE mixed product	814
Surfactants	1500
Methanol	300
Butanol	1000
Propanol	300
Bio-oil	175
Lignin	400
Xylonic acid	1000
FDCA	1500
Gasoline	1337
Diesel	1177
Stillage for animal feed	100
	€/kWh
Electricity	0.04
Heat	0.024

5.7 ENVIRONMENT

The environmental sub-model was created by partners JR and JRC. The environmental model generated environmental profiles for the 27 concepts under consideration. The model was built in Excel and included the following impact categories (87, 163, 164):

- Particles - This is a measure of the particulate matter emitted to the atmosphere which has a potential impact on health.

- Abiotic depletion – Abiotic resources are natural resources such as iron ore and crude oil, which are regarded as non-living. Abiotic depletion is calculated based on the reserves and rates of extraction to indicate the level of resource depletion.
- Acidification potential – This measures the potential of the biorefinery to produce acidifying pollutants. Acidifying pollutants have an impact on the soil, groundwater, surface water, biological eco-systems and materials. The major acidifying pollutants are SO_2, NO_x and NH_x.
- Eutrophication potential – This measures the potential impact of the biorefinery delivering excessively high levels of nutrients to the atmosphere. The most important of these nutrients being nitrogen and phosphorous. Excessive levels of nutrients in the environment cause unwanted and elevated biomass production in aquatic and terrestrial ecosystems.
- Global warming potential – This measures the potential of the biorefinery to produce emissions likely to enhance heat radiation absorption of the atmosphere, causing the earth's surface temperature to rise.
- Ozone layer depletion potential – This refers to the emissions from the biorefinery that impact on the thinning of the stratospheric ozone layer. The thinning of the ozone layer allows a greater fraction of solar UV-B radiation to reach the earth's surface, with potentially harmful impacts on the health of organisms, plants and other materials.
- Photochemical ozone creation potential – This is a measure of the air pollutants released that form reactive compounds, such as ozone, by the action of sunlight.
- Primary energy demand (fossil) – This is the direct net energy (LHV) use at the source of materials or supply to the biorefinery. It is desired to use as little fossil energy as possible to obtain the maximum environmental benefits.

The environmental assessments were made for the 27 defined biorefinery concepts only. A summary of the results are given in Section 10.2.4. It was not possible to create environmental assessments of any combination of modules, so the environmental model did not provide the same level of flexibility.

As part of the environmental assessment, JR and JRC compared the biorefinery concepts to conventional routes for production of the same products and services. This made it possible to identify the real environmental benefits and impacts of the biorefinery plants. The results are summarised in Section 10.2.4 and further in the detailed reports by Bird et al. (163,164).

5.8 SOCIO-ECONOMIC

The socio-economic model was created by Patricia Thornley (Aston University) and gave a generalised view of the impact a biorefinery plant had on a particular country (88, 161). The aim of the socio-economic model was to quantify socio-economic parameters for the different biorefinery concepts. The development and operation of a biorefinery facility as well as the feedstock supply chain has an impact on socio-economic factors. Many of these factors will vary depending on the geographic location of the plant. The socio-economic impacts of the biorefinery complexes were analysed for different EU member states chosen and the results included in the evaluation of the most promising biorefineries.

Five countries were chosen by the Biosynergy project for evaluation:

- United Kingdom
- Spain
- Poland
- Netherlands
- Germany

The full summary of potential socio-economic impacts and the level of assessment are shown in Table 5.15. The key focus for the model created was employment and the socio-economic interfaces to existing agricultural and land-use patterns (88).The assessment model was built based on a plant processing 500,000 tonnes per year of dry biomass but could assess any scale chosen by the user.

The impacts were chosen in consultation with project partners to provide an assessment of the relative significance of biorefinery development to regional and national activities for different member states in order to evaluate the potential for development of those sectors.

Table 5.15. Summary of socio-economic impacts (88)

Biorefinery interface	Potential socio-economic impacts	Extent of assessment
Feedstock resource	Impacts on existing market availability and market prices for the feedstock	High level overview
	Viability of feedstock supply	High level overview
Fuel supply	Transport	Detailed assessment
	Logistics	High level overview
	Infrastructure	Not included as assessment required is too site specific for a generic model
Employment	Job creation	Detailed assessment
	Diversification	Not included as assessment required is too location specific for a generic model
	Skills	High level overview
Ecological	Fuel supply	Not included as assessment required is too geographically specific
	Airborne emission	Not included as accounted for in LCA work being carried out by partners
	Noise	Not included as development specific
	Visual impact	Not included as development specific
Public interfaces	Public perceptions	Not included as site/development specific
	Public objections	Not included as site/development specific
Local economy	Contribution to strategic plans	High level overview
	Standard of living	Not included as site specific
	Skills & competitiveness	High level overview
Markets	Products/by-products	Semi-quantitative assessment owing to limited data availability and prediction capacity
	Trade potential	Semi-quantitative as linked to products/by-products assessment
Others	Energy security	Not considered as too site/application specific
	Land-use	Detailed assessment
	Agricultural/industrial interfaces	Detailed assessment

Due to the flexible nature of the biorefinery configurations, this assessment does not consider the variations to staffing patterns that may occur with varying process configurations. It was expected that these would only have a minor impact on the results so generic estimates were made for manning levels of facilities at this scale.

The Excel based socio-economic model was integrated into the Biosynergy Process Synthesis Model (Appendix 5) to create a single spreadsheet based model to provide process and socio-economic results. When choices were made in the process synthesis user interface, the calculations in the socio-economic model updated and generated the socio-economic results. The results of the socio-economic model for the 27 concepts can be found in Section 10.2.5.

6 PROCESS MODULE DESCRIPTIONS AND MODELS

6.1 PROCESS MODULE DESCRIPTIONS

Each processing step was modelled as a separate process module, as described earlier in Section 3.3 and 5.1. The modules are connected to form the complete biorefinery concepts using the process synthesis user interface described in Section 7.1. Each module describes the processing step and takes account of all materials and energy necessary for the operation of that module (see Figure 6.1). In this way, the methodology is more flexible than a case by case biorefinery analysis. If more technologies are to be studied, a new module is developed, rather than a new complete biorefinery model. Each module is flexible; the scale or other process parameters may easily be changed; the module recalculates the balances depending on the adjusted values.

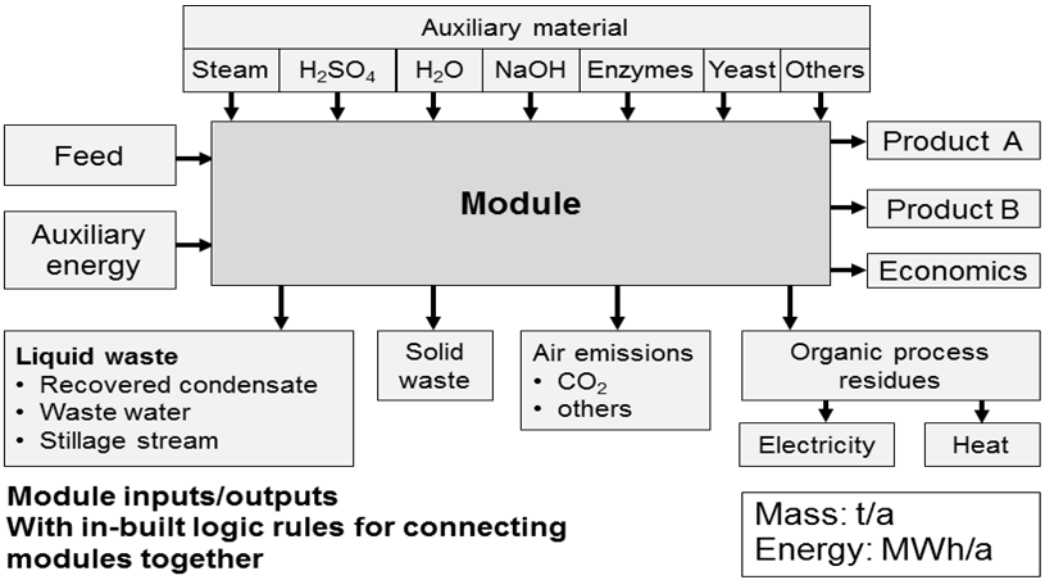

Figure 6.1 – Process module diagram

The information to build the modules was supplied by the project partners over the duration of the project. The information from partners was frequently updated and modified as new developments were made. Where project partners could not provide the information, it was taken from the literature and validated with cross checks. Where partners were studying a particular process, they assisted in the validation and optimisation of the module to ensure that it correctly represented that particular process. It was the decision of the Biosynergy project that the data from the partners used to build the models should be future or anticipated (see Section 5.5 for more details on data collection and validation).

The process steps or modules were created based on the requirement of the project to study defined biorefinery concepts. There were 27 concepts in total shown in Table 6.1; these were broken down into process modules.

Table 6.1 – Full list of all concepts considered

	Feed	Pretreatment	C5	C6	Lignin
0	Straw	Mechanical/alkaline fractionation	Furfural	Ethanol	Bio-oil phenolic fractionation
1	Straw	Steam explosion	Furfural	Ethanol	Bio-oil phenolic fractionation
2	Softwood	Steam explosion	Furfural	Ethanol	Bio-oil phenolic fractionation
3	Straw	Gasification	Syngas to ethanol/ mixed alcohols		
4	Straw	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
5	Straw	Steam explosion	Ethanol	Ethanol	Gasification to ethanol
6	Straw	AVIDEL	Surfactants	Ethanol	Bio-oil phenolic fractionation
7	Straw	Organosolv	Ethanol	Ethanol	Bio-oil phenolic fractionation
8	Softwood	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
9	Straw	Steam explosion	Furfural	Ethanol	Pyrolysis to bio-oil
10	Straw	Steam explosion	ABE	Ethanol	Bio-oil phenolic fractionation
11	Straw	Mech/alk fractionation	ABE fermentation	Ethanol	Dry lignin product
12	Straw	Mech/alk fractionation	ABE fermentation		Dry lignin product
13	Straw	Mech/alk fractionation	Furfural	Ethanol	Dry lignin product
14	Straw	Aquathermolysis + further processes	Bio-oil phenolic fractionation, furfural		
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
16	Straw	Steam explosion	ABE fermentation		Dry lignin product
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
18	Straw	Organosolv	Surfactants	Ethanol	Dry lignin product
19	Straw	Organosolv	Surfactants	FDCA	Dry lignin product
20	Straw	AVIDEL	Furfural	FDCA	Dry lignin product
21	Straw	Fast pyrolysis	Bio-oil for heat and power		
22	Softwood	Gasification	Fischer-Tropsch synthesis to hydrocarbons		
23	Straw	Fast pyrolysis	Bio-oil gasification → alcohol synthesis		
24	Straw	Mech/alk fractionation	Ethanol		Dry lignin product
25	Straw	Steam explosion	Ethanol, stillage to animal feed		Lignin combusted
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

Each module was integrated as far as possible for energy, water and chemical usages. It was not as comprehensive as whole plant optimisation, but this was not possible using the modular methodology. The aim of the modelling was to give indicative figures, not to carry out intensive process design.

In the following sections each module model is described. A block diagram of the process showing main process flows and a process description are given. Detailed process flow diagrams were not included for each module due to the size and complexity of the diagrams. The main assumptions are displayed in a data table for each module and the data source identified.

The modules are connected using the process synthesis user interface described in Section7.1, where the user chooses which technologies are to be included in the analysis. There were logic rules built into the connection of the modules so only feasible connections are made, and to ensure that the correct conversions, mass, energy and economics are calculated. The inbuilt logic rules and process synthesis operations are described in Section 7.2.

6.1.1 FEEDSTOCK RECEPTION, PREPARATION, STORAGE AND HANDLING

This module was included in all of the biorefinery concepts, as all delivered biomass needs to be received, cleaned and stored before being processed further. The block diagram for this module is shown in Figure 6.2. This module was built based on work carried out by Toft (89) and the main assumptions are shown in Table 6.2.

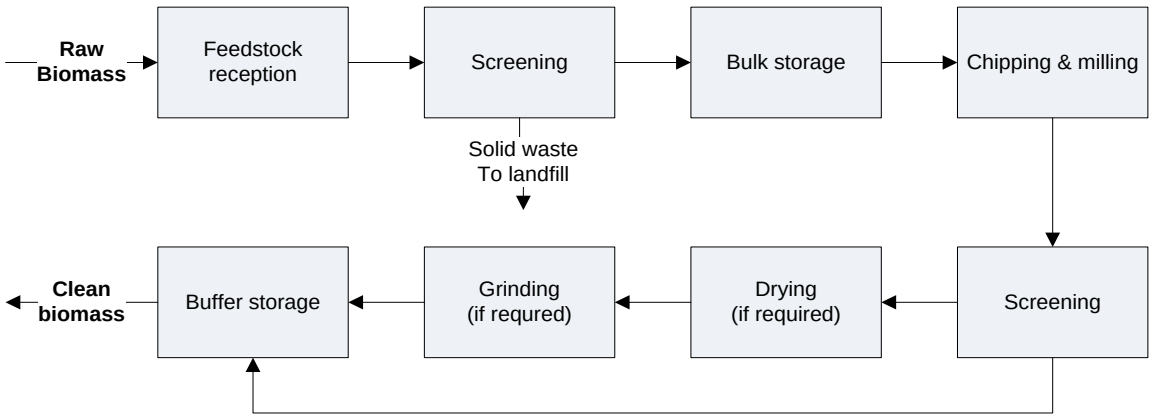

Figure 6.2 - Feedstock, reception, storage and handling block diagram

Following initial feedstock reception is a screening step to remove stones, metal and other debris. It was assumed that 0.5% of the dry biomass input is waste and this solid waste is sent to landfill for disposal. After screening the biomass is sent to bulk storage. There is enough biomass stored in bulk storage to operate the plant for 3 days. From bulk storage the biomass is sent for milling, with the biomass milled depending on particle size requirement of the next step. There is a post mill screen included in which any oversize material is recycled to pass through the size reduction step again. The next step is drying (if required). This is optional and only included if required for subsequent processing steps

(generally drying is required if a thermochemical module is to follow). The moisture level required is dependent on the subsequent module; 35% for combustion, 15% for gasification and 10% for pyrolysis. The heat is provided by hot flue gases (if available) or by low pressure steam. Following drying is an optional grinding step in which particle size can be further reduced; this is required for fast pyrolysis. The final part of this module is buffer storage. There is enough buffer storage for the equivalent of 4 hours operation. From here the biomass is sent to the next process module.

Table 6.2 – Feedstock reception, storage and handling data table (89)

Reception step
Receives enough biomass to operate the plant, plus enough excess to maintain bulk storage of 3 days operation
Screening
For the removal of stones, metal etc
Waste sent to landfill
Assumed that 0.5wt% of dry biomass feed is waste material
Bulk storage
Enough biomass in bulk storage to maintain 3 days plant operation
Chipping and milling
To chip biomass to required size
Post chipping screening
Oversized material is recycled to chipping and milling
Drying
Only required if subsequent processes are thermochemical. Moisture requirement 35% for combustion, 15% for gasification, 10% for pyrolysis
Rotary dryers assumed with maximum capacity of 20 tonnes water/h evaporation load
Grinding
To further reduce particle size after drying. Required if pyrolysis chosen as subsequent module
Buffer storage
Buffer storage capacity equivalent to 4 hours operation

6.1.2 STEAM EXPLOSION

Steam explosion is a thermochemical pretreatment method, which increases the accessibility of cellulose to hydrolysis. It is one of the most commonly used pretreatment processes, due to its low use of chemicals and energy (104). Steam explosion helps break down the lignin matrix that shields the cellulosic fibres and solubilises the hemicellulose (90) to pentose sugars. In this case the steam explosion is catalysed by the addition of dilute H_2SO_4. The block diagram for this module is shown in Figure 6.3. The reactions, conversion rates and other process data are shown in Table 6.3. This module was built based on information supplied by ABNT and taken from the literature (137).

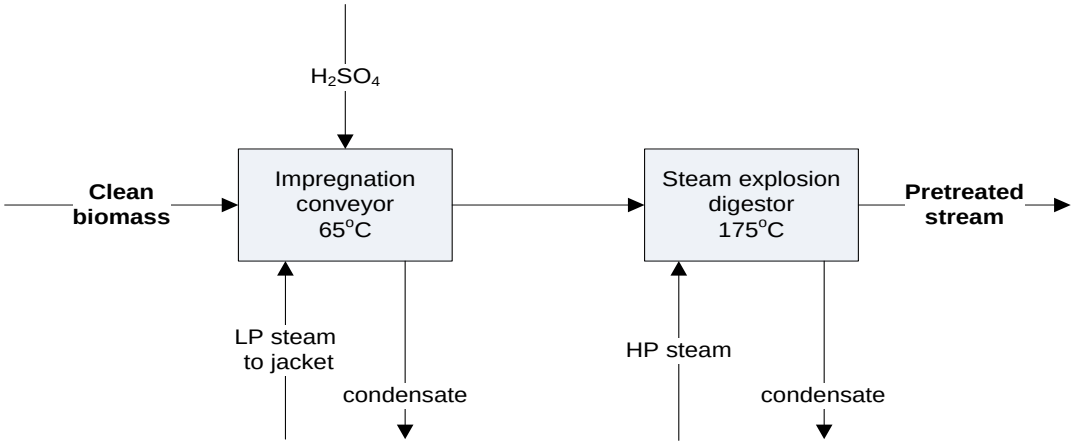

Figure 6.3 – Steam explosion block diagram

Cleaned biomass from the reception, storage and handling module is fed into an acid impregnation conveyor. In the screw conveyor a solution of sulphuric acid is injected and low pressure steam is used to increase the temperature to 65°C. The acid and elevated temperature accelerates the breakdown of the carbohydrate lignin complex. After the straw is well impregnated with diluted acid solution it is fed into batch digesters where the steam explosion occurs. Biomass is held in the digester and high pressure steam is injected which raises the temperature to 150-200°C. The pressure is held and then suddenly released causing an explosive decompression. This breaks down the internal structure of the biomass, releasing the hemicellulose sugars. The hemicellulose is depolymerised and solubilised and then hydrolysed to xylose (91). The process opens up the structure of the biomass allowing better digestion of the cellulose by enzymes (91).

Table 6.3: Steam explosion data table (ABNT, 137)

Impregnation conveyor	
Operating temperature	65°C
H_2SO_4 addition	0.38kg/kg biomass feed
Acid concentration	1% H_2SO_4
Steam explosion digester	
Operating temperature	175°C
Operating pressure	16 bar
Steam input	0.69kg steam/kg feed
Recovered condensate	80% of steam input
Reactions	**Fraction converted**
$(cellulose)_n + {}_nH_2O \rightarrow$ glucose	0.07
$(hemicellulose)_n + {}_nH_2O \rightarrow$ xylose	0.8
$(hemicellulose)_n \rightarrow {}_n$furfural $+ 2_nH_2O$	0.05
$(lignin)_n \rightarrow {}_n$Soluble lignin	0.02

6.1.2.1 VALIDATION

As well as validation by the partners, validation data was collected from the literature and is shown in Table 6.4. The values taken from the literature compare well with the values

used in the module model. The main differences can be seen in comparing the results from Ballesteros et al. (93) to the module and other literature. This can be explained because in the Ballesteros process (93) a stronger acid concentration was used to catalyze the reaction. This led to an improvement in cellulose hydrolysis, but a negative effect on hemicellulose hydrolysis, as the stronger acid caused the production of degradation products such as furfural and acetic acid from hemicellulose, rather than xylose. In addition the ethanol conversions are lower in the Ballesteros work than in the module model and other literature sources. This was due to Ballesteros only carrying out fermentation of the solid cellulose residue and not the liquid hemicellulose sugars.

Table 6.4 – Steam explosion validation data

	Pretreatment		Enzymatic hydrolysis		Fermentation to ethanol		Conversion efficiency		Notes
	Cellulose to glucose	Hemi-cellulose to xylose	Cellulose to glucose	Hemi-cellulose to xylose	Glucose	Xylose	Energy	Mass	
	%	%	%		%	%	%	%	
Module	7%	80%	90%		95%*	85%*	39%	23%	
Sassner et al., 2008 (145)					90%	90%	40%	25%	Salix, SO2 catalysed
Sassner et al., 2009 (145)					90%	90%	42%	24%	Corn stover, SO2 catalysed
Sassner et al., 2010 (145)					90%	90%	45%	30%	Spruce, SO2 catalysed
Piccolo et al., 2009 (14)		75%	80%		92%	80%		27%	Hardwood, dilute acid
Linde et al, 2008 (92)	5%	72%	92%	87%	88%		33%	20%	Wheat straw, dilute acid
Ballesteros et al. (93)	19%		66%	~			17%	10%	Higher conc. acid, only cellulose underwent EH and fermentation

* Taken from fermentation modules

The closest match in terms of processing conditions was the work by Linde et al. (92) and their work confirms that the values used in the module models are reasonable. In the enzymatic hydrolysis of the streams from steam explosion all values compare well, as do the subsequent fermentation conversions. This gives confidence when using the module model, as it compares well to other published work.

6.1.3 FRACTIONATION

The fractionation module follows the steam explosion module and consists of a series of operations to separate the steam exploded biomass into a C5 stream and a C6/lignin stream, or into separate C5, C6 and lignin fractions. The choice of whether to include lignin fractionation is made by the user in the process synthesis user interface (see Section

7.1). The block diagram for this module is shown in Figure 6.4. The lignin dissolution and lignin precipitation steps are optional. This module was based on information supplied by ABNT, and information taken from the literature, specifically papers by Li et al. (95) and Nguyen and Saddler (94). The main process data is shown in Table 6.5

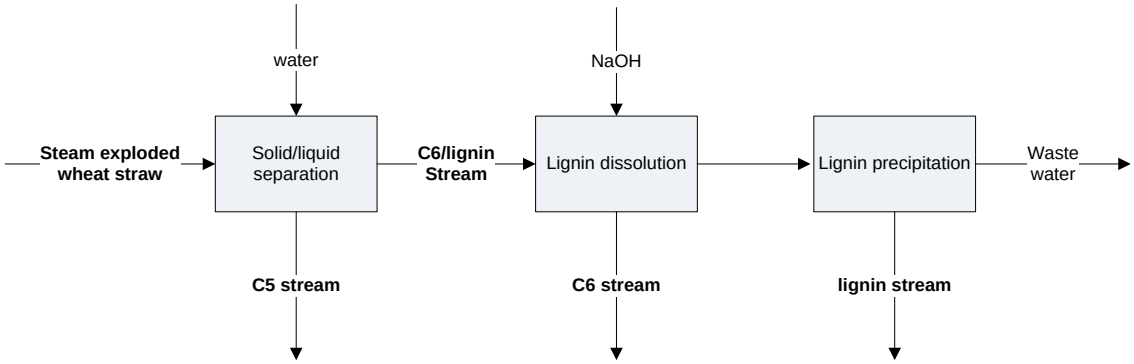

Figure 6.4 – Fractionation block diagram

The steam exploded biomass first undergoes a solid liquid separation in which the liquid C5 stream is separated from the solid cellulose/lignin stream by a counter current washing operation. The C5 enriched stream is then sent to a C5 processing module. The next step for the separation of cellulose (C6) and lignin is optional. It is possible to send the C6/lignin stream to the next module without any additional fractionation or to carry out further operations to result in the separation of the cellulose and lignin.

Where further fractionation is desired the C6/lignin stream first undergoes lignin dissolution. This consists of a caustic wash where a considerable amount of lignin is dissolved. Following this a solid liquid separation takes place in order to separate the C6 rich solid from the lignin rich filtrate. The lignin rich liquid is then sent to a lignin precipitation step. In this step dilute sulphuric acid is added which causes the lignin to precipitate out of solution and the lignin granules are recovered by means of a filter.

Table 6.5 – Fractionation data table (94, 95, 90)

Solid/liquid separation	
Water addition	5.86 kg water/kg feed
Xylose recovery in C5 stream	99%
All soluble lignin in C5 stream	
99% of H_2SO_4 leaves in C5 stream	
Cellulose, hemicellulose and lignin recovery in C6/lignin stream	99%
C5 stream	95wt% water
C6/lignin stream	60wt% water
Lignin dissolution	
Lignin dissolved	85wt%
NaOH addition	0.12kg/kg feed
NaOH concentration	5wt%
Cellulose stream	
Cellulose and hemicellulose recovery	90wt%
Water	60wt%
Lignin precipitation	
H_2SO_4 addition	0.1712kg/kg input to lignin precipitation
H_2SO_4 concentration	88wt%
Lignin product stream	
Water	45wt%
Lignin	54wt%
Other	1wt%

6.1.4 AVIDEL

AVIDEL is a pretreatment method which allows the extraction of raw cellulose by the solubilisation of lignin and hemicellulose in an organic solution of acetic and formic acid. This extraction helps to recover the cellulose without degradation of the lignin to lignosulfonates and hemicellulose to furfural. The block diagram for this process is shown in Figure 6.5. The information to build this module was supplied by ARD and the main process data is shown in Table 6.6.

The biomass stream from the RSH module is first mixed with the organic acids and heated to 105^{o}C using low pressure (LP) steam. The acids cause the solubilisation of the lignin and hemicellulose, leaving the cellulose solids intact. Following the organic acid extractor the stream is sent to a filter, where the solid cellulose stream is recovered. The solid cellulose stream is further washed with recycled acids, followed by a solid liquid separation. This leaves a clean solid cellulose stream and organic acids which are recycled back to the organic acid extraction step.

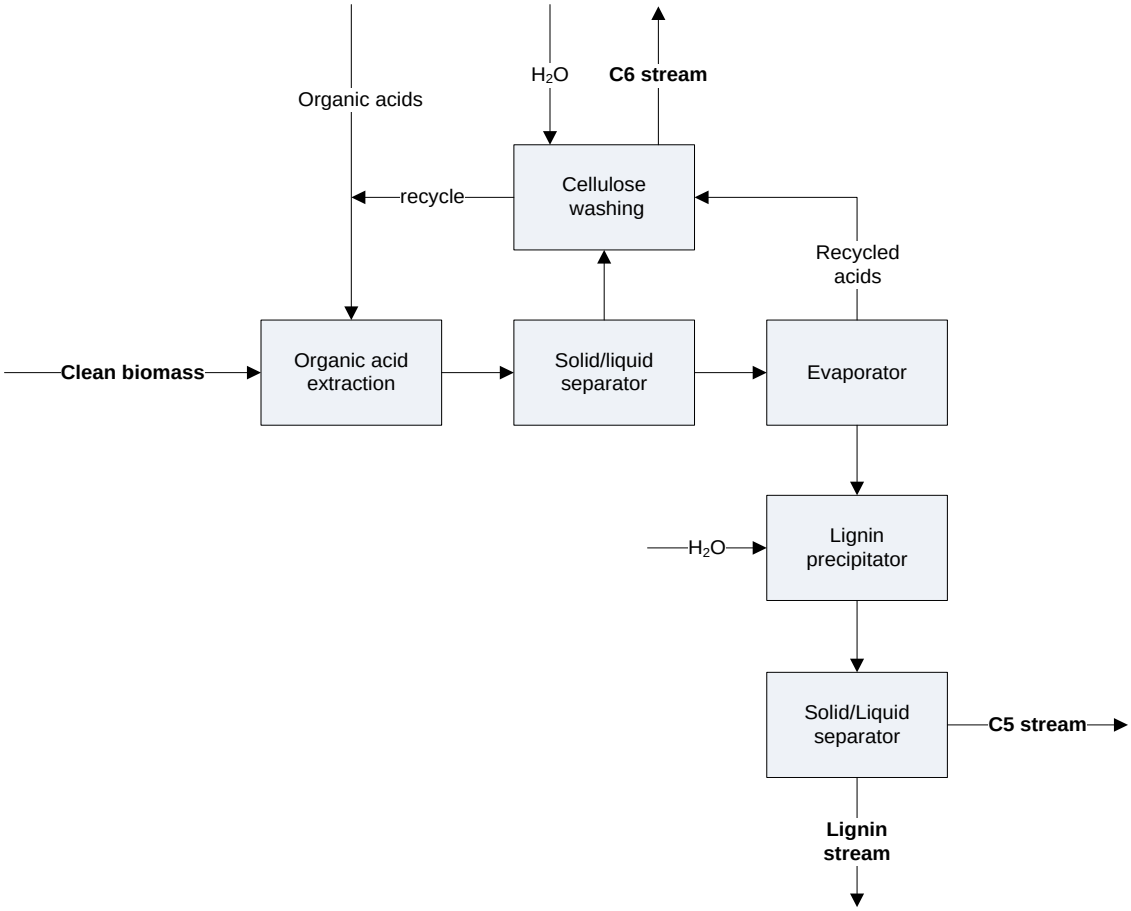

Figure 6.5 – AVIDEL block diagram

The liquid stream containing the solubilised hemicellulose and lignin is concentrated under vacuum to 65% solids to remove the majority of the organic acids. The concentrated liquor is sent to a lignin recovery step which consists of water addition and strong agitation, causing the lignin to precipitate, followed by solid/liquid separation. This leaves a solid lignin stream and C5 rich liquid stream available for further processing (96, 97).

Table 6.6 – AVIDEL data table (ARD)

Organic acid extractor (band extractor)	
Operating temperature	105oC
Operating pressure	Atmospheric
Organic acid addition	5 times biomass input
Acid recovery	98%
Acid composition:	By weight
Acetic acid	50%
Formic acid	30%
Water	20%
Cellulose separation (screw press)	
Operating temperature	Atmospheric
Cellulose recovery	92wt% of cellulose input
Cellulose washing	
Cellulose composition (after wash)	**wt%**
Water	43.3
Cellulose	41.8
Xylans	7.8
Lignin	1.6
Organic acids	4.7
Other	0.9
Juice concentration	
Vacuum concentrator	65oC
Acids recovered from incoming stream	99.9wt%
Lignin precipitation	
Reactor with strong agitation	
Water addition	1kg/kg input
Lignin extraction (screw press)	
Lignin precipitated and recovered	95wt% of lignin input to lignin precipitation
Overall recoveries	
Cellulose recovery	92% of total cellulose input
Hemicellulose to xylose (recovered)	34% of total hemicellulose input
Lignin recovery	88% of total lignin input

6.1.5 ORGANOSOLV

The aim of Organosolv pretreatment is to dissolve the lignin content of the lignocellulosic biomass in order to release the sugar rich hemicellulose and cellulose fractions, and make them easily hydrolysable. Organosolv uses a combination of an organic solvent (ethanol) and water to dissolve the lignin. Removal and recovery of the solvent is required to help reduce the cost, and also because the solvent can act as an inhibitor for the subsequent processes (104). The block diagram for this process is shown in Figure 6.6. The information to build this module was supplied by ECN. The main data points are shown in Table 6.7.

The biomass and solvent are heated to 200^{o}C and pressurised to 32bar before being sent to the Organosolv reactor. Lignin and hemicellulose dissolution occur and the resulting stream undergoes a solid liquid separation. This separates the solid cellulose from the liquid fraction containing lignin and dissolved sugars. The cellulose rich stream is sent to a

flash vessel to recover the ethanol solvent. The ethanol is recycled to the process and the cellulose rich stream is then processed in a subsequent module.

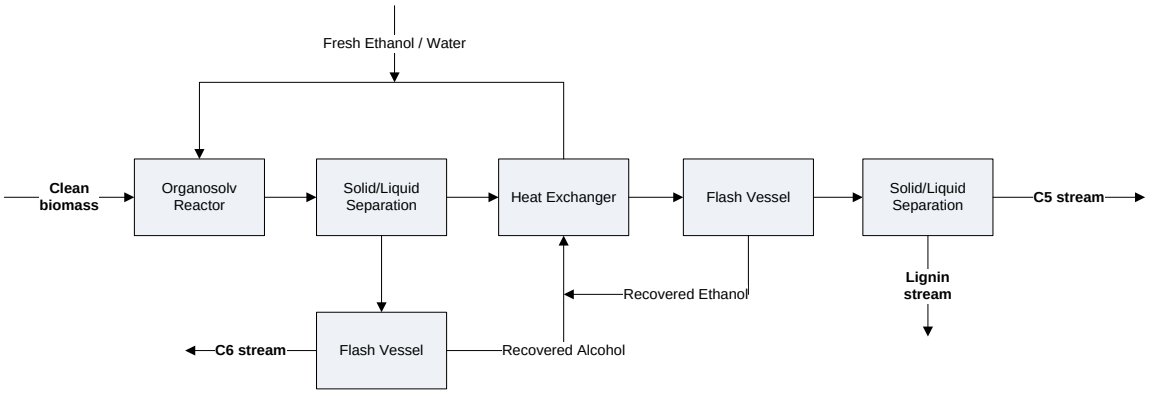

Figure 6.6 – Organosolv block diagram

The liquid stream containing C5 sugars and dissolved lignin is sent to a multistage flash to recover the majority of the ethanol which is recycled to the Organosolv reactor. The lignin and C5 sugar rich solution is sent to a second reactor to undergo lignin precipitation. Water is added, which lowers the ethanol concentration and the lignin precipitates. There follows a filtration in which the solid lignin stream is separated from the C5 rich stream.

Table 6.7 – Organosolv data table (ECN)

Organosolv reactor	
Operating temperature	200^{o}C
Operating pressure	32bar
Ratio of solids: solvent	1 kg solids for 5 litres ethanol (60wt%)
Delignification	80%
Hemicellulose/xylan hydrolysis	50%
Cellulose hydrolysis (in Organosolv reactor)	5%
Other sugar polymer hydrolysis	50%

6.1.5.1 VALIDATION

As well as validation by the partners supplying the data, the module was compared to data taken from the literature. This data is shown in Table 6.8.

The lignin removal achieved in the module is slightly higher than previously achieved in the literature, but this is balanced by the relatively low hemicellulose recovery compared to the literature. The cellulose recovery achieved in the module is comparable to the literature. The enzymatic hydrolysis of the glucose is low compared to that stated in the literature. This is due to experimental results being used in the model, the partners did not feel confident that a higher level could be achieved in the near future (98). In general the module compares well with the validation data.

Table 6.8 – Organosolv validation data

	Lignin removal	Cellulose recovery	Hemicellulose recovery	Enzymatic hydrolysis, glucose conversion	Notes
	%	%	%	%	
Module	80%	90%	50%	66%	
Zhang et al. 2007 (99)	50%	95%	79%		Corn stover, H_3PO_4/acetone
Carioca et al. 1985 (100)	70%		90%	95%	Elephant grass, ethanol
Pan et al., 2006 (101)	74%	88%		90%	Chopped poplar, ethanol, H_2SO_4
Sun et al., 2007 (102)	70%	98%	50%	92%	Wheat straw, glycerol
Papatheonous et al., 1995 (103)	>70%	98%	75%		Wheat straw, ethanol, H_2SO_4

6.1.6 MECHANICAL/ALKALINE FRACTIONATION

This pretreatment method involves performing mechanical and chemical pretreatment in one step (104). This improves the accessibility of cellulose to enzymes, resulting in higher delignification and improved enzymatic hydrolysis (104). The combination of chemical and mechanical action increases the efficiency of the pretreatment with the moderate operating temperatures helping to prevent the formation of degradation and oxidation products. Alkaline pretreatment is excellent for delignification and improvement of enzymatic degradability but less effective for the separation of C5 and C6 fractions (105). The block diagram for the mechanical alkaline fractionation is shown in Figure 6.7. The information required for the construction of this module was provided by A&F and the main process data is shown in Table 6.9.

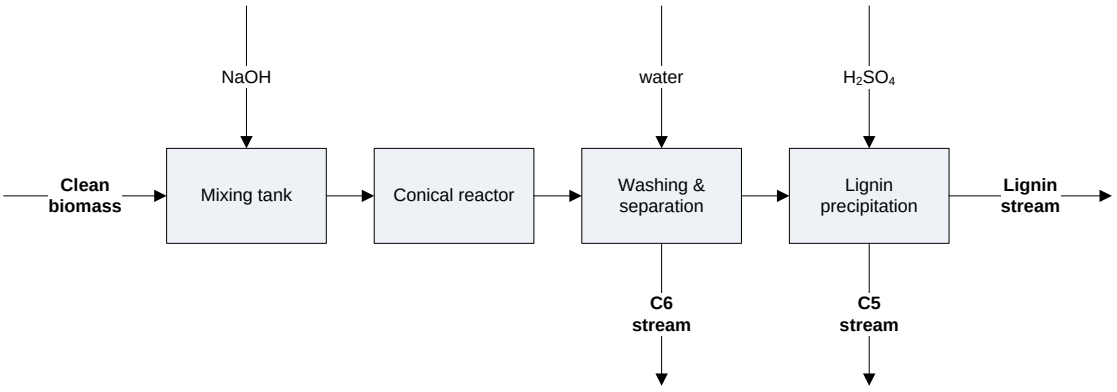

Figure 6.7 – Mechanical/alkaline fractionation block diagram

In the first step the cleaned biomass is mixed with NaOH. Following this the mixture is sent to a conical reactor where it is held at 95^{o}C. The reactor contains a rotating screw running at approximately 60rpm which leads to excellent mixing of the contents and some mechanical breakdown of the biomass (105). In the reactor lignin is dissolved and a small

amount of the hemicellulose converted to xylose. The reacted mixture is sent to a water washing and solid/liquid separation step, resulting in a cellulose rich solid stream to be sent on to further processing, and a C5/dissolved lignin stream. This liquid stream undergoes a lignin precipitation step in which H_2SO_4 is added, causing the lignin to precipitate out of solution. Finally this is filtered to result in a solid lignin stream and a liquid stream rich in C5.

Table 6.9 – Mechanical/alkaline fractionation data table (A&F)

Mixing tank	
Amount of NaOH based on dry biomass content	6wt%
Conical reactor	
Operating temperature	95°C
Operating pressure	Atmospheric
Reactions	Fractional conversion
Hemicellulose → xylose	21%
Solid lignin → dissolve lignin	61%
Ash → dissolved ash	85%
Solid others → dissolved others	50%
Washing and solid/liquid separation	
Water	0.092kg water/ kg reacted stream
Lignin precipitation	
H_2SO_4 addition	0.038kg/kg liquor stream
H_2SO_4 concentration	98wt%
Dissolved lignin precipitated	85wt%
Lignin stream	40wt% water

6.1.6.1 VALIDATION

As well as validation by the partners researching mechanical/alkaline fractionation (106) validation data was collected from the literature about alkaline pre-treatment (Table 6.10) and also mechanical/alkaline pre-treatment (Table 6.11). Mechanical alkaline pretreatment is a relatively new innovation, so literature data was limited. When compared to literature validation data, the conversions achieved in the module model are similar to levels of cellulose, hemicellulose and lignin removal being reported. This reduces the level if uncertainty in using this module model.

Table 6.10 – Alkaline fractionation validation data

	Feed	**Solvent**	**Cellulose yield**	**Hemicellulose removal**	**Lignin removal**	**EH cellulose conversion**
			%	**%**	**%**	**%**
Zhao, Wang et al.., 2008 (107)	Spruce chips	NaOH / urea	91%	40%	19%	70%
Chen, Sharma-Shivappa et al.., 2007 (108)	Barley and wheat straw	NaOH	70-90%	7-40%	20-85%	
Bjerre et al. 1996 (109)	Wheat straw	NaOH		50%	65%	85%

Table 6.11 – Mechanical/alkaline fractionation validation data

	Feed	Solvent	Cellulose yield	Hemicellulose removal	Lignin removal	EH cellulose conversion
			%	%	%	%
Module	Wheat straw	NaOH	99%	22%	61%	86%
Vrije, De Haas et al. 2002 (110)	Miscanthus	NaOH	>95%	44%	77%	69%

6.1.7 CONCENTRATED HCL PRETREATMENT

In this pretreatment method concentrated hydrochloric acid (HCl) is employed as a powerful agent for cellulose hydrolysis. The block diagram for this process is shown in Figure 6.8. The information to construct this module was supplied by Bioref and the main assumptions are shown in Table 6.12.

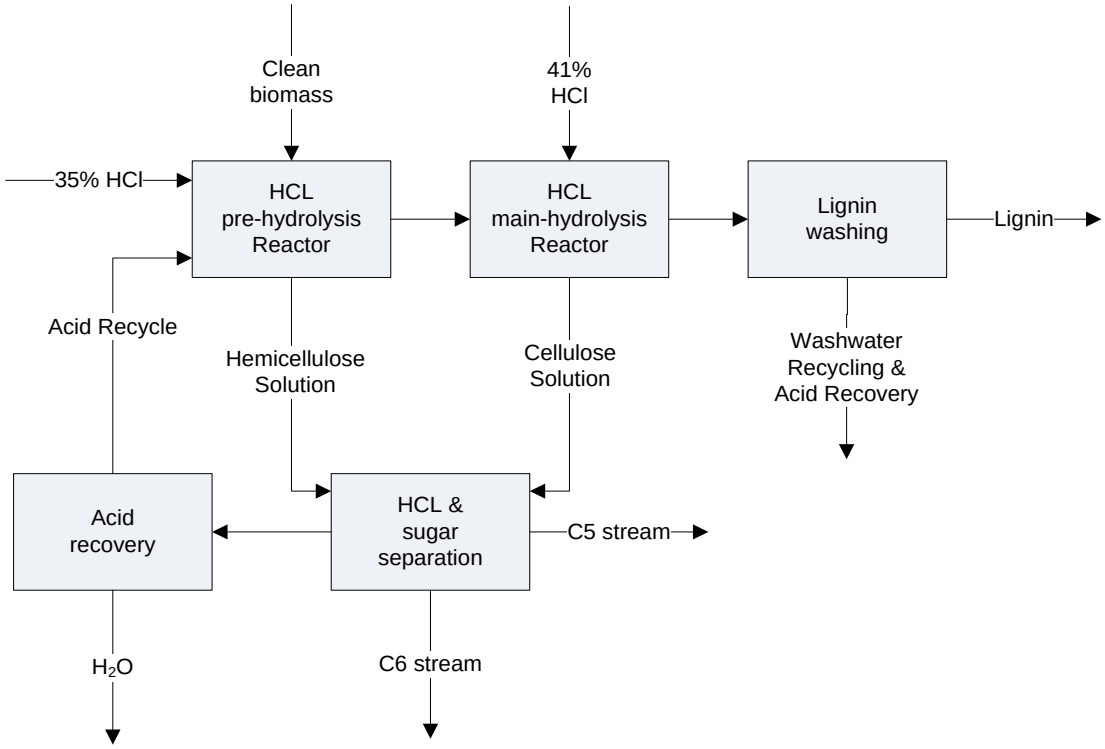

Figure 6.8 – Conc. HCl pretreatment block diagram

The first step in concentrated HCl pretreatment is pre-hydrolysis. In this step hemicellulose sugars are released from the biomass by the addition of HCl (35% concentration). In this pre-hydrolysis step 70% of the hemicellulose is hydrolysed to C5 sugars. The reactor is maintained at a temperature of 20-22^{o}C by means of a cooling jacket. The liquid C5 rich stream is separated from the remaining solid cellulose and lignin. The liquid stream is sent to HCl recovery steps whilst the solid stream proceeds to the main hydrolysis step.

In the main hydrolysis step acid at 41% concentration is added to the cellulose/lignin stream. In the reactor cellulose hydrolysis occurs with 80% of the cellulose converted to glucose and 70% of the remaining hemicellulose converted to xylose. The liquids and solids from this main hydrolysis step are separated to give a C6 rich liquid stream and a lignin rich solid stream. The solid lignin stream undergoes a washing step to further recover sugars and acid, leaving the final lignin product. The HCl is recovered from the C5, C6 and lignin streams by means of vacuum distillation at 45^{o}, 50mbar. The HCl is recycled to reduce the overall operating costs, and to prevent inhibition in subsequent process steps. Once the HCl has been removed the C5, C6 and lignin streams are ready for further processing. One big disadvantage of this process is the use of the strong acid with the negative impacts associated (e.g. toxicity, corrosiveness) (111).

Table 6.12 – Concentrated HCl pretreatment data table (Bioref)

Pre-hydrolysis	
Acid addition	1.25kg/kg feed
HCl concentration	35%
Hemicellulose → xylose	60-80%
Operating temperature	20-22^{o}C
C5 stream	30wt% water
Main hydrolysis	
Acid addition	0.54 kg/kg feed
HCl concentration	37-40%
Cellulose → glucose	80%
Remaining hemicellulose → xylose	70%
Operating temperature	20-22^{o}C
C6 stream	30wt% water
Lignin washing and recovery	
Washwater required	0.5 kg/kg feed
Lignin product	40wt% water
HCl in recycled washwater	2wt%
HCl separation and recycle	
Vacuum distillation	45^{o}C, 50mbar
Based on HCl input, recovery achieved:	
HCl recovered as gas (95% conc.)	45%
HCl recovered as liquid (23.5% conc.)	35%
HCl recovered as liquid (16.2% conc.)	10%
Remaining HCl in sugar streams	10%

6.1.7.1 VALIDATION

As well as validation by the partners supplying the information to build this module, validation data was collected from the literature about concentrated HCl pretreatment. This data is shown in Table 6.13. All values in the literature compare well to the values used in the module model. This indicates that the module model is representative of the concentrated HCl pretreatment method and the results generated can be used with confidence.

Table 6.13 – Concentrated HCl validation data

	Cellulose conversion to glucose	Hemicellulose conversion to xylose	Sugars to ethanol	Acid recovery rate
	%	%	% theoretical *	%
Module	80%	91%	77%	95%
Sivers et al., 1994 (112)	92%	88%	80%	
Hamelinck et al., 2005 (75)	90%	90%		80-97%
Hayes., 2009 (11)	87%	95%		

* Theoretical ethanol yield 0.51kg ethanol/ kg sugars

6.1.8 AQUATHERMOLYSIS

Aquathermolysis involves the treatment of biomass with hot pressurised water. In this process the hemicellulose is removed from the biomass, whereas the cellulose and lignin are relatively unaffected by the treatment. Aquathermolysis focuses on the production of furfural from the hemicellulose (113) leaving a solid residue suitable for further processing, in Concept 14 by fast pyrolysis. A block scheme for this process is shown in Figure 6.9. This module was built using information supplied by ECN and the main assumptions are shown in Table 6.14.

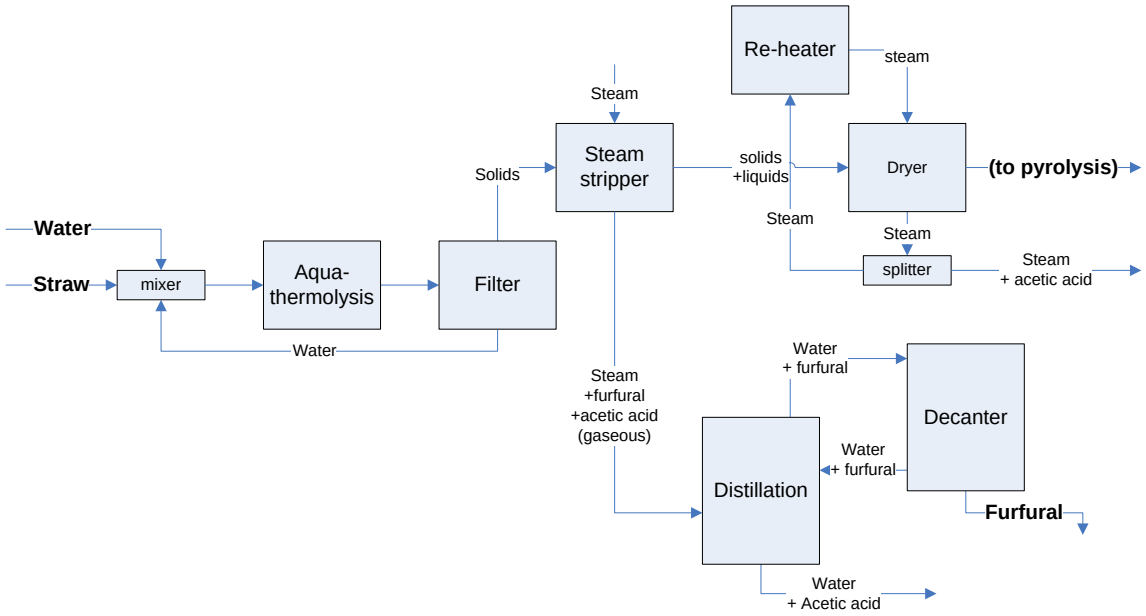

Figure 6.9 - Aquathermolysis block scheme

The first step involves biomass and water being held at 200°C in the reactor. After leaving the reactor the stream is filtered, with the liquid filtrate, consisting mostly of water, recycled back to the aquathermolysis reactor. The "wet solids" stream is sent to a steam stripper to selectively remove the furfural and some acetic acid also entrained into the furfural/water stream. The liquid furfural/water stream from the strippers is sent to a distillation column, where it is split into a furfural product stream and a wastewater stream

(consisting mostly of water). As well as a distillation column, there are two decanters, to help remove the water and improve the purity of the furfural product stream. The solids remaining after the steam stripper are sent to a dryer to result in a lignocellulosic residue, consisting mostly of cellulose and lignin, suitable for further processing in this case by fast pyrolysis.

Table 6.14 – Aquathermolysis data table (ECN)

Aquathermolysis reactor	
Dilution in reactor to	40wt% water
Operating temperature	200°C
Operating pressure	17 bar
Solids to steam stripper	50wt% solids
Reactions	Fraction hemicellulose converted
$C_5H_8O_4 \rightarrow C_5H_4O_2 + 2H_2O$	62.5wt%
$2\ C_5H_8O_4 + 2H_2O \rightarrow 5CH_3OOH$	17.6wt%
Steam stripper	
Steam requirement	0.13kg/kg feed
Furfural removal	100wt%
Acetic acid removal	5wt%
Water removal	25wt%
Distillation of furfural/water stream	
Furfural recovery	99.9wt%
Furfural product stream	99% purity
Solids drying	
Solids dried to	10wt% water

6.1.9 GASIFICATION AND GAS CLEAN UP (FLUIDISED BED)

In this module dried biomass is fed into an indirectly heated circulating fluidised bed (CFB) gasifier. The block diagram for this module is shown in Figure 6.10. This module was built based on information supplied by ABNT and ECN, and from the literature (120,121,122,114). The main assumptions and data are shown in Table 6.15.

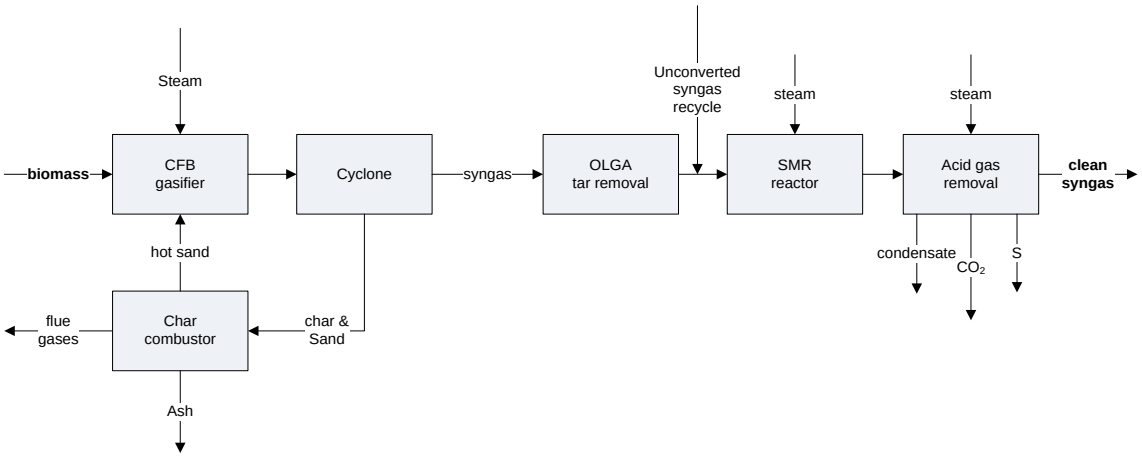

Figure 6.10 – Gasification and gas clean up block diagram

In the gasifier biomass is converted into syngas, tar and char. The indirectly heated CFB employs sand as the fluidising medium and heat carrier. The gasifier operates between 820-900^{o}C and low pressure steam is employed as the gasifying agent. The mass ratio of steam/biomass is 0.4 kg steam /kg dry biomass.

The syngas leaving the gasifier contains various contaminants such as tar and acid gases, which need to be removed before further processing. These contaminants need to be removed to prevent poisoning of the catalysts employed in syngas processing. Directly following gasification the product stream goes through a cyclone to remove char and sand. The char and sand are then sent to the char combustor, where the char is combusted to heat the sand before the sand is sent back to the gasifier. It is assumed that the gasifier is operated in a balanced way, so that all the heat required comes from char combustion.

Following the removal of char and sand the syngas is sent to a tar removal process. The tar is removed by means of washing with an organic fluid (OLGA process). The product gas is cooled, causing the liquid tars to condense and the gaseous tars are absorbed by the scrubbing liquid at this lower temperature (115). The liquid tars are separated from the scrubbing liquid and returned to the char combustor to provide additional energy.

The tar free syngas stream leaving the OLGA tar removal process is sent to a filter to have fine particles and alkalis removed. After this, the gas stream which has been cooled to 60-70^{o}C is compressed to 10-15 bar by means of a multistage compressor. The compressed syngas is sent to a steam methane reforming unit (SMR). This adapts the ratio of H_2/CO by converting the non-reacted gases (mainly methane and other light hydrocarbons) to syngas (CO, H_2) (115). As a result of the SMR process about 70% of methane is converted into carbon monoxide and hydrogen. The equation for this:

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

After the SMR the syngas stream is compressed up to a pressure higher than 75 bar by means of a multi-stage compressor with intermediate refrigeration before entering the final stage of the gas cleaning; the acid gas removal.

In order to avoid poisoning of the catalysts in subsequent processing modules, acid gases such as H_2S and CO_2 need to be eliminated from the syngas stream. The process consists of absorbing the acid compound at high pressure by means of a solvent, which is afterward regenerated. As a result, more than 80% of the H_2S is removed from the incoming stream. The H_2S is converted to elemental sulphur and the CO_2 emitted to atmosphere.

Table 6.15 – Gasification and gas clean up assumptions and data table (ABNT,ECN,120,121,122,114)

Indirect CFB gasifier	
Operating temperature	820-900°C
Steam as fluidizing medium	0.4kg/kg dry biomass
Sand recirculation	27kg/kg biomass
Fresh sand (to account for losses)	0.01% of circulating rate
Cyclone	99.9% of sand and char removed
OLGA tar removal	
Operating temperature	320°C
Operating pressure	2.5 bar
Tar removal	95wt%
Steam methane reformer (SMR)	
Operating pressure	12.5bar
CH4 conversion	70wt%
Steam addition	0.8kg/kg dry biomass input
Acid gas removal	
H_2S in stream removed	80%
CO_2 in stream removed	59%

6.1.10 GASIFICATION AND GAS CLEAN UP (DIRECT) WITH FISCHER-TROPSCH TO HYDROCARBON FUELS

This module was based on the work by Kreutz et al. (116) and Bechtel (117) and consists of high pressure oxygen blown fluidised bed gasification. This module was created specifically for Concept 22 which is the BtL concept based on a softwood feedstock. The block diagram for this module is shown in Figure 6.11 and the main information and assumptions shown in Table 6.16.

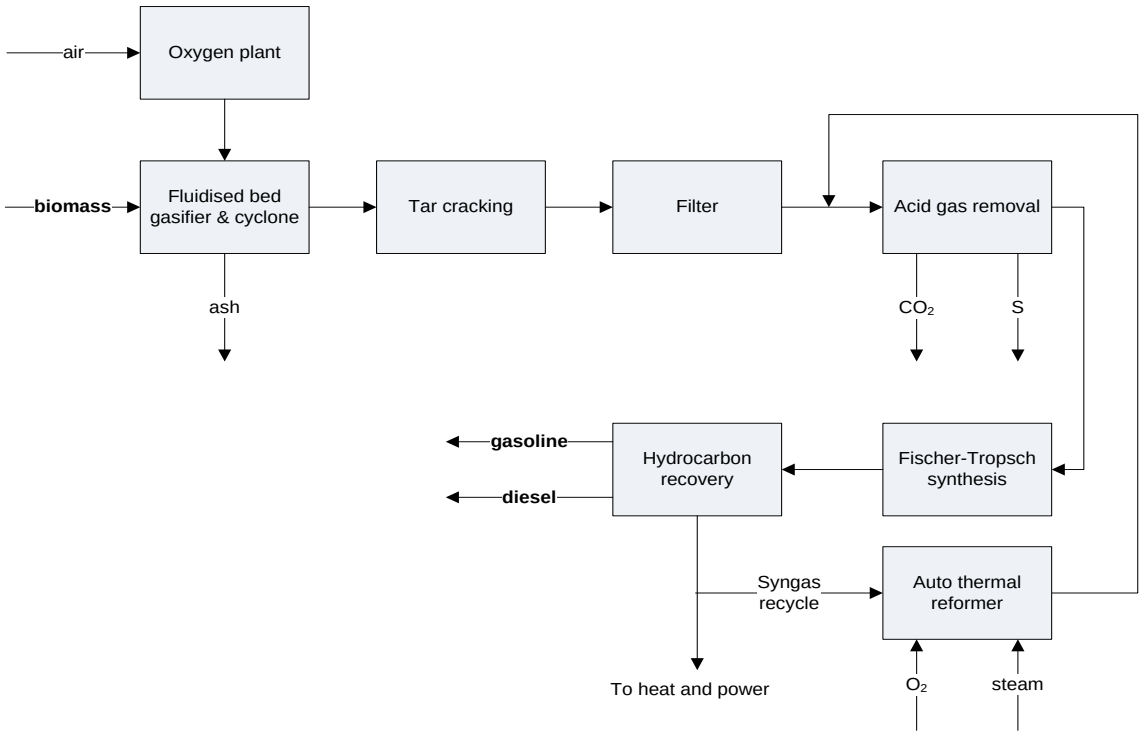

Figure 6.11 - Gasification, FT synthesis block diagram

Table 6.16 – Gasification and Fischer-Tropsch assumptions and data table (116, 117)

Oxygen blown fluidised bed gasifier	
CO_2 to feed hopper	0.1 x dry biomass input
Steam: dry biomass (wt ratio)	0.25
Carbon conversion	96%
Air separation unit (ASU)	
O_2 purity required	99.5%
O_2:dry biomass (wt ratio)	0.3
Tar cracker	
Operating pressure	28.8bar
Operating temperature	800^oC
Acid gas removal	
Operating temperature	40^oC
CO_2 removal	97%
H_2S removal	100%
Slurry phase FT reactor	
CO converted	99%
Product split	**CO converted to products, wt%**
CO_2	30.5
CH_4	18.9
C_4H_{10}	1.9
C_9H_{20}	4.4
$C_{15}H_{32}$	2.4
$C_{21}H_{44}$	14.4
C_4H_8	10.5
C_9H_{18}	11.0
$C_{15}H_{30}$	5.7
CH_3OH	0.3
Auto thermal reformer (for syngas recycle)	
Steam to carbon mol ratio	0.3

The biomass is fed to the gasifier via a CO_2 pressurised lock hopper, with oxygen being blown into the gasifier from an air separation unit (ASU). In the gasifier sand is used as the bed material and the temperature reaches around 1000^oC. Before the syngas can be processed further into useful products, any contaminants are removed through a number of gas cleaning steps.

Directly following the gasifier a cyclone separates the resulting syngas from the entrained ash and unconverted char. The syngas is then processed in a tar cracker to convert any residual tar to light hydrocarbon gases. The syngas is cooled to 350^oC in a fire tube cooler, raising steam for use within the process. Particulates are removed by a filter with further cooling before the acid gas removal step. The CO_2 is removed to improve the kinetics and economics of the further processes and the H_2S is removed to avoid poisoning of the catalysts. The H_2S is converted to elemental sulphur and the CO_2 is vented to atmosphere.

The clean syngas is then sent to a slurry phase FT synthesis reactor for conversion into hydrocarbons. A slurry phase Fischer-Tropsch (FT) reactor with an iron catalyst is employed to convert the syngas to hydrocarbons. In a slurry phase reactor the syngas is

bubbled through a liquid in which the catalyst particles are suspended (116). The reactions generate a lot of heat which is removed by boiler tubes running through the reactor.

The product stream from the FT reactor contains a mixture of hydrocarbons and gases. The light gases (unconverted syngas and C1-C4 gases) are first separated from the liquid fraction. A portion of the unconverted syngas is recycled to the process to increase the yield of hydrocarbons, with the remainder of unconverted syngas being sent to generate heat and power. The recycled syngas is passed through an autothermal reformer, to produce a mixture primarily of CO, H_2 and CO_2 before being fed back into the process. The mixed hydrocarbon liquid passes through distillation and refining steps to result in diesel and gasoline a as the finished products.

6.1.10.1 VALIDATION

This module was built based on data taken from the literature. Validation data was collected from other literature sources to ensure that the values assumed were correct. The validation data is shown in Table 6.17. The energy conversion (LHV basis) achieved by the module model of 29% compared well with other values reported in the literature, as did the CO conversion per pass assumed in the Fischer-Tropsch synthesis reactor.

Table 6.17 – Biomass hydrocarbon fuels validation data

	Energy conversion efficiency (LHV)	**CO conversion per pass**	**Notes**
	%	**%**	
Module	29%	40%	fuels only
Larson et al., 2009 (118)	34.10%		
Tijmensen et al., 2002 (119)	33-40%	40%	atmospheric gasification, fuels and electricity
Tijmensen et al., 2002 (119)	42-50%	40%	pressurised gasification, fuels and electricity
Boerrigter et al, 2004 (162)	25.9%		indirect gasification
Boerrigter et al., 2004 (162)	37.4%		atmospheric gasification O2 blown
Boerrigter et al., 2004 (162)	19.8%		Pressurised gasification, O2 blown
Boerrigter et al., 2004 (162)	55.4%		entrained flow

6.1.11 MIXED ALCOHOL SYNTHESIS

In this module cleaned syngas from gasification is reacted in the presence of a catalyst to produce a mixed alcohol stream containing methanol, ethanol, butanol, pentanol, and propanol. The block diagram for this module is shown in Figure 6.12. The module for mixed alcohol synthesis was based on the work by Phillips et al. (120,121) and from information given by ABNT. The main data points are shown in Table 6.18

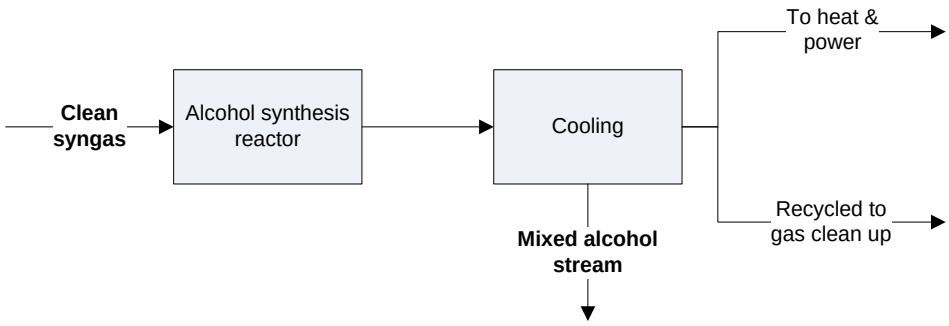

Figure 6.12 – Mixed alcohol synthesis block diagram

The syngas is preheated to 280-350^{o}C before entering the synthesis reactor. The reactor consists of a multi-tube fixed bed reactor using a modified Fischer Tropsch catalyst (121). In here, the syngas is converted via high pressure catalytic synthesis into methanol, ethanol, other higher alcohols, water, methane and small amounts of other hydrocarbon products. The water-gas shift reaction occurs simultaneously, consuming CO from the syngas and water produced in the synthesis reactions (121). The heat of reaction is removed by generating steam. By means of catalytic synthesis, about 40% CO per pass is converted; leaving a high quantity of CO unreacted. Approximately 40% of converted CO (carbon basis) is turned into ethanol whereas the rest is converted into methanol, other higher alcohols, CO_2, methane and ethane. The reaction for alcohol synthesis can be summarised as (122):

$$nCO + 2nH_2 \rightarrow C_nH_{2n+1} + (n-1)H_2O$$

The reactor outlet stream is cooled to 93^{o}C by internal recovery and further to 60^{o}C by air cooled exchangers and finally to 40^{o}C by cooling water (120). Cooling the syngas to this level causes the alcohols to condense and they are collected from the unconverted syngas. The liquid alcohol stream is sent to the mixed alcohol distillation module for product separation and recovery. A portion of the unreacted syngas is recycled back to the gas clean up section (to be found in the gasification and gas clean up module); the rest is sent to the heat and power plant, to help fuel the process. The unreacted gas stream is mixed with the process syngas stream prior to the SMR due to the high levels of methane to be found in the unreacted syngas.

Table 6.18 – Mixed alcohol synthesis assumptions and data table (ABNT, 120, 121)

Alcohol synthesis reactor	
Total CO conversion per pass	40%
Selectivity	**%**
CO2	34.43
Methanol	3.25
Methane	2.54
Ethanol	39.41
Ethane	2.36
Propanol	14.71
n-butanol	2.8
Pentanol +	0.5
95% unreacted syngas recycled	

6.1.11.1 VALIDATION

In addition to the validation carried out by the partners supplying data to build the module model, validation data was collected from the literature on the process of gasification followed by mixed alcohol synthesis. This data is shown in Table 6.19. It was difficult to collect data as many of the cases were for long term projections. The module model values compared well with the literature data for near term projected performance. The module model can be used with confidence but the user should be aware of the differences between performances used in much of the literature. There was a greater level of uncertainty associated with this module.

Table 6.19 – Gasification and mixed alcohol synthesis validation data

	Conversion efficiency (mass basis)	**Conversion efficiency (LHV basis)**	**CO conversion per pass**	**Notes**
	%	**%**	**%**	
Module	15.10%	28.60%	40%	ABNT projected case
Wei et al.., 2009 (15)	18.87%	26.94%		
Phillips., 2007 (120)		~43%	60%	Projected case
Phillips., 2007 (120)			10-40%	Literature case
Dutta et al.., 2010 (122)	42%	37.10%		Projected case

6.1.12 MIXED ALCOHOL DISTILLATION

This module follows on from mixed alcohol synthesis in which the mixed alcohol stream is distilled into separate alcohol product streams. The block diagram is shown in Figure 6.13.

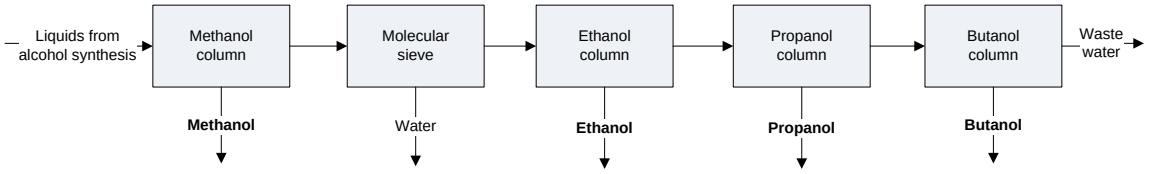

Figure 6.13 – Mixed alcohol distillation block diagram

The outlet from mixed alcohol synthesis is cooled down to 20-35^{o}C in order to condense the alcohols in the liquid phase. This stream is sent to a "stabilizing column" where methanol and other volatile components are separated in the top, while water and other alcohols are obtained in the bottom stream. The stream is evaporated at 150^{o}C and afterwards sent to molecular sieves in order to remove the water from the alcohol mixture. Finally the C3, C4 and C5 alcohols are separated by means of distillation towers (115). The information to build this module was supplied by ABNT and the main data is shown in Table 6.20.

Table 6.20 – Mixed alcohol distillation assumptions and data table (ABNT)

Mixed alcohol distillation	
Methanol column	
Methanol recovered in distillate	90%
Ethanol recovered in distillate	0.1%
Molecular sieve	
Water removed	95%
Ethanol column	
Ethanol recovered in distillate	95%
Propanol recovered in distillate	2%
Propanol column	
Propanol recovered in distillate	80%
Butanol recovered in distillate	2%
Butanol column	
Butanol recovered in distillate	80%
Pentanol recovered in distillate	2%

6.1.13 C5 TO ETHANOL

In this module a C5 rich stream from a pretreatment module undergoes fermentation to ethanol. The block diagram for this module is shown in Figure 6.14. The information needed to build this module was supplied by ABNT and taken from the paper by Aden et al. (137). The data and assumptions are shown in Table 6.21.

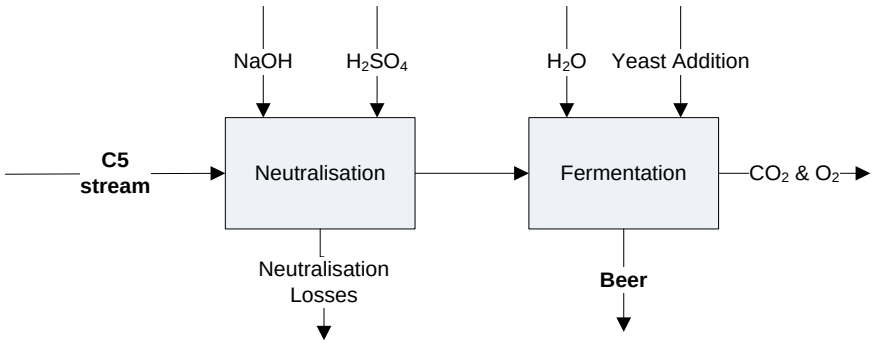

Figure 6.14 – C5 fermentation to ethanol block diagram

Some of the pretreatment methods prior to this module are strongly acidic or basic. This is not desirable for this module as fermentation must occur under neutral conditions, so the

first step is neutralisation of the incoming C5 rich stream (if required). In the neutralisation process acid or base is added to neutralise the C5 stream. The solids are removed from the stream before it is sent to the fermentation reactor.

In the fermentation reactor water is added along with yeast. The C5 sugars (mostly xylose) are then converted to ethanol. The reaction is represented by the equation: $3C_5H_{10}O_5 \xrightarrow{yeast} 5CO_2 + 5C_2OH_6$

The conversion achieved is approximately 85% of the xylose fed into the fermentation (123). The fermentation gases, consisting mostly of CO_2, are extracted from the fermentation reactor and vented to atmosphere. The fermented mixture is then sent to the ethanol distillation module for product recovery.

Table 6.21 – C5 fermentation assumptions and data table (ABNT, 137)

C5 fermentation	
High water content maintained of	>90wt% water
Yeast addition	2g/kg input
Reactions	**Fraction converted**
3xylose → 5CO2 + 5ethanol	0.85
3xylose + 5 H2O → 5glycerol + 2.5O2	0.003
Xylose + H2O → xylitol + 0.5O2	0.046
3xylose + 5CO2 → 5succinic acid + 2.5O2	0.009
3xylose → 5lactic acid	0.002
2xylose → 5 acetic acid	0.014

6.1.14 C5 TO ABE

In this module a C5 rich stream from a pretreatment module undergoes fermentation to acetone, butanol and ethanol (ABE). There are two different ABE recovery methods built into the module model. These depend on the sugar concentration in the fermented stream. If the sugar concentration <5wt% then distillation is used, if the sugar concentration >5wt% then pervaporation is used. The block diagrams for this module are shown in Figure 6.15 and Figure 6.16 with the main assumptions and data shown in Table 6.22. The information needed to build this module was supplied by IFP.

Similar to the C5 fermentation to ethanol, a neutral stream is required. Therefore the C5 stream first undergoes a neutralisation step (if required). The solids are removed from the neutralised stream and the stream diluted to maintain a high water content before being sent to the vessel. In the fermentation vessel yeast is added and the C5 stream undergoes fermentation to ABE. Fermentation gases (CO_2 and O_2) were removed from the vessel and vented to atmosphere.

If the sugar concentration in the fermented stream is less than 5wt% the fermented stream undergoes a two step distillation in order to recover the ABE product (Figure 6.15).

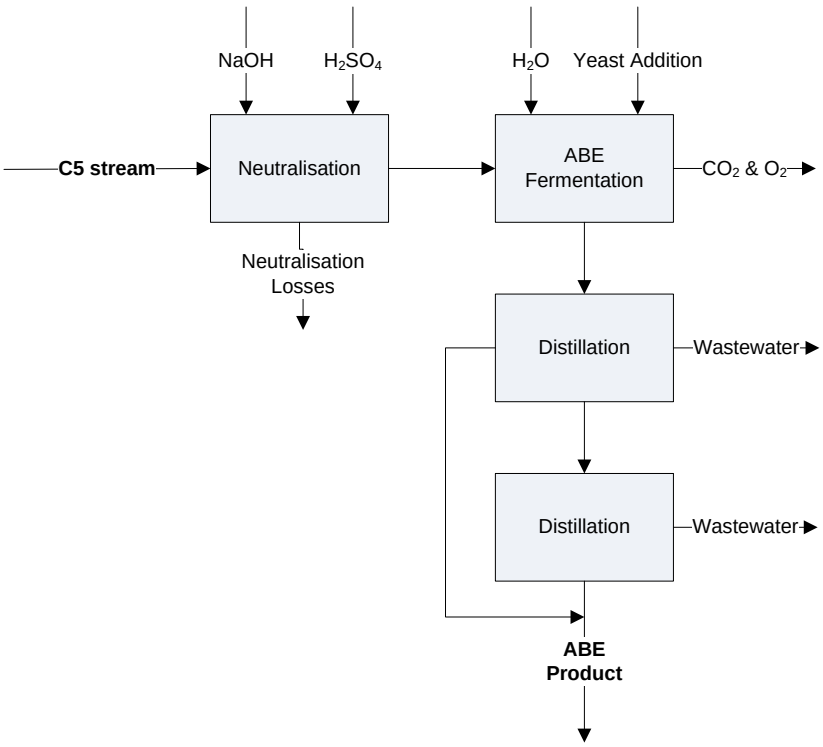

Figure 6.15 - C5 fermentation to ABE block diagram (sugar concentration <5wt %)

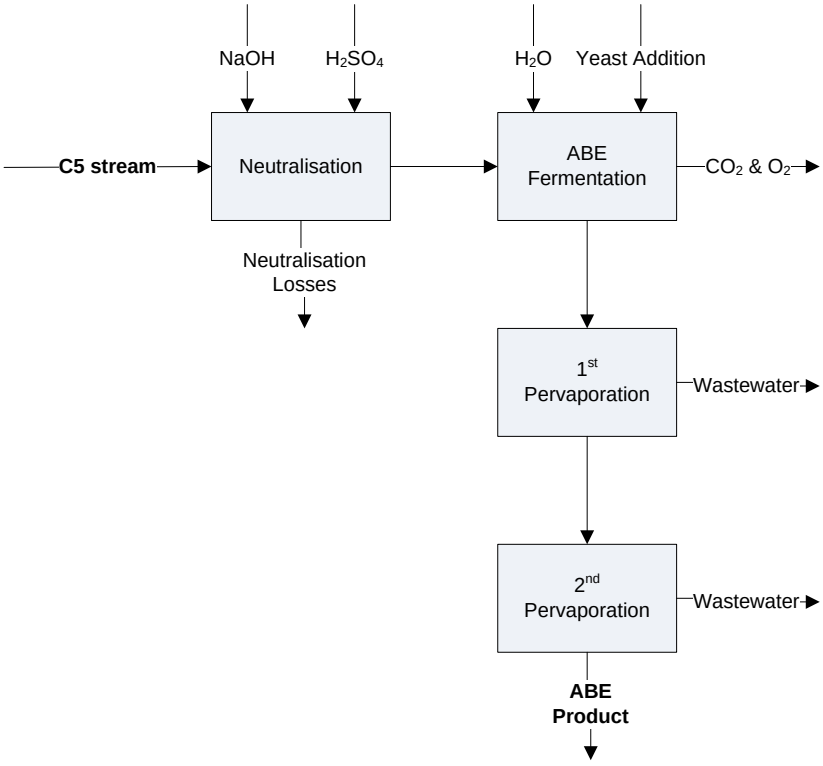

Figure 6.16 – C5 fermentation to ABE block diagram (sugar concentration >5wt %)

If the sugar concentration in the fermented stream is greater than 5wt% then the process includes continuous extraction of the product by pervaporation (Figure 6.16). The condensed pervaporate goes through a second pervaporation membrane to give the final product. If the sugar concentration in the fermented stream is less than 5wt% then a two stage distillation follows the fermentation in order to recover the ABE product.

Table 6.22 – C5 fermentation to ABE assumptions and data table (IFP)

Neutralisation	
Sugar losses	4%
Fermentation	
Yeast	2g/kg input
Xylose consumed	90wt%
Glucose consumed	95wt%
Of this:	40wt% converted to ABE in proportions:
Acetone	37wt%
Butanol	61wt%
Ethanol	2wt%
H_2 production	0.025kg/kg sugar consumed
CO_2 production	0.59kg/kg sugar consumed

6.1.15 C5 TO FURFURAL

In this module a C5 stream from a pretreatment module is reacted with steam and acid to produce furfural. A separation and distillation step then follows to result in the final furfural product stream. The block diagram for this module is shown in Figure 6.17. The information to create this module was supplied by TUD and the main assumptions are shown in Table 6.23.

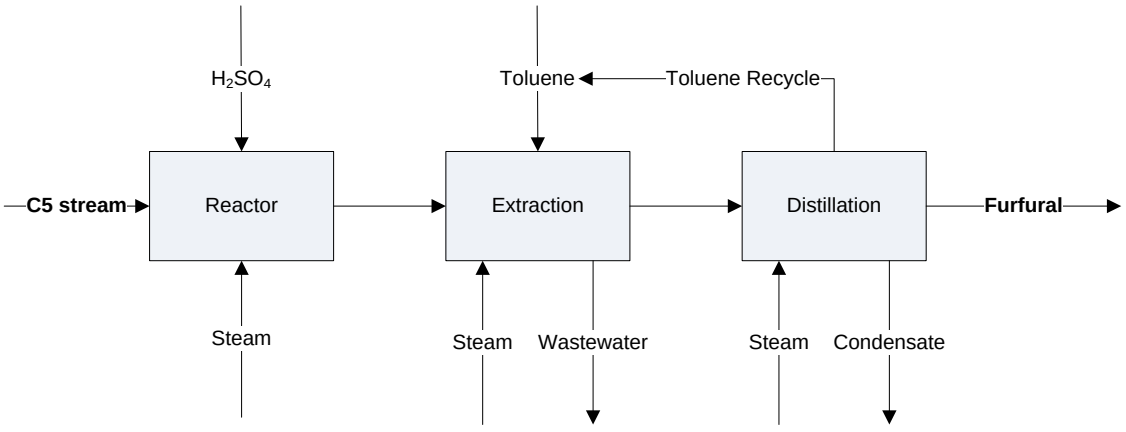

Figure 6.17 – C5 to furfural block diagram

The C5 stream from a pretreatment module is diluted to maintain a high water content of >85wt% and a small amount of H_2SO_4 is added to bring the acid concentration in the reactor to approximately 1wt%. The high water content is maintained to minimise side reactions and the formation of insoluble organic materials. Steam is added to the reactor to

increase the temperature to ~175°C. In the reactor the C5 sugars are converted to furfural, as represented by the following equation:

$$C_5H_{10}O_5 \rightarrow C_5H_4O_2 + 3H_2O$$

The molar conversion of C5 sugars to furfural achieved in the reactor is 0.75. Following the reactor the solid residues are removed and the liquid stream, containing the furfural, is sent to a liquid-liquid extraction. Toluene is used in the extraction as it has a lower heat of vaporisation than water, and hence reduces energy consumption. The extracted liquid is then sent to a distillation step to further purify the furfural and obtain the final furfural product. The toluene is recovered and recycled back to the process in an effort to reduce costs.

Table 6.23 – C5 to furfural assumptions and data table (TUD)

Reactor	
Operating temperature	175°C
Maintain high water content	>85wt%
Acid concentration	1wt%
Molar conversion C5 sugars → furfural	0.75
Steam addition (for reactor and extraction steps)	2kg/kg furfural
Liquid-liquid extraction	
Toluene to furfural mass ratio after extraction	5:1
Toluene loss in extraction	5%
Furfural recovery	100%
Distillation	
Steam usage	2kg/kg furfural
Furfural recovery	99%

6.1.15.1 VALIDATION

In order to ensure that the assumptions used in the module model for furfural production were correct, validation data was collected from the literature. Only limited information was found about furfural yield from C5 sugars. This is shown in Table 6.24. The table shows the potential or theoretical yield of furfural and the attainable yield. The potential yield of 136 kg furfural/tonne dry feed from the module compares well with values reported for bagasse, olive stones and sorghum straw. This was the expected result as these feedstocks are similar in composition to wheat straw. The attainable yield from the module model was higher than that reported by the literature but this can be explained as these were projected results and not actual results, as given by Montane et al. (124) for olive stones.

Table 6.24 – C5 to furfural validation data

	Potential yield kg furfural/tonne feed	Attainable yield kg furfural/tonne feed	Notes
Module	136	104	wheat straw - steam explosion
Montane et al., 2002 (124)	220		corn cobs
Montane et al., 2002 (124)	120		bagasse
Montane et al., 2002 (124)	170		corn stalks
Montane et al., 2002 (124)	160		sunflower hulls
Montane et al., 2002 (124)	160		hardwoods
Montane et al., 2002 (124)	135	54-95	olive stones
Vazquez et al., 2007 (125)	134		sorghum straw

6.1.16 C5 TO SURFACTANTS

In this module a C5 stream from a preceding pretreatment module is converted into a bio-based surfactant by glycosylation. The glycosylation of the C5 sugars obtained from hemicelluloses leads to alkyl polypentoside surfactants. The block diagram for this process is shown in Figure 6.18. The information to build this module was supplied by ARD with the main assumptions shown in Table 6.25.

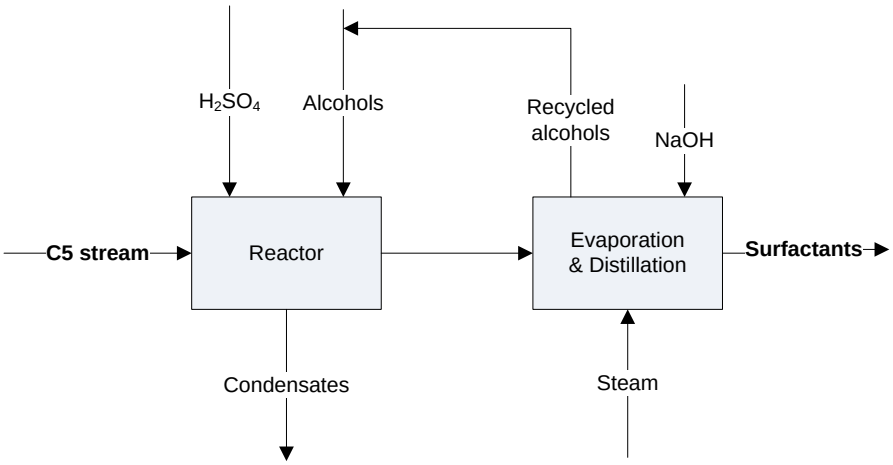

Figure 6.18 – C5 to surfactants block diagram

The C5 stream is first sent to the glycosylation reactor. Butanol and acid are fed to the reactor which is maintained at a temperature of 125^{o}C and has strong agitation. Natural fatty alcohols are used in the alkyl-polyglycoside synthesis to build up the hydrophobic part of the molecule (126). The acid acts as a catalyst for the reaction. The reacted stream then undergoes evaporation and distillation to recover the surfactant product. The condensates, consisting mostly of water and butanol are recycled to the glycosylation reactor.

Table 6.25 – C5 to surfactants assumptions and data table (ARD)

Reactor	
Operating temperature	125°C
Butanol feed	0.6 * total C5 input
H_2SO_4 addition	0.1 * xylose in C5 stream
Surfactant recovery	
Continuous evaporation with short path distillation	
Operating temperature	160°C
Surfactant recovery	100%
NaOH addition	1kgNaOH/kg H_2SO_4

6.1.17 C5 TO XYLONATE (XYLONIC ACID)

This module involves the microbial production of xylonic acid or xylonate from the C5 sugar; xylose. The block diagram for this module is shown in Figure 6.19 and data in Table 6.26. Information for this module was supplied by VTT.

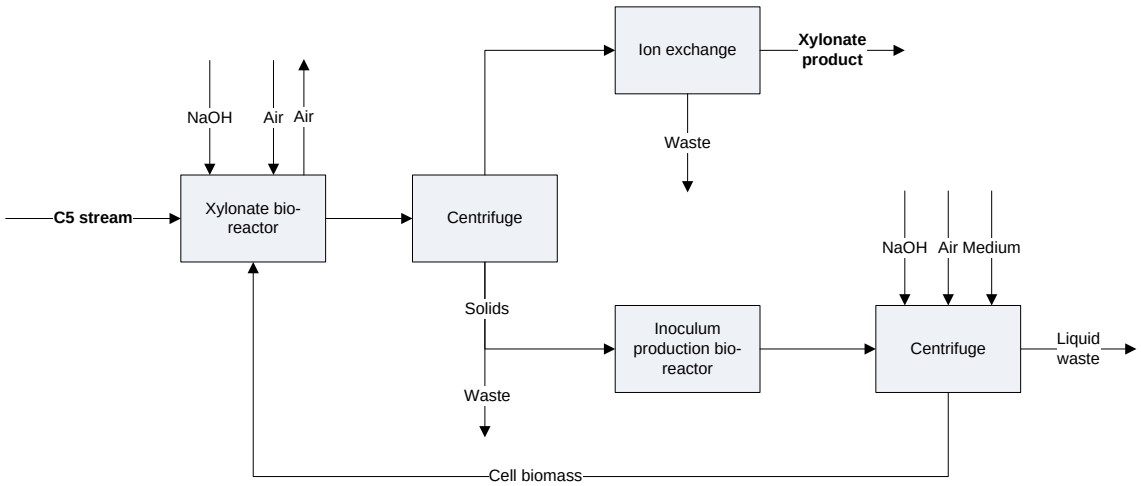

Figure 6.19 – C5 xylonate (xylonic acid) production block diagram

The C5 stream is fed into the xylonate bioreactor along with air, NaOH to maintain the pH and inoculum (from the inoculum bioreactor described later in this section). In the reactor the C5 sugars and also any C6 sugars present in the stream are converted to xylonate and gluconate respectively.

The conversion achieved is 100% according to the reactions:

$$2C_5H_{10}O_5 + O_2 \rightarrow 2C_5H_{10}O_6$$

$$2C_6H_{12}O_6 + O_2 \rightarrow 2C_6H_{12}O_6$$

Once the reactions are completed the stream is sent to a centrifuge to remove the solid biomass residues. A portion of the solid residue is sent to the inoculum production bioreactor. This portion of biomass residue containing some inoculum is fed into the inoculum production reactor along with air, NaOH and growth medium. The contents of

the reactor are then centrifuged to give a liquid waste and the inoculum stream is sent to the xylonate bioreactor.

The supernatant stream rich in xylonate from the centrifuge undergoes ion exchange in order to recover the final xylonate product. The recovery method was not researched as part of this project, so after discussion with VTT ion exchange was assumed for xylonic acid recovery.

Table 6.26 – C5 to xylonic acid assumptions and data table (VTT)

Xylonate bio-reactor	
Operating temperature	30°C
Operating pressure	1bar
NaOH addition	0.1 x xylonate produced (kg)
Inoculum addition	$3.57x10^{-4}$ x total C5 input stream
Xylose to xylonate	100%
Inoculum production	
Growth medium additions	312.5kg/kg inoculum
Recycled biomass/inoculums	0.05kg/kg inoculum
NaOH addition	0.34kg/kg inoculums produced
Product recovery	
Xylonate recovery	100%

6.1.18 C6 ENZYMATIC HYDROLYSIS AND FERMENTATION

Following pretreatment modules the C6 steam may undergo enzymatic hydrolysis and fermentation. The product of this module is a beer stream containing ethanol. The block diagram for this module is shown in Figure 6.20. The information for this module was supplied by ABNT and taken from the literature (145,137).

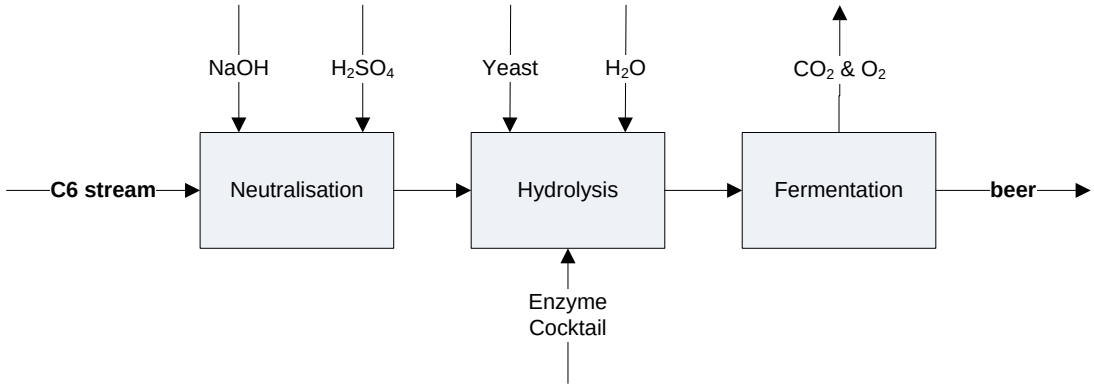

Figure 6.20 – C6 enzymatic hydrolysis and fermentation block diagram

The enzymatic hydrolysis process is favoured by a low temperature of 40°C and neutral conditions, so the first step in this module is cooling and neutralisation. The stream is first cooled to 40°C before sodium hydroxide and/or H_2SO_4 is added to neutralise the C6 stream. This occurs depending on the pretreatment method employed prior to this module.

Following this is enzymatic hydrolysis in which the cellulose is converted to glucose by means of an enzyme. The enzyme helps to break down the cellulose structure to release the sugars. The conversion of cellulose to glucose achieved is dependent on the effectiveness of the previous pretreatment module. The different conversions achieved depending on the pretreatment method are shown in Table 6.27. Following enzymatic hydrolysis the stream undergoes fermentation where the glucose is converted to ethanol. The conversion of glucose to ethanol that can be achieved is 95%, and it is carried out by yeast called *Saccharomyces cerevisiae*. The fermented stream or beer is then sent to the beer well. This stream contains the ethanol plus water, yeast, enzymes and unconverted biomass.

Table 6.27 – C6 enzymatic hydrolysis and fermentation assumptions and data table (ABNT, 145, 137)

Enzymatic hydrolysis	
Operating temperature	40°C
Enzyme dosage	17g enzyme/kg cellulose
Enzyme in cocktail	34wt%
Dilution to maintain high water content	>85wt% water
Reaction	
Cellulose + H_2O → glucose	
Pretreatment prior to hydrolysis	**Cellulose hydrolysis (wt %)**
Steam explosion	90%
AVIDEL	48%
Organosolv	66%
Mechanical/alkaline	86%
Conc. HCl	60%
Fermentation	
Yeast addition	2g/kg input
Reactions	Glucose fraction converted
glucose → 2ethanol + $2CO_2$	0.95
glucose + $2H_2O$ → 2glycerol + $2O_2$	0.004
glucose + $2CO_2$ → 2succinic acid + O_2	0.006
glucose → 3acetic acid	0.0015
glucose → 2lactic acid	0.006

6.1.18.1 VALIDATION

The performance of enzymatic hydrolysis and fermentation is dependent on the pretreatment method employed prior to the hydrolysis. For this reason the hydrolysis and fermentation validation is dealt with within the pretreatment module descriptions.

6.1.19 C6 (&C5) FERMENTATION TO ABE

There are two different processing options within this module for processing C6 to ABE, or C5 and C6 to ABE. The fermentation must take place under neutral conditions, so if steam explosion with acid is the preceding module, then the C5 stream must first undergo a neutralisation step. The process for the production of ABE following steam explosion is

shown in Figure 6.21. The modules for ABE from C6 (and C5 is required) were built based on information supplied by IFP (127).

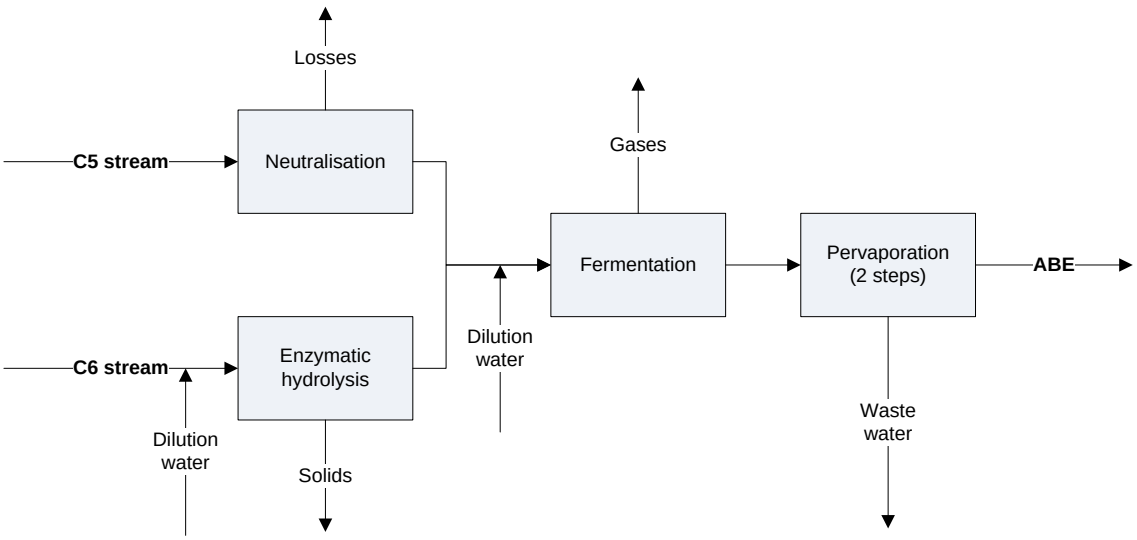

Figure 6.21 – C6 (&C5) to ABE, following steam explosion

If C5 and C6 streams are to be fermented then the C5 stream must first be neutralised due to the high levels of acid. Without neutralisation the acid would inhibit the fermentation. It is assumed that there are losses of 4% (by mass) in the neutralisation step. The C6 stream is diluted and then undergoes enzymatic hydrolysis. In this step the cellulose is broken down into glucose by enzymatic action. As before in previous enzymatic hydrolysis processes the level of cellulose hydrolysis is dependent on the pretreatment method employed. The values used relating to pretreatment method are shown in Table 6.28. The solid residues are removed from the hydrolysed stream before it is mixed with the neutralised C5 stream and sent to the fermentation step. In the fermentation reactor the sugars are fermented to acetone, butanol and ethanol (ABE). This mixture then undergoes continuous extraction of the product via pervaporation. The condensed pervaporate then goes through a second pervaporation membrane to give the final product. The performance for the first membrane was based on laboratory results. For the second pervaporation, literature data was used (128).

Table 6.28 – Cellulose hydrolysis based on pretreatment method (A&F, ABNT, ECN, Bioref, ARD)

Pretreatment method	Cellulose hydrolysis (wt %)
Steam explosion	90
AVIDEL	48
Organosolv	66
Mechanical/alkaline	86
Conc. HCl	60

The process for ABE fermentation following all other pretreatment methods apart from steam explosion is shown in Figure 6.22. A cooling step is included prior to the enzymatic hydrolysis, if the input streams were at a temperature of greater than 40^{o}C. At temperatures higher than this the enzymatic hydrolysis is not successful. If C5 and C6 are to be fermented to ABE then the C5 stream is used for dilution of the C6 stream prior to enzymatic hydrolysis. This saves water and also gives a more concentrated stream for the fermentation. As described previously, the stream then undergoes enzymatic hydrolysis to hydrolyse the cellulose to glucose. The solid residues are removed from the stream before it is sent to fermentation. The sugars are fermented to a mixture of acetone, butanol and ethanol. This stream undergoes two pervaporation steps to result in a purified ABE product.

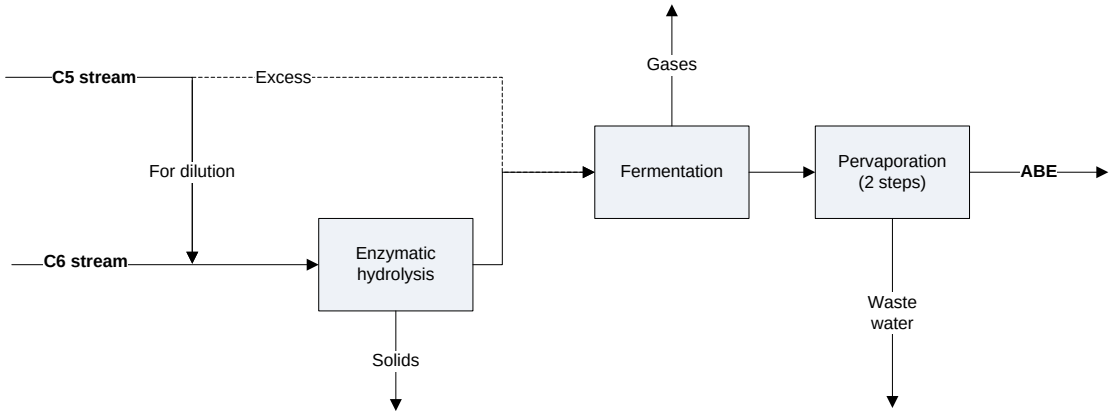

Figure 6.22 – C6 (&C5) to ABE following other pretreatment methods

Table 6.29 – ABE module data table (IFP)

Enzymatic hydrolysis	
Enzyme addition	17g/kg cellulose
Enzyme in cocktail	34wt%
Solids removal	90wt%
Liquids in solids removed	1wt%
Fermentation	
Yeast addition	2g/kg input
Xylose consumed	90%
Glucose consumed	95%
Of which: To ABE	 34%
Acetone	37wt%
Butanol	61wt%
Ethanol	2wt%
Gases produced:	
H_2	0.025kg/kg sugar consumed
CO_2	0.59kg/kg sugar consumed

6.1.19.1 VALIDATION

In order to ensure the accuracy of the module model, data was collected from the literature and compared to the values utilised in the module model. The module model and data collected from the literature is shown in Table 6.30. For the conversion of sugars to ABE a value of 36% was used in the module model. This compared well with the values reported in the literature which ranged between 34-44%. The mass and energy conversion efficiency achieved in the module model was dependent on the pretreatment method employed, as this dictated the amount of sugars available for fermentation. In the module model values between 14-37% were achieved with a value of 35% reported in the literature. The values achieved in the module were lower, but this was due to the pretreatment module, rather than errors in the ABE module; some pretreatment methods were better at releasing the sugars than others. When those pretreatment methods were utilised, with good sugar release, comparable conversion efficiencies are reported.

Table 6.30 – ABE fermentation validation data

	Sugars to ABE	**Mass conversion efficiency**	**Energy conversion efficiency**	**Notes**
	%	**%**	**%**	
Module	36%	11-18% *	14-37% *	Wheat straw
Pfromm et al., 2010 (129)	34%	23%	35%	
Qureshi et al., 2010 (130)	43%			Barley straw, acid hydrolysed
Qureshi et al., 2010 (131)	44%			Corn stover
Qureshi et al., 2010 (131)	39%			Switchgrass

Depending on pretreatment method employed

6.1.20 C6 TO FDCA

The first step in the production of 2, 5-Furandicarboxylic acid (FDCA) is the enzymatic hydrolysis of the C6 stream followed by the dehydration of sugars to hydroxymethylfurfural (HMF) with the final step of the oxidation of HMF to FDCA. The block diagram is shown in Figure 6.23 with the main assumptions and data shown in Table 6.31. The data for this module was supplied by Bioref.

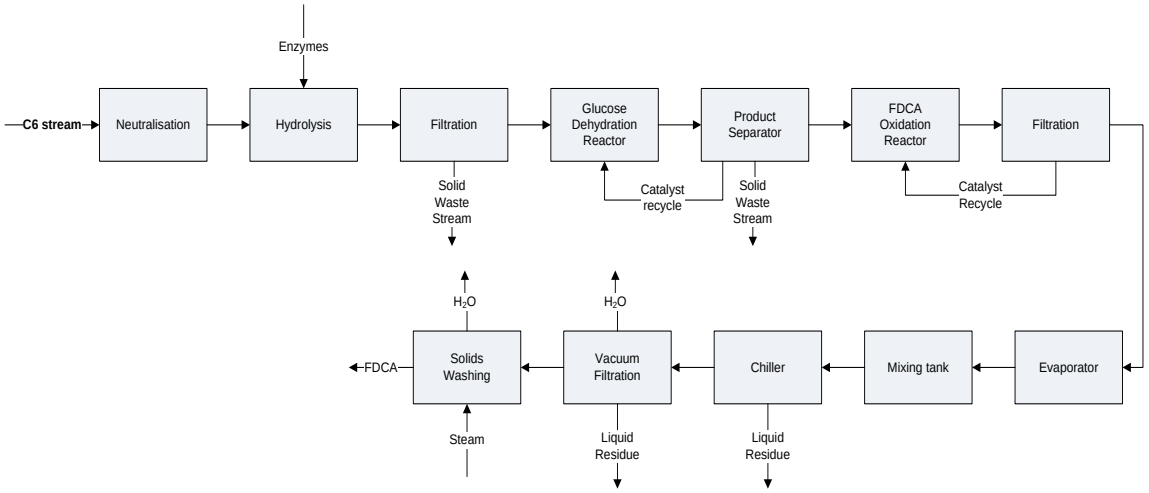

Figure 6.23 – C6 to FDCA block diagram

The temperature of the incoming C6 stream must be in the region of 40^{o}C, so if it is higher than this the stream is cooled. The cooling water is re-used later in the process for dilution to try and reduce overall water usage. In a similar way to other modules containing enzymatic hydrolysis, the incoming C6 stream may require neutralisation, as a strongly acid or alkali environment inhibits the enzymes used to enzymatic hydrolysis. The levels of cellulose hydrolysis achieved vary depending on the pretreatment method employed (see Table 6.28). Solids are removed from the stream before it is sent to the glucose dehydration reactor. The cellulose is dissolved in an ionic liquid. Hydrochloric acid catalyses the conversion of dissolved cellulose into glucose and HMF is produced from cellulose with yields up to 54%. This process uses inexpensive catalysts for the transformation of cellulose into valuable products at high yields (132). Following reaction the catalyst is removed by filtration and sent back to the reactor. The HMF rich stream is then sent to the oxidation reactor. (133)

The HMF oxidation occurs in a heated reactor which is filled with a mixture of HMF, water and catalyst. There is a continuous addition of NaOH to maintain a constant pH and the mixture is maintained at a temperature of 70^{o}C. Following the reactor the reaction mixture is filtered in order to recycle the catalyst. The solution is concentrated to half its initial reaction volume using an evaporator. Hydrochloric acid at 32%w/v is added to the residue whilst being stirred to cause the crystals to precipitate. The acidic solution is cooled to 4^{o}C and filtered under vacuum. The solid residue is washed with water and then finally dried to constant weight. The reaction yield is 97% with respect to HMF.

Table 6.31 – FDCA production data table (Bioref)

Enzymatic hydrolysis	
Enzyme addition	17g/kg cellulose
Enzyme in cocktail	34wt%
Operating temperature	40oC
Dilution to maintain high water content	>70wt%
Dehydration of glucose to HMF	
Ionic liquid	9kg/kg glucose
Catalyst	0.1kg/kg glucose
Operating temperature	100oC
Glucose to HMF	71wt%
Recovery of HMF	70%
Oxidation of HMF to FDCA	
Water addition	56.5kg/kg HMF
Catalyst	0.59kg/kg HMF
NaOH	2.26kg/kg HMF
HMF conversion to FDCA	97%
Air addition	4722litres/hour/kg HMF
Evaporator	
Reduces volume by half	
Mixing tank	
32%w/v HCl	2.66kg/kg FDCA
Chiller to cool solution to:	4^{o}C
Vacuum filtration	
Solids removed	99%
Solid residue washing	
Water	7.3kg/kg FDCA
Filtration	
Solids removed	99%
Drying	
Product dried to constant moisture at 60oC	
Product	7wt% water

6.1.21 ETHANOL DISTILLATION

Beer streams from C6 and/or C5 fermentation are the input into for this module used to obtain the final ethanol product stream. The block diagram is shown in Figure 6.24. Information to create this module was supplied by ABNT and IFP.

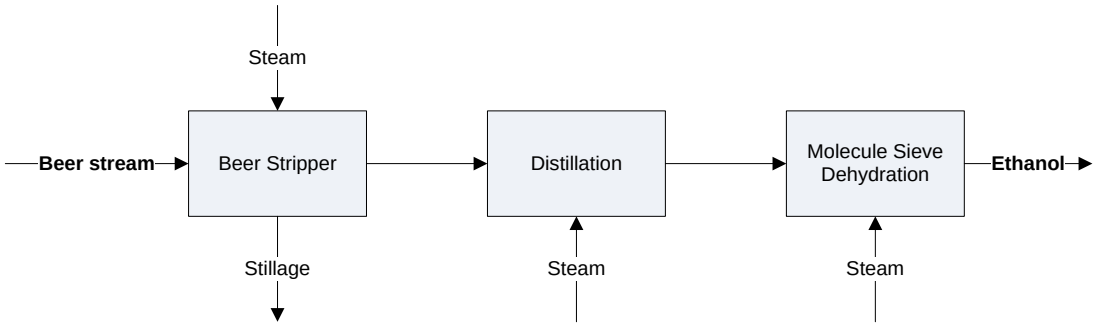

Figure 6.24 – Ethanol distillation block diagram

The first stage in the recovery of ethanol takes place in the beer stripper in which steam is directly injected to distil the ethanol. This separates the liquid ethanol product stream from the resulting solids. The solid residue can be processed further, or can be combusted to

provide heat (and power) for the biorefinery. The ethanol product stream from the beer stripper contains about 40% w/w ethanol (123). This stream then undergoes distillation to achieve an ethanol stream near the azeotropic point (95% w/w ethanol). Following distillation the ethanol goes through a molecular sieve dehydrator that dries the ethanol in the vapour phase. When ethanol vapour passes through the bed, the desiccant absorbs the water molecules, but not the ethanol molecules. Commercial ethanol with over 99.5% purity is achieved with the molecular sieve (90).

Table 6.32 – Ethanol distillation data table (ABNT, IFP)

Beer stripper	
Ethanol stream	40wt% ethanol
Distillation	
Ethanol stream	92wt% ethanol
Molecular sieve	
Ethanol stream	99wt%

6.1.22 PYROLYSIS

In this module biomass undergoes fast pyrolysis to result in bio-oil, which may be further processed or sold as a product As well as fresh biomass feed, the lignin stream remaining after pretreatment may undergo fast pyrolysis to produce bio-oil The block diagram for this module is shown in Figure 6.25. Information to build this module was supplied by Aston (AVB) and ECN. The main assumptions are shown in Table 6.33.

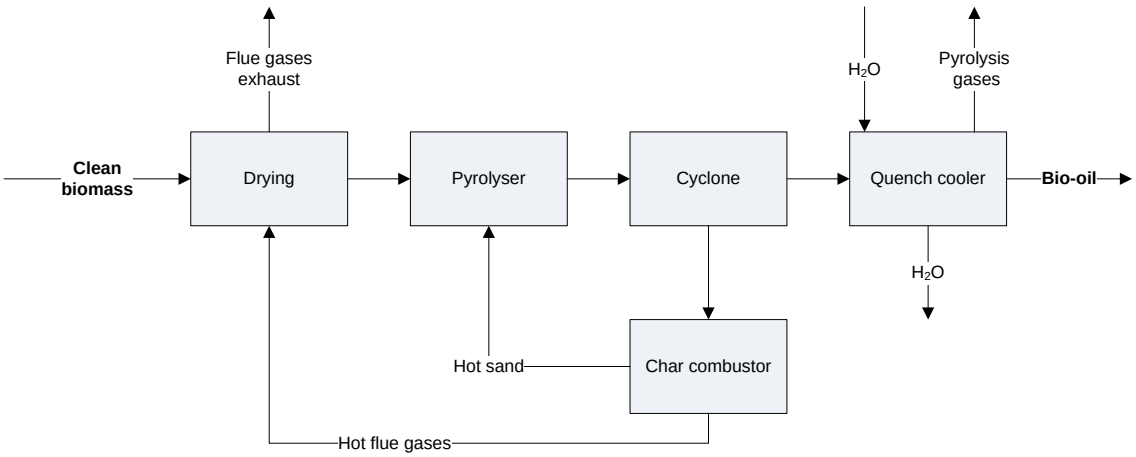

Figure 6.25 – Pyrolysis block diagram

Before entering the fast pyrolysis reactor, the feed must be dried to 10wt% water. This helps improve conversion and reduces water content in the final product. In fast pyrolysis biomass is decomposed rapidly at a very high temperature in the absence of an oxidising agent. The biomass is decomposed to mostly vapours and aerosols and some charcoal, which on condensing forms a dark brown liquid called bio-oil (134). In this module the

incoming stream is fed to a bubbling fluidised bed fast pyrolysis reactor. The product split between gas, liquid and char depends on the feedstock. The spilt is shown in Table 6.33. Following pyrolysis the hot vapours and char are sent to a cyclone. The char and sand are removed and sent to a char combustor. The char is combusted and heats the sand, before it is sent back to the fluidised bed reactor. This provides the heat for the reactions. The hot vapours are sent to a quench cooler. In the quench the vapours were cooled from approximately 400^{O}C to 25^{o}C, causing the liquids to condensate and resulting in the bio-oil product. The pyrolysis gases are sent to the heat and power module to be combusted and provide heat for the process. The bio-oil may be sold as the final product (potentially to conventional petro-chemical refineries as a bio-based intermediate) or may undergo further processing to obtain value added products.

Table 6.33 – Pyrolysis data table (AVB, ECN)

CFB pyrolyser			
Operating temperature	500^{o}C		
Feed water content	10wt%		
Product composition depends on feedstock			
wt% products	Gas	Liquid	Char
Straw	20	65	15
Wood	12	73	15
Lignin	30	30	40
Cyclone			
Removes all sand, ash and char			
Quench			
Cools products from ~400^{o}C to 25^{o}C			
Condenses all liquids			

6.1.23 LIGNIN DRYING

One of the choices for lignin processing is to dry it, and sell it as a fuel or a product for further processing. In this module the lignin stream is dried to the required moisture content of 16wt% as defined by ABNT (115). The wet lignin stream is fed into a rotary dryer. Heat is supplied by steam and the evaporated water sent to atmosphere. The information for this module was taken from the thesis by Toft (89) with the specification of the lignin product from ABNT. The block diagram is shown in Figure 6.26.

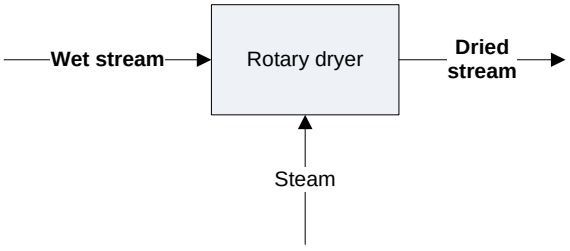

Figure 6.26 – Drying block diagram

6.1.24 STILLAGE DRYING

This module is included as part of the ABNT base case, Concept 25. In the base case the solid residues from fermentation (stillage) are dried and sold as animal feed. The block diagram for this module is shown in Figure 6.27. The information to build this module was supplied by ABNT and the main assumptions are shown in Table 6.34.

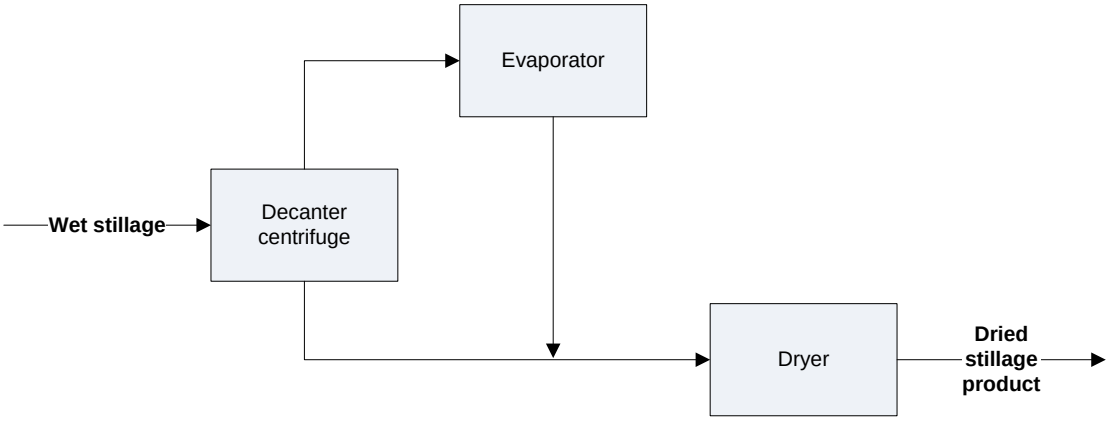

Figure 6.27 – Stillage drying block diagram

The wet stillage from the beer stripper is first sent to a decanter centrifuge. This removes water to a moisture content of 70%. The liquids removed are sent to an evaporator to further recover solids. The liquid stream is reduced to 27.5% solids. This dried stream is then mixed with the centrifuge bottoms before being sent to the final drying step which consists of a rotary dryer where the stream is dried to 23% moisture.

Table 6.34 – Stillage drying data table (115)

Decanter centrifuge	
Removes water to moisture content	70wt%
Evaporator	
Reduces water content to:	72.5wt%
Evaporator efficiency	90%
Dryer	
Reduces water content to:	22wt%
Dryer efficiency	50%

6.1.25 BIO-OIL FRACTIONATION

The objective of this module is to derive a phenolic rich bio-oil fraction suitable for direct application in the resins and wood preservative industry (135).The target product is for the (partial) replacement of conventional phenol in phenol-formaldehyde resins. These resins are primarily used in the manufacture of wood panels (135). The block diagram is shown in Figure 6.28. The information to build this module was supplied by BTG and the main assumptions are shown in Table 6.35.

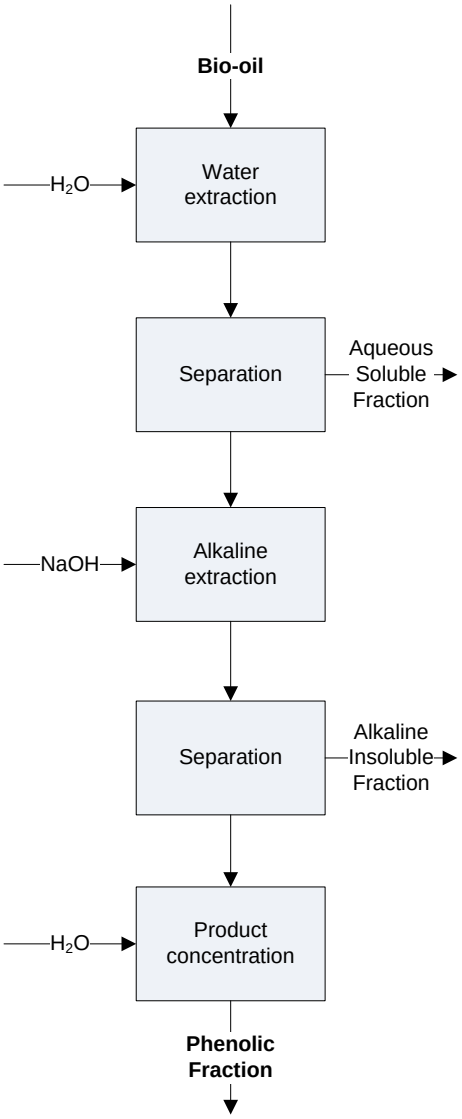

Figure 6.28 – Bio-oil fractionation block diagram

The bio-oil from fast pyrolysis is mixed with water in order to separate the water soluble fraction and the water insoluble fraction. The water soluble fraction contains mainly sugars, acids, alcohols and water. The water insoluble fraction contains phenolics and a neutral lignin fraction plus approximately 10wt% water. The separation is achieved using decanters.

The water insoluble fraction is mixed with sodium hydroxide to separate the charged fraction from the neutral fraction. Since phenols are slightly acidic, they dissolve in the sodium hydroxide (135) leaving the neutrals undissolved. The dissolved phenolics are then separated from the solid neutrals. Finally the dissolved phenolics undergo a distillation step to remove the remaining water and leave the phenolic fraction.

Table 6.35 – Phenolic fractionation data table (BTG)

Water extraction	
Water addition	1kg/kg bio-oil
Alkaline extraction	
NaOH addition	2.5kg/kg insoluble phase
NaOH concentration	1M
Phenolic fraction	
~85wt% solids	

6.1.26 BIO-OIL FOR HEAT AND POWER

In this module bio-oil is combusted in a modified boiler along with other process residues to generate heat, in the form of steam. The generated steam then passed through a steam turbine to generate electricity. The idea is to have this plant alongside a conventional petrochemical refinery to meet some of the heat and power demand for the refinery. In this way the overall fossil fuel demand and emissions from the plant are reduced. This is one way for biorefineries to be integrated into conventional petrochemical refineries. The assumptions to build this module were provided by JR and Aston.

6.1.27 BIO-OIL GASIFICATION AND GAS CLEAN UP

In this module the bio-oil is gasified in oxygen blown, slagging entrained flow gasifier. The block diagram for this module is shown in Figure 6.29. This module was based on communications with ECN and the paper by Drift et al. (136).

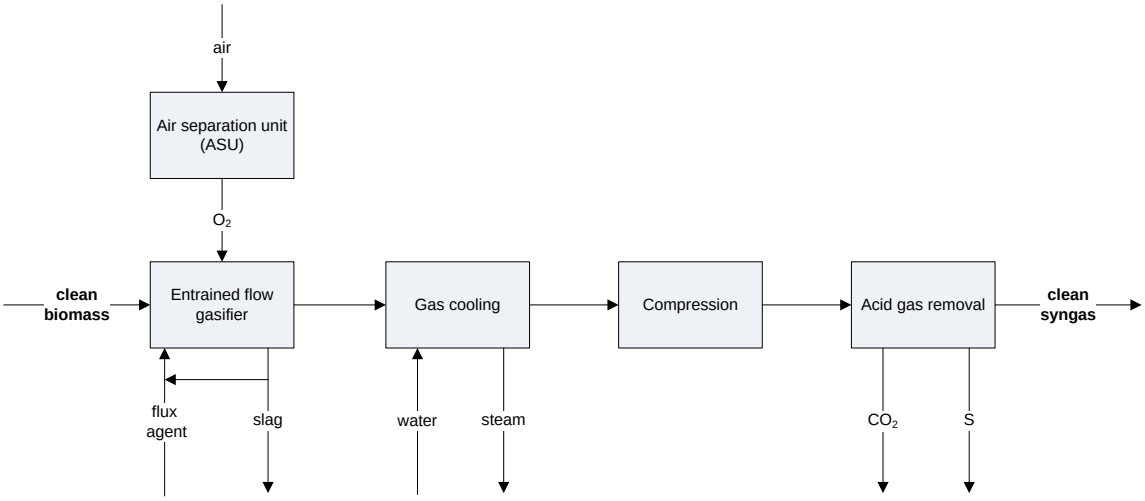

Figure 6.29 – Bio-oil gasification block diagram

The biomass is fed into the gasifier, along with a flux agent and a small amount of slag recycle. In the gasifier ash forming components melt and condensate on the gasifier walls. A slagging gasifier helps prevent this problem by removing the melted components as a liquid slag. In a slagging gasifier the slag acts as a protective layer on the gasifier wall, and the liquid slag is removed from the bottom of the gasifier. A flux agent is added to generate

the liquid slag at the operating temperature of the gasifier. The gasifier runs at approximately 1300^{o}C. In this gasifier silica is added as the flux agent with a ratio of 0.6-1.2 kg/kg fuel ash. To maintain good wall coverage in the gasifier, the slag and flux agent are recycled. The formation of soot is suppressed by the addition of steam with the oxygen at the rate of 0.1kg steam per kg oxygen (136).

Following the gasifier the syngas is cooled to 900^{o}C with a cold syngas quench, followed by cooling in a fire tube boiler producing steam at 60 bar (136). The cooled syngas (500^{o}C) is then sent to gas clean-up steps. Gasification of bio-oil produces a tar and methane free syngas, so tar removal and steam-methane reforming are not required. The syngas is compressed before being sent to acid gas removal, described in Section 6.1.9. The CO_2 is emitted to atmosphere and the elemental sulphur sent to landfill. The clean syngas is then ready for conversion into ethanol and other alcohols.

Table 6.36 – Bio-oil gasification data table (ECN, 136)

Entrained flow gasifier	
Operating temperature	>1200^{o}C
Flux addition	0.08kg/kg bio-oil
O_2 supply	0.521kg/kg bio-oil
O_2 purity	99%
Gas output composition	wt%
CO	38.52
H_2	26.44
CO_2	11.2
H_2O	23.56
N_2	0.24
H_2S	0.04
Compression train	
Multistage compression	>75bar
Acid gas removal	
Steam requirement	0.408kg steam/kg gas input
H_2S removal	80%
CO_2 removal	59%

6.1.28 WATER AND RESIDUES

This is a calculation module created in an effort to integrate water usage and waste residue collection across the biorefinery concept. High water usage is known to be a common problem in biorefineries, so this module aims to reduce water usage by recycling as much as possible. The main assumptions are shown in Table 6.38.

The worksheet first looks at steam requirements for each module and also any condensate collected. In any process plant the condensate would be collected and reused in the boiler feedwater system. This module mimics this and calculates how much fresh boiler water would be required to meet steam requirements of the entire biorefinery whilst recycling as

much condensate as possible. It is assumed that there is a 5% loss in the condensate system.

The second part of this module looks at process water requirements for each module plus any cooling water returns. These figures in combination with the process water returning from the wastewater treatment plant are used to calculate the amount of fresh water required by the biorefinery. This kind of integrated water system would exist in a biorefinery plant so these calculations aim to mimic this level of integration.

The final part of this module looks at the waste residues from each module. The liquid residues are first dewatered with any organic solid residues sent to provide heat or to landfill. The liquid stream remaining is sent to the wastewater treatment module.

Also included in this sheet are the volatile gaseous waste streams including the biogas generated in the wastewater treatment module. These are sent to be combusted to provide heat for the biorefinery.

Table 6.37 – Water and residues data table (137)

Condensate collection
Assumed 5% losses
Waste dewatering
95% solids removal

6.1.29 WASTEWATER

The wastewater treatment plant is based on the model used by Aden et al. (137) in the techno-economic analysis of a lignocellulosic bioethanol plant. The block diagram for this module is shown in Figure 6.30 with the main assumptions shown in Table 6.38.

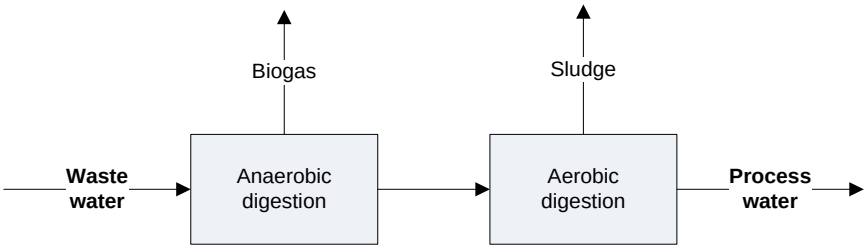

Figure 6.30 – Wastewater block diagram

Table 6.38 – Wastewater module data table (137)

Anaerobic digestion	
CH_4 production	0.229kg/kg COD removed
CO_2 production	1 mol CO_2 per 3 mols; CH_4
Cell mass production	30g for each 1kg COD removed
COD removal	93%
Nutrient addition	37g per kg COD
Biogas composition:	
CH_4	75wt% dry basis
CO_2	25wt% dry basis
Aerobic digestion	
90% of remaining soluble organics converted	
Total COD reduction	99.4%

The wastewater first undergoes anaerobic digestion in which 90% of the organic components are converted to methane and CO_2. The produced biogas is then sent to the heat and power module for fuel. The anaerobic digestion process results in a 93% removal of COD. The liquid from the anaerobic digestion is then sent to aerobic lagoons, where 90% of the remaining soluble organics are converted. The total COD reduction achieved in this wastewater treatment plant is 99.4%. The cleaned water is then sent back to the process or discharged if not required.

6.1.30 HEAT AND POWER

In this module the heat and power requirements for the biorefinery are produced from process residues and additional biomass. The biomass and residues are combusted in a boiler to generate steam. The steam then passes through a steam turbine to generate electricity. This module was based on information supplied by Aston (AVB), JR and from the thesis by Toft (89). Additional biomass is only utilised if the process residues cannot provide all of the heat requirements of the plant. The aim of the heat and power module is to provide exactly enough steam to make the biorefinery self sufficient. In general more electricity is produced than is required by the plant. The surplus electricity is sold to the grid providing additional income for the biorefinery. The efficiencies are shown in Table 6.39

Table 6.39 – Heat and power module data table (Aston, JR, 89)

Efficiencies	
Heat production efficiency	70%
Electrical power generation efficiency	30%
Combustion efficiency	90%

6.1.31 HEAT ONLY

In this module only the heat requirements of the biorefinery are met by process residues and biomass; no electricity is generated. The residues and/or biomass are combusted in a

boiler to generate steam for the biorefinery. The electricity requirement is met by purchasing electricity from the grid. The efficiencies assumed are the same as for the heat and power module, see Table 6.39.

6.1.32 NO HEAT AND POWER

This module is used if the user chooses not to heat or power the biorefinery using process residues and biomass in the process synthesis user interface. The heat and power is provided purely from fossil sources. Natural gas is used in a gas boiler to generate the steam requirements and electricity is purchased from the grid. The combustion efficiency of natural gas is assumed to be 90% (115).

7 PROCESS SYNTHESIS APPLIED TO PROCESS MODULES

This chapter describes the application of process synthesis, described in Chapter 4, to the modules created in the modelling step (Chapter 6). A hybrid process synthesis method was applied, combining elements of expert systems and heuristics or rules. This chapter describes the creation of the process synthesis user interface, the links created between the modules (logic rules etc) and how logic rules were incorporated to allow only feasible concepts to be created.

The process synthesis element of the project was built during and after the creation of each process module. It couldn't be completed and constructed without first having the module models to link together. Once the process synthesis user interface and modules were completed this formed the completed process synthesis model. This was created using Excel and also integrated the socio-economic models.

Each of the process steps was modelled separately as a 'module' (see Chapters 5 and 6). The modules were linked together by the user through the process synthesis user interface page (see Section 7.1). Each module looked to this page for input, and applied the IF logic rule; based on the choice made by the user the modules calculated by choosing data from the correct preceding module and applying the correct assumptions. The results generated were then used in subsequent analysis and comparison of biorefinery concepts (see Chapter 10).

7.1 USER INTERFACE

One of the objectives of the project was to make the methodologies created user friendly and accessible to the project partners. The methods/models had to include a level of flexibility to allow the user to generate biorefinery chains for themselves, and not be fixed to just the 27 chosen concepts. To facilitate this, a user interface was created in which the user was guided through a number of steps to generate a complete biorefinery process chain. In addition the user interface and complete model was created so that the finished system could be used externally to the project to provide a long lasting tool.

The mechanics of the modular process synthesis methodology enable the user to make choices from those displayed in the interface; beginning with the scale, feedstock and pretreatment steps. Logic and in-built relationships populate the subsequent options made available to the user. This continues until a complete process chain is generated from feedstock to product. As the user moves through the user interface making choices, behind this page the module models are generating data about the chosen process steps. Once the

user has completed the module choice they click on “Create summary” to generate the output file. A more detailed user manual can be found in Appendix 3. This methodology provides a way to logically and methodologically generate and analyse biorefinery process concepts.

The user begins by entering the amount of biomass (kg/h dry) to be processed in the biorefinery (see Figure 7.1). The user then chooses the country where the plant is to be located from the drop down menu; there are the choices of UK, Spain, Germany, Netherlands and Poland. Moving down the page the user can change the annual operating hours if they wish and can see the annual biomass processing rate. The next step involves choosing the feedstock from the dropdown menu; wheat straw or softwood followed by the choice of pretreatment method. Depending on the choice made here different options are displayed on the page from which the user makes the choice of subsequent processing steps. The user continues through the sheet until the process has been defined. The final choice to be made by the user is for heat and power provision of the plant. The user has to choose whether power and/or heat is to be provided by biomass. There are 3 options available; heat and power from biomass, heat from biomass and power from the grid or heat from natural gas and power from the grid.

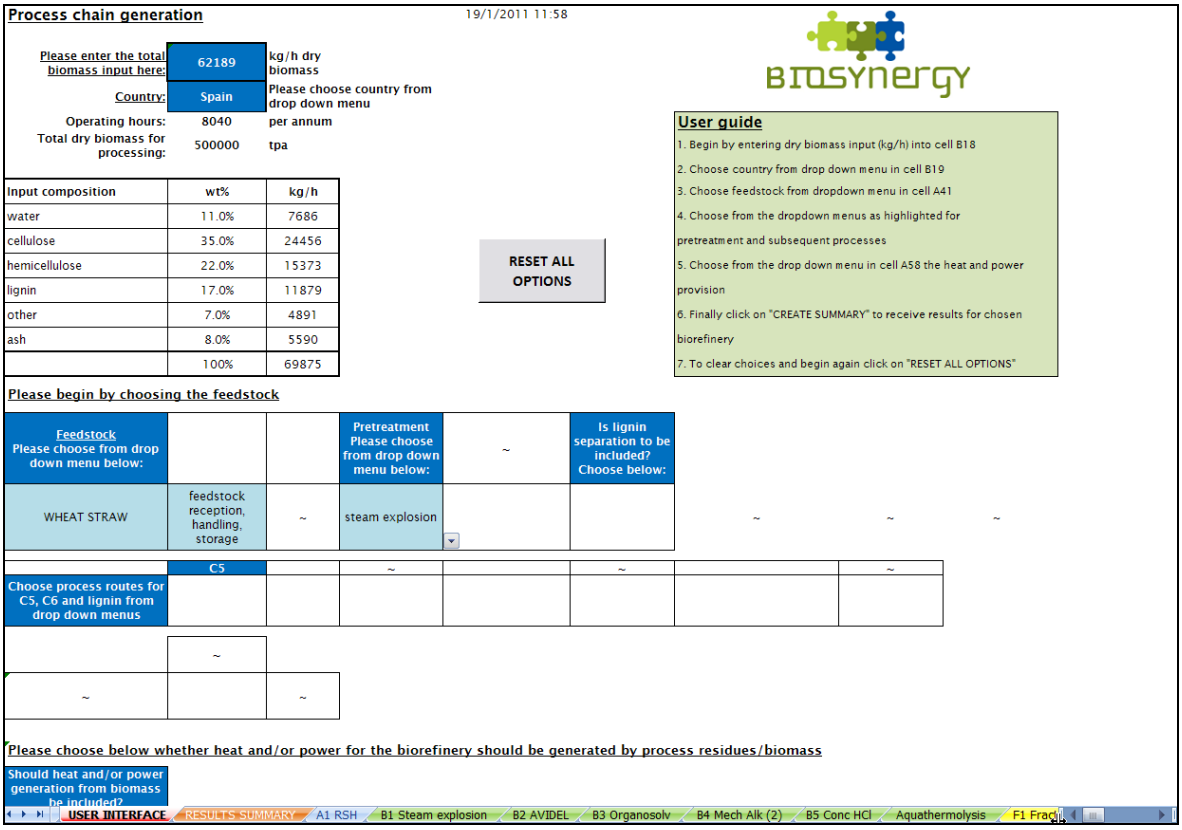

Figure 7.1 – User interface screen grab 1

A summary of the chosen process is given at the bottom of the page plus a button to create summary (see Figure 7.2). Once the user has fully defined the configuration to be investigated this button is pressed to generate a data file about that particular biorefinery. This file contains a full description of the process in terms of mass and energy flows, cost estimations and socio-economic factors. This file contains all the information needed to carry out subsequent analysis and comparison. An example of the summary file is given in Appendix 4. To begin again the user clicks on the "Reset all options" button to clear their previous choices and prepare the system for subsequent biorefinery chains.

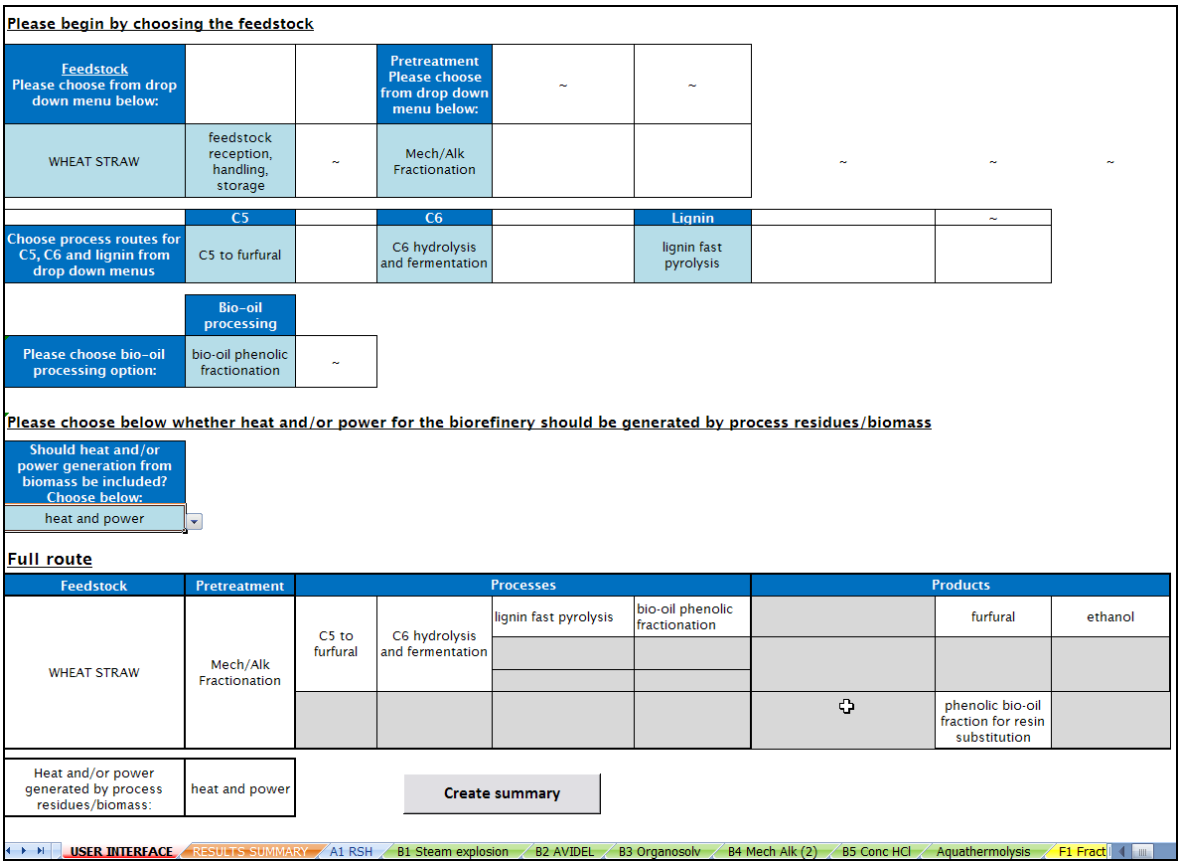

Figure 7.2 – User interface screen grab 2

7.2 LINKING OF PROCESS MODULES

Depending on the choices made in the user interface, different modules are connected and module information calculated. This all happens "behind the scenes" within the process module models. The user controls the linking of the modules using only the interface. In this way, the accuracy of the model can be assured and those in possession of this version of the methodology know that they are all using the same version. This is particularly useful considering the large number of partners involved in the project. It is possible for users to make some adjustments to the modules. They are able to change the assumptions highlighted in blue bold text within each module, but cannot edit the underlying

calculations. The logic and relationships between the modules are described in the following sections.

Within the process model there are numerous possible connections between modules (see Figure 7.3) but for this thesis and the Biosynergy project the creation of the methodology focussed on 27 defined biorefinery process chains (see Table 6.1). It is possible to create many more biorefinery process chains, but the focus for accurate results was on these 27.

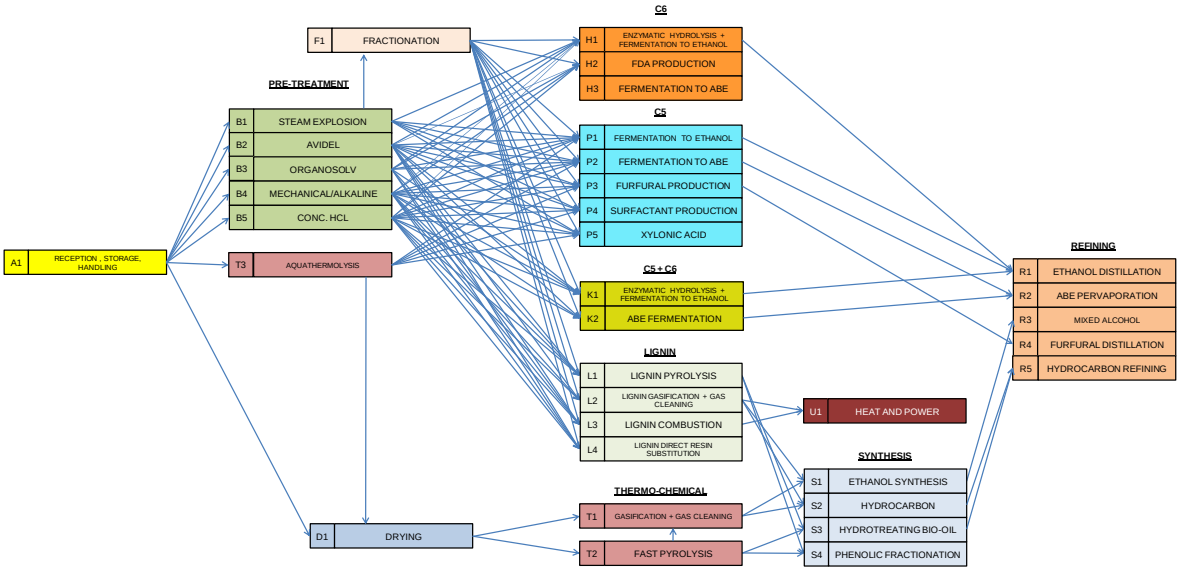

Figure 7.3 – Module spider diagram

The user interface controls which modules are linked and all modules look to this sheet for reference. The majority of the logic rules were built using the IF logic function within Excel. For example, looking at Concept 0 (wheat straw, mechanical/alkaline pretreatment, furfural, ethanol and phenolic fraction of bio-oil products), straw was chosen as the feedstock, so within the RSH module the function IF wheat straw chosen THEN wheat straw composition used. Following this within the mechanical/alkaline fractionation module, IF mechanical/alkaline pretreatment chosen in the user interface page THEN mechanical/alkaline module looks to the RSH module for input flow and composition. This logic continues throughout the modules and if modules are not chosen in the user interface then the module inputs and outputs remain at zero and no calculations are performed.

7.2.1 FEEDSTOCK RECEPTION, STORAGE AND HANDLING (RSH)

All biorefinery concepts begin with the feedstock reception, storage and handling module (RDH). In this module the biomass is received, cleaned, chopped and stored ready for processing. If a thermochemical process (i.e. gasification or fast pyrolysis) is chosen by the user to follow then this module includes a drying step to remove water to the required

moisture content. If fast pyrolysis is chosen by the user, then an extra grinding step is included to reduce the biomass to the required particle size. No modules can precede the feedstock, reception, storage and handling module but there a number of modules which may follow it (see

Table 7.2).

The inbuilt logic rules for this module:

- Depending on the feedstock chosen in the user interface the input composition changes (see Table 7.1). The solid rejects assumption also changes depending on the feedstock; 0.5wt% for wheat straw and 1% for softwood. The reject level was provided by ABNT (97, 115) for wheat straw and an arbitrary value was assumed for softwood.
- The module calculates the total biomass required based on the figure input by the user and any additional requirement for power and/or heat (this value taken from the heat and power or heat only modules).
- If gasification or pyrolysis is chosen by the user as the subsequent module then a drying step is included.
  - Depending on the conversion process a different drying requirement is used in the model (gasification feed 15wt% water, pyrolysis feed 10wt% water)
  - An additional grinding step is included if fast pyrolysis has been chosen to follow, as a smaller particle size is required for this process.
- Depending on the location chosen by the user, the location factor (see Table 5.11) changes in the Fixed Capital Investment (FCI) calculations.
- Depending on the scale chosen by the user, the FCI calculation automatically adjusts.

Table 7.1 – Feedstock composition

	Wheat straw	**Softwood**
	Wt% wet basis	**Wt% wet basis**
Water	11%	30%
Cellulose	35%	31%
Hemicellulose	22%	17%
Lignin	17%	20%
Ash	8%	1%
Other	7%	2%

Table 7.2 – Feedstock reception, preparation, storage and handling module connections

Preceding module/s	Subsequent module/s
N/A	AVIDEL
	Mechanical/alkaline fractionation
	Aquathermolysis
	Pyrolysis
	Steam explosion
	Organosolv
	Conc. HCl pretreatment
	Gasification

7.2.2 STEAM EXPLOSION

Steam explosion is a thermochemical pretreatment method. The biomass is impregnated with sulphuric acid before being fed to digesters. Here high pressure steam is added and the steam explosion occurs. The explosion breaks down the internal structures of the biomass and releases the hemi-cellulose sugars. The RSH module precedes the steam explosion module and the fractionation module always follows (see Table 7.3)

If steam explosion or ABNT base case is chosen as the pretreatment method by the user:

- Steam explosion module looks to the RSH module for the biomass input and composition.
- Depending on the location chosen by the user, the location factor changes in the FCI calculations.
- Depending on the scale chosen by the user, the FCI calculation automatically adjusts

Table 7.3 – Steam explosion module connections

Preceding module/s	Subsequent module/s
RSH	Fractionation

7.2.3 FRACTIONATION

The fractionation module always follows the steam explosion pre-treatment module and includes two steps; a solid/liquid separation resulting in a cellulose/lignin stream and C5 stream follower by a further optional lignin separation step (see Figure 5.2). If the user choose steam explosion then the next option displayed “Is lignin separation to be included?”. The user makes the choice of yes or no from the drop down menu. This includes or excludes lignin separation from the fractionation module. The possible connections for this module are shown in Table 7.4.

If steam explosion followed by no lignin separation or the ABNT bas case is chosen in the user interface:

- The input flow and composition is imported from the steam explosion module.

- The solid/liquid separation part of the module is completed.
- The output of this module with no lignin separation is a cellulose/lignin stream and a C5 stream.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts and if lignin separation is not chosen by the user, then this is removed from the cost calculations.

If steam explosion followed by lignin separation is chosen:

- The input flow and composition is imported from the steam explosion module.
- The solid/liquid separation part of the module is completed.
- The cellulose/lignin stream undergoes further processing to separate the lignin.
- The output of this module when fractionation is chosen is separate cellulose, lignin and C5 streams.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.4 – Fractionation module connections

Preceding module/s	Subsequent module/s
Steam explosion	C5 to ethanol
	C5 to ABE
	C5 to furfural
	C5 to surfactants
	C5 to xylonic acid
	C6 to ethanol
	C6 to ABE
	C6 to FDCA
	Lignin pyrolysis*
	Lignin drying*
	Lignin gasification*

*only if lignin fractionation included

7.2.4 AVIDEL

AVIDEL is a pretreatment method in which cellulose is extracted by the solubilisation of lignin and hemicellulose. The solubilisation is carried out by a solution of organic acids. This gives C5, C6 and lignin streams for further processing. The possible connections for this module are shown in Table 7.5.

If AVIDEL is chosen as the pretreatment method in the user interface page:

- AVIDEL module looks to the RSH module for the biomass input and composition.

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI automatically adjusts.

Table 7.5 – AVIDEL module connections

Preceding module/s	Subsequent module/s
RSH	C5 to ethanol
	C5 to ABE
	C5 to furfural
	C5 to surfactants
	C5 to xylonic acid
	C6 to ethanol
	C6 to ABE
	C6 to FDCA
	Lignin pyrolysis
	Lignin drying
	Lignin gasification

7.2.5 ORGANOSOLV

The aim of the Organosolv pretreatment is to dissolve the lignin in order to release the sugar fractions and make them more hydrolysable. The biomass is heated in the presence of a solvent, leading to the dissolution of the lignin fraction; various separations then follow, to result in three streams; C5, C6 and lignin. The possible connections for this module are shown in Table 7.6.

If Organosolv is chosen as the pretreatment method in the user interface page:

- Organosolv module looks to the RSH module for the biomass input and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI automatically adjusts.

Table 7.6 – Organosolv module connections

Preceding module/s	Subsequent module/s
RSH	C5 to ethanol
	C5 to ABE
	C5 to furfural
	C5 to surfactants
	C5 to xylonic acid
	C6 to ethanol
	C6 to ABE
	C6 to FDCA
	Lignin pyrolysis
	Lignin drying
	Lignin gasification

7.2.6 MECHANICAL/ALKALINE FRACTIONATION

Within this pretreatment method the biomass is both mechanically and chemically pre-treated. The biomass is soaked in NaOH and placed in a conical reactor with vigorous agitation. There follows a number of separation steps in order to obtain the separate C5, C6 and lignin fractions. The possible module connections for mechanical alkaline fractionation are shown in Table 7.7.

If mechanical/alkaline fractionation is chosen in the user interface page:

- Mechanical/alkaline fractionation module looks to the RSH module for the biomass input and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.7 – Mechanical/alkaline fractionation module connections

Preceding module/s	Subsequent module/s
RSH	C5 to ethanol
	C5 to ABE
	C5 to furfural
	C5 to surfactants
	C5 to xylonic acid
	C6 to ethanol
	C6 to ABE
	C6 to FDCA
	Lignin pyrolysis
	Lignin drying
	Lignin gasification

7.2.7 CONCENTRATED HCL PRETREATMENT

In this pretreatment method the biomass is treated with a concentrated solution of HCl. This leads to the hydrolysis of cellulose and hemicellulose to sugars. The solid lignin stream is separated to result in a C5 rich stream, a C6 rich stream and a lignin stream for further processing. The possible module connections are shown in Table 7.8.

If concentrated HCl pretreatment is chosen as the pretreatment method by the user in the user interface page:

- HCl pretreatment module looks to the RSH module for the biomass input and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.8 – Concentrated HCl pretreatment module connections

Preceding module/s	Subsequent module/s
RSH	C5 to ethanol
	C5 to ABE
	C5 to furfural
	C5 to surfactants
	C5 to xylonic acid
	C6 to ethanol
	C6 to ABE
	C6 to FDCA
	Lignin pyrolysis
	Lignin drying
	Lignin gasification

7.2.8 AQUATHERMOLYSIS

In this module the biomass is treated with hot pressurised water. The hemicellulose is removed with the cellulose and lignin relatively unaffected. The hemicellulose fraction is then used to produce furfural, whereas the cellulose/lignin is recovered as a residue which is dried and processed using fast pyrolysis. The possible module connections are shown in Table 7.9.

If aquathermolysis is chosen as the pretreatment method by the user in the user interface page:

- Aquathermolysis module looks to the RSH module for the biomass input and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.9 – Aquathermolysis module connections

Preceding module/s	Subsequent module/s
RSH	Fast pyrolysis

7.2.9 GASIFICATION AND GAS CLEAN UP (FLUIDISED BED)

In this module dried biomass is fed into a circulating fluidised bed gasifier with steam as the gasifying agent. The resulting gasification products are cleaned to remove contaminants such as tar and acid gases, to leave a clean syngas suitable for further processing. The possible module connections are shown in Table 7.10.

If gasification followed by mixed alcohol synthesis is chosen by the user in the user interface page:

- In the RSH module, drying calculations are included.

- Gasification and gas clean up (fluidised bed) module looks to the RSH module for the dried biomass input and composition.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.10 – Gasification and gas clean-up (pre alcohol synthesis) module connections

Preceding module/s	Subsequent module/s
RSH	Mixed alcohol synthesis
Fractionation (lignin stream)	
AVIDEL (lignin stream)	
Mechanical/alkaline fractionation (lignin stream)	
Organosolv (lignin stream)	
Conc. HCl pretreatment (lignin stream)	

7.2.10 GASIFICATION AND GAS CLEAN UP (DIRECT) WITH FISCHER-TROPSCH TO HYDROCARBON FUELS

In this module the biomass is gasified in a high pressure oxygen blown fluidised bed. Following gasification are gas clean up steps to remove contaminants such as tar and particulates from the syngas. The syngas is then processed in a slurry phase Fischer-Tropsch synthesis reactor for conversion into hydrocarbons and resulting in diesel and gasoline as finished products. The possible module connections are shown in Table 7.11.

If gasification followed by Fischer-Tropsch synthesis to hydrocarbon fuels is chosen in the user interface page:

- In the RSH module, drying calculations are included.
- Gasification and gas clean up with Fischer-Tropsch to hydrocarbon fuels module looks to the RSH module for the dried biomass input and composition.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.11 – Gasification and gas clean up (BtL) module connections

Preceding module/s	Subsequent module/s
RSH	N/A

7.2.11 MIXED ALCOHOL SYNTHESIS

In this module clean syngas from the gasification modules is reacted in the presence of a catalyst to produce a mixed alcohol stream containing methanol, ethanol, propanol, butanol and pentanol. The possible module connections are shown in Table 7.12.

If gasification followed by mixed alcohol synthesis is chosen in the user interface:

- Mixed alcohol synthesis module looks to gasification and gas clean up (fluidised bed) module for input flow and composition.

If bio-oil gasification has been chosen then the only option available for processing the syngas is mixed alcohol synthesis:

- The mixed alcohol synthesis module looks to the bio-oil gasification module for input flow and composition.

For biomass and bio-oil gasification:

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.12 – Mixed alcohol synthesis module connections

Preceding module/s	Subsequent module/s
Gasification and gas clean up	Mixed alcohol distillation

7.2.12 MIXED ALCOHOL DISTILLATION

This module automatically follows the mixed alcohol synthesis module if this has been chosen by the user. The mixed alcohol stream is distilled into separate alcohol product streams. The possible module connections are shown in Table 7.13.

If mixed alcohol synthesis is chosen following gasification and gas clean up (fluidised bed) or bio-oil gasification:

- The input flow and composition is imported from the mixed alcohol synthesis module.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.13 – Mixed alcohol distillation module connections

Preceding module/s	Subsequent module/s
Mixed alcohol synthesis	N/A

7.2.13 C5 TO ETHANOL

In this module the C5 rich stream from a pretreatment module is fermented to ethanol. The product of this module is a beer stream, which is sent to distillation to obtain the final ethanol product. The possible module connections are shown in Table 7.14.

If C5 to ethanol or ABNT base case is chosen in the user interface page:

- Depending on the pretreatment module preceding, the C5 to ethanol module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C5 stream flow and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.14 – C5 to ethanol module connections

Preceding module/s	Subsequent module/s
Fractionation	Ethanol distillation
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.14 C5 TO ABE

In this module a C5 rich stream from a pretreatment module is fermented to produce an acetone-butanol-ethanol (ABE) mixture. This module includes continuous extraction of the product mixture by pervaporation. The possible module connections are shown in Table 7.15.

If C5 to ABE is chosen in the user interface page:

- Depending on the pretreatment module chosen by the user, the C5 to ABE module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C5 stream flow and composition.
- The C5 to ABE module looks to the preceding pretreatment module for the stream temperature. This determines whether a cooling step is included in the calculations. If the stream is >40^{o}C it requires cooling.
- If mechanical/alkaline fractionation is the preceding pretreatment module then a neutralisation step is included.
- If the concentration of sugars in the stream to fermentation is <5%, distillation is the product recovery process utilised in the module. If the sugar concentration is >5% then pervaporation is the recovery process.
- The cost estimation is automatically adjusted depending on the product recovery method (distillation or pervaporation).
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

If C5 to ABE and C6 to ABE are chosen in the user interface then the C5 stream is redirected to the C6 to ABE module; the C5 to ABE module remains blank. The combined C5 and C6 to ABE module rules are included in the C6 to ABE module (Section 7.2.19).

Table 7.15 – C5 to ABE module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.15 C5 TO FURFURAL

A C5 rich stream from a pretreatment module is converted into furfural in this module. The module involves the reaction of the C5 stream with steam and acid to produce furfural. A separation and distillation step is included to result in the final furfural product stream. The possible module connections are shown in Table 7.16.

If C5 to furfural is chosen following a pretreatment module in the user interface page:

- Depending on the pretreatment module chosen by the user, the C5 to furfural module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C5 stream flow and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.16 – C5 to furfural module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.16 C5 TO SURFACTANTS

In this module a C5 stream from a pretreatment module is converted into bio-based surfactants by glycosylation. The reaction involves heating of the C5 stream in the presence of alcohols. The surfactant product is then recovered by evaporation. The possible module connections are shown in Table 7.17

If C5 to surfactants is chosen in the user interface page:

- Depending on the pretreatment module chosen by the user, the C5 to surfactants module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C5 stream flow and composition
- The C5 to ABE module looks to the appropriate pretreatment module for the stream temperature. This determines the level of preheating that can be achieved by exchange with the recycled condensates.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.17 – C5 to surfactants module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.17 C5 TO XYLONATE (XYLONIC ACID)

In this module xylonic acid is produced from the C5 sugars contained in the C5 stream following pretreatment. This module includes product recovery to result in the finished xylonic acid product. The possible module connections are shown in Table 7.18.

If C5 to xylonic acid is chosen following a pretreatment module in the user interface page:

- Depending on the pretreatment process chosen by the user, the C5 to xylonic acid module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C5 stream flow and composition
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.18 – C5 to xylonate module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.18 C6 ENZYMATIC HYDROLYSIS AND FERMENTATION

In this module the C6 stream from a pretreatment module undergoes enzymatic hydrolysis and fermentation to produce ethanol. The product of this module is a low ethanol concentration "beer" stream containing the product alcohol. This is sent onto the distillation module for product recovery. The possible module connections are shown in Table 7.20.

If C6 enzymatic hydrolysis and fermentation to ethanol or the ABNT base case is chosen in the user interface page:

- Depending on the pretreatment module, the C6 to ethanol module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C6 stream flow and composition.
- The C6 to ethanol module looks to the appropriate pretreatment module for the stream temperature. This determines whether a cooling step is included in the calculations. If the stream is >40^{o}C it requires cooling.
- Depending on the pretreatment module prior to this module a different cellulose hydrolysis efficiency is used. The different efficiencies are shown in Table 7.19.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.19 – C6 to ethanol module cellulose hydrolysis assumption

Pretreatment	Cellulose hydrolysis, %
AVIDEL	48%
Conc. HCl	60%
Mech/Alk Fractionation	86%
Organosolv	66%
Steam explosion	90%

Table 7.20 – C6 to ethanol module connections

Preceding module/s	Subsequent module/s
Fractionation	Ethanol distillation
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.19 C6 (&C5) FERMENTATION TO ABE

In this module either the C6 stream from a pretreatment module, or both the C5 and the C6 streams are fermented to acetone-butanol-ethanol (ABE). This module also includes product recovery to give a finished ABE mixture. The possible module connections are shown in Table 7.21.

If C6 fermentation to ABE is chosen in the user interface page:

- Depending on the pretreatment process module, the C6 to ABE module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C6 stream flow and composition.
- If C5 to ABE has also been chosen then the C6 to ABE module looks to the C5 to ABE module for the C5 flow and composition.
- If steam explosion is the pretreatment module then a different model (within the module) is utilised as the stream first has to be neutralised before undergoing hydrolysis and fermentation (see Figure 6.21)
- The neutralised C6 stream then undergoes enzymatic hydrolysis, is mixed with the C5 stream (if included) and is fermented to ABE.
- For all other pretreatments preceding the module the C6 and C5 stream (if included) are mixed before undergoing enzymatic hydrolysis, fermentation and product recovery (see Figure 6.22)
- Depending on the pretreatment module prior to this module a different cellulose hydrolysis efficiency is used. The different efficiencies are shown in Table 7.19.
- Depending on the steps included in the module model, the cost estimations update automatically to include/exclude process steps.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.21 – C5 to ABE module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.20 C6 TO FDCA

This module involves the enzymatic hydrolysis of the C6 stream from a pretreatment module, followed by dehydration and oxidation to result in FDCA. The possible module connections are shown in Table 7.22.

If C6 to FDCA is chosen in the user interface page:

- Depending on the pretreatment module chosen by the user, the C6 to FDCA module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the C6 stream flow and composition.

- The C6 to FDCA module looks to the appropriate pretreatment for the stream temperature. This determines whether a cooling step is included in the calculations. If the stream is >40^{o}C it requires cooling.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.22 – C6 to FDA module connections

Preceding module/s	Subsequent module/s
Fractionation	N/A
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.21 ETHANOL DISTILLATION

Beer streams from C6 and/or C5 fermentation are the input to this module to recover the final ethanol product stream. The possible module connections are shown in Table 7.23.

If C5 to ethanol and/or C6 to ethanol are chosen by the user in the user interface page:

- If C5 to ethanol has been chosen then the ethanol distillation module looks to the C5 to ethanol module for input flow and composition.
- If C6 to ethanol has been chosen then the ethanol distillation module looks to the C5 to ethanol module for input flow and composition.
- If C5 to ethanol and C6 to ethanol have been chosen, the ethanol distillation module will look to both these modules for input flow and composition.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.23 – Ethanol distillation module connections

Preceding module/s	Subsequent module/s
C5 to ethanol	N/A
C6 to ethanol	

7.2.22 PYROLYSIS

In this module raw biomass, the dry solid residue from aquathermolysis or a dried lignin stream from a pretreatment module undergoes fast pyrolysis. This results in bio-oil which may be sold as a finished product or processed in further modules. The possible module connections are shown in Table 7.24.

If pyrolysis of the whole biomass is chosen by the user in the user interface page:

- Drying and grinding calculations are included in the RSH module.
- The pyrolysis module takes the dry biomass input flow and composition from the RSH module.

If pyrolysis of the lignin fraction is chosen after a pretreatment step:

- Depending on the pretreatment process chosen by the user, the pyrolysis module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the lignin flow and composition.

If the aquathermolysis module is chosen in the user interface:

- The pyrolysis module looks to the aquathermolysis module for the solid residue flow and composition.

In both cases:

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.24 – Fast pyrolysis module connections

Preceding module/s	Subsequent module/s
RSH	Bio-oil phenolic fractionation
Drying	Bio-oil heat and power plant
Aquathermolysis	

7.2.23 LIGNIN DRYING

In this module lignin from a pretreatment module is dried, to obtain dry lignin suitable for sale or further processing. The possible module connections are shown in Table 7.25.

If lignin gasification, dry lignin product or the ABNT base case is chosen by the user in the user interface page:

- Depending on the pretreatment module, the lignin drying module looks to the fractionation, AVIDEL, mechanical/alkaline fractionation, Organosolv or concentrated HCl pretreatment module for the lignin flow and composition.
- The lignin drying module extracts the lignin stream temperature from the appropriate pretreatment, as this has an impact on the heat required by the module to dry the lignin.
- Depending on the process chosen for the lignin, different moisture requirement levels are used; lignin for sale 16wt%, lignin for gasification or pyrolysis 10wt%.

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation adjusts.

Table 7.25 – Lignin drying module connections

Preceding module/s	Subsequent module/s
Fractionation	Fast pyrolysis
AVIDEL	
Mechanical/alkaline fractionation	
Organosolv	
Conc. HCl pretreatment	

7.2.24 STILLAGE DRYING

When the ABNT base case is chosen in the user interface, then this module is automatically included. In this module the stillage from the fermentation process is dried to give a finished product which may be sold as animal feed or as a fuel. The stillage contains a high proportion of lignin, as no lignin fractionation follows steam explosion. The whole cellulose/lignin stream is sent for fermentation. The possible module connections are shown in Table 7.26.

If the ABNT base case is chosen in the user interface page:

- The stillage drying module takes the stillage flow and composition from the ethanol distillation module.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.26 – Stillage drying module connections

Preceding module/s	Subsequent module/s
Ethanol distillation	N/A

7.2.25 BIO-OIL FRACTIONATION

In this module bio-oil from the fast-pyrolysis module undergoes a fractionation process, to obtain a phenolic fraction. This process involves water and alkali addition, fractionation and evaporation. The phenolic fraction may then be sold as a direct substitute for phenol in phenol-formaldehyde resins. The possible module connections are shown in Table 7.27.

If bio-oil fractionation is chosen following fast pyrolysis in the user interface page:

- The bio-oil fractionation module takes the bio-oil flow and composition from the pyrolysis module.

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.27 – Bio-oil fractionation module connections

Preceding module/s	Subsequent module/s
Fast pyrolysis	N/A

7.2.26 BIO-OIL FOR HEAT AND POWER

The bio-oil from fast pyrolysis along with any combustible process residues is processed in this module to generate heat and power. The bio-oil is combusted to generate steam which passes through a turbine to generate power. This heat and power may be used to meet the biorefinery requirements and it has the potential to be integrated into a conventional petrochemical refinery in order to reduce fossil based heat and power demand. The possible module connections are shown in Table 7.28.

If bio-oil for heat and power is chosen to followed fast pyrolysis in the user interface page:

- The bio-oil composition is taken from the water and residues module (the flow and composition is included in this module if bio-oil gasification has been chosen by the user).
- The total steam requirement for the biorefinery is taken from the water and residues module and used to calculate the remaining process heat to be utilised.
- The total electricity requirement of the biorefinery is taken from the water and residues module and used to calculate the remaining electricity to be utilised.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.28 – Bio-oil for heat and power module connections

Preceding module/s	Subsequent module/s
Fast pyrolysis	N/A

7.2.27 BIO-OIL GASIFICATION AND GAS CLEAN-UP

Bio-oil from the fast pyrolysis module is gasified in this module to produce syngas for further processing. The bio-oil is gasified in an oxygen blown entrained flow gasifier followed by acid gas removal to provide clean syngas for further processing. The possible module connections are shown in Table 7.29.

If bio-oil gasification is chosen by the user in the user interface page:

- The bio-oil flow and composition is taken from the pyrolysis module.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

Table 7.29 – Bio-oil for heat and power module connections

Preceding module/s	Subsequent module/s
RSH	Alcohol synthesis

7.2.28 WATER AND RESIDUES

This module is included in all biorefinery concepts. This module brings together information from all other modules on steam usage, condensate collection, steam generated by modules, freshwater requirement, cooling water return, liquid and gaseous residues. This module is connected to all others and data is automatically collected through the links. From this module the overall steam requirement, freshwater requirement, wastewater to treatment plant and residues to the heat and power module are calculated.

7.2.29 WASTEWATER

This module is included in all biorefinery concepts. The wastewater flow and composition are taken from the water and residues module.

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

7.2.30 HEAT AND POWER

In this module process residues and biomass are used to provide heat and power for the biorefinery concept. The residues and biomass are combusted to generate steam. The steam then passes through a turbine in order to generate electricity.

If the user chooses that heat and electricity for the biorefinery concept are to be provided by biomass and process residues:

- The total steam requirement for the biorefinery is taken from the water and residues module.
- The total electricity requirement is taken from the summary page. The amount of surplus electricity, once the needs of the biorefinery have been met, is calculated.

- The flow and composition of process residues is taken from the water and residues module and used to calculate if extra biomass is required in order to meet the heat demand of the biorefinery concept.
- The module feeds back to the RSH module the amount of extra biomass required for heat and power.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

7.2.31 HEAT ONLY

In this module process residues and biomass are used to provide heat for the biorefinery concept. The residues and biomass are combusted to generate steam. The electricity requirement is purchased from the grid.

If the user chooses on the user interface page that heat for the concept is to be provided by biomass and process residues:

- The total steam requirement for the biorefinery is taken from the water and residues module.
- The total electricity requirement is taken from the summary page
- The flow and composition of process residues is taken from the water and residues module and used to calculate if extra biomass is required in order to meet the heat demand of the biorefinery concept.
- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

7.2.32 NO HEAT AND POWER

In this module heat and power is supplied from non-renewable sources. Natural gas is combusted to provide the steam and the electricity is purchased from the grid.

If the user chooses that heat and power for the biorefinery is not to be provided by biomass and process residues:

- The total steam requirement for the biorefinery is taken from the water and residues module and the amount of natural gas required to produce this is calculated.
- The total electricity requirement is taken from the summary page to calculate the cost of purchasing this from the grid.

- Depending on the location chosen in the user interface the location factor changes in the FCI calculations.
- Depending on the scale the FCI calculation automatically adjusts.

7.2.32.1 SUMMARY MODULE

This module provides an overall summary of the biorefinery concept. It is connected to all other modules and is used to display the results of the chosen biorefinery concept. It includes calculations the overall costs, profit/loss, efficiency and the totalised results for the biorefinery. An example of this summary page can be found in Appendix 4.

8 REVIEW OF BIOREFINERY EVALUATION METHODS

This chapter focuses on the final step in the methodology – biorefinery chain evaluation and comparison. The specification for the full methodology and the part that the evaluation step plays is described in Section 3.5. A technique was required to utilise the results generated in the process model to compare the biorefinery concepts on the basis of cost, efficiency, environment, socio-economic and other criteria. The comparison method had to consider all criteria in a flexible, transparent and repeatable way in order to rank the biorefineries and identify the most promising.

In this chapter the literature is reviewed to assess current evaluation methods for the identification of promising biorefinery processes. The different literature evaluations are described according to the criteria included as for this thesis an evaluation method was required that would allow criteria to be included or excluded in a flexible way. To begin the chapter in Section 8.1 the main characteristics of the methodology required for the evaluation of biorefineries are defined. The evaluation method was required to assess the biorefinery options in order to identify the "best" option, where best could mean the most profitable, efficient, environmentally or socio-economically beneficial or a good performance from a combination of these factors. Once reviewed in Section 8.2, the suitability of the evaluation methods found in the literature to this project is discussed in Section 8.3.

8.1 REQUIRED CHARACTERISTICS OF EVALUATION METHODOLOGY

An evaluation method was required to evaluate the 27 biorefinery concepts, and from the evaluation the most promising biorefinery concepts had to be identified. The methodology for biorefinery evaluation was required to have the following characteristics.

- The methodology needed to be consistent with the same defined methodology applied to each evaluation.
- The methodology had to be easily reapplied to investigate different scenarios with results generated quickly.
- The method for using the modelling results to evaluate and rank the biorefinery concepts had to be transparent and easy to explain and justify.
- The ability to consider a range of criteria. From the process modelling step data was available about processing efficiency, process economics, environmental impact and

socio-economic impacts. The chosen methodology had to be capable of evaluating any combination of these criteria.

- The ability to set the objectives of the analysis as different stakeholder groups have different objectives for the biorefinery analysis. For example, industrial stakeholders may be interested in the most cost effective biorefineries, whereas environmentalists would be interested in the most environmentally friendly biorefinery concepts. Therefore the methodology chosen had to be capable of reapplying the analysis according to a group's particular interest.
- The ability to reapply the methodology as new information was added or as new biorefinery concepts were to be considered. As well as the requirement to reapply the analysis according to stakeholder's interests, there was also the requirement of flexibility to include more information or concepts as they were generated.

The key requirements for the evaluation methodology were flexibility and consistency. A methodology was required that would allow the users to quickly compare and analyse biorefinery concepts for some or all of the criteria with varying objectives. The biorefinery concepts had to be evaluated technically, economically, environmentally and in terms of socio-economics. The extent and depth of the evaluation possible was not to be limited by the evaluation method chosen. Although the evaluation method was required for 27 concepts, it was not to be limited by this number and had to be flexible enough to be reapplied to any number of biorefinery concepts.

8.2 REVIEW OF CONVENTIONAL METHODS FOR BIOREFINERY EVALUATION

It became clear from the literature that biorefinery evaluations differed from paper to paper, with some work focussing on the technical aspects, economics, environmental impacts, markets or any combination of these criteria. For this thesis an evaluation method was required that would allow the user to include or exclude criteria. The method chosen was to allow the increase or decrease in importance of criterion in the overall ranking.

Numerous evaluations have been carried out in the literature, some examples are given in Table 8.1 which also lists the criteria that are included in the evaluation; technical, economic, environmental, market. The majority of the evaluation work focussed on ethanol based processes (137, 42, 22, 75) as can be demonstrated by the work listed in Table 8.1 but there is also the need to consider other product portfolios and processing technologies. The majority of evaluation studies were techno-economic, with a relatively small number including other criteria such as environmental performance or an assessment of the market

situation for the biorefinery products. No work was found that included socio-economic evaluation in conjunction with the other criteria. In the following sections different biorefinery evaluations, including some or all of the criteria, are described and the potential application to this project discussed.

8.2.1 TECHNICAL EVALUATION

Technical evaluations of biorefineries focus on the operation and efficiency of the processes or describe specific processing areas in great technical detail. The technical evaluations in the literature tended to be reviews of the technologies available for processing of biomass, or for recovery of products. These were normally descriptive and in general did not focus on identifying the best option, but in some cases the writer did state their own opinion of the most promising options. Within the literature there have been technical reviews of products from gasification (12), the products from biomass(40, 41), biorefinery processes (21), different product separation technologies (142, 119) but mostly about the production of ethanol (74, 144, 15).

An example of a technical evaluation is the work by Huang et al. (142). Huang (142) gives a critical technical review of separation methods related to biorefineries. These included the extraction of sugars through different pretreatment methods and product separation and recovery. The focus of the review were processes involved in ethanol based biorefineries and gave details of the processes involved in terms of recovery, yields and operating conditions. Based on the critical review of the techniques, Huang then identified the two key steps in a biorefinery that offer the biggest opportunities and challenges in terms of separation. These were the detoxification of the streams for ethanol fermentation and ethanol product recovery. Huang identified these processes as having the most potential and promise for further research and development. This choice was made purely based on the knowledge of the writers and the information they had collected. A disadvantage of this type of review is that the whole plant is not evaluated; only component parts of a theoretical plant. It was very difficult to evaluate how these technologies would perform as part of a whole plant and which technologies should be included. It was not possible to quickly carry out this kind of analysis and a simple technical review would not be suitable for the detailed evaluation of the 27 biorefinery concepts. The methodology used to evaluate the processes did not follow a defined methodology and so would not be repeatable by another group of researchers.

Table 8.1 – Biorefinery evaluations in the literature

Author	Topic	Technical	Economic	Environment	Market
Balat et al. (43)	Feedstocks, pretreatments	✓			
Balat et al. (138)	Fuels & chemicals from pyrolysis	✓			
Black and Veatch (25)	Lignocellulosic ethanol plants	✓	✓	✓	✓
Boerrigter et al. (162)	Co-production of FT fuels & substitute natural gas	✓	✓	✓	
Bridgwater (86)	Thermal processing of biomass	✓	✓		
Cardona and Sanchez (42)	Ethanol	✓	✓		
Cardona and Sanchez (74)	Ethanol, energy consumption	✓			
Cherubini et al. (139)	Ethanol biorefinery			✓	
Cherubini et al. (140)	Biofuel & bioenergy systems			✓	
Corma et al. (41)	Chemical products from biomass	✓			✓
Demirbas (21)	Biorefinery processes	✓			
Deverell et al. (45)	Ethanol production	✓	✓		
Dutta and Phillips (122)	Thermochemical ethanol	✓	✓		
Foust et al. (22)	Ethanol biochemical vs. thermochemical		✓	✓	
Hamelinck and Faaij (76)	Biofuels, now vs. future	✓	✓		
Hamelinck et al (75)	Ethanol short, medium & long term	✓	✓		
Hamelinck et al.(141)	FT fuels from biomass	✓	✓		
Holladay et al. (38)	Biorefinery lignin products	✓	✓		✓
Huang et al. (24)	Ethanol, biomass & plant size	✓	✓		
Huang et al. (142)	Review of separation technologies	✓			
Huber et al. (40)	Fuel products from biomass	✓			✓
Kazi et al. (23)	Ethanol, pretreatment methods	✓	✓		
Larson et al. (118)	Gasification, fuels and electricity	✓	✓		
Lynd et al. (4)	Biorefineries (succinic acid)		✓		✓
Mu et al. (143)	Biochemical vs. thermochemical ethanol			✓	
Phillips et al. (120)	Gasification, mixed alcohols	✓	✓		
Piccolo and Bezzo (14)	Ethanol biochemical vs. thermochemical	✓	✓		
Ptasinski (12)	Gasification and biofuels	✓			
Sanchez and Cardona (144)	Ethanol from different feedstocks	✓			
Sassner et al. (145)	Ethanol, different feedstocks	✓	✓		
Seiler et al. (146)	BtL processes	✓	✓		
Sendich et al. (147)	Ethanol biorefineries		✓	✓	
Sivers and Zacchi (112)	Ethanol production processes	✓	✓		
Sun and Cheng (111)	Ethanol production	✓			
Tijmensen et al. (119)	Review of separation technologies	✓			
Uihlein and Schebek (10)	Lignocellulosic biorefinery			✓	
Vliet et al. (148)	FT diesel well-to-wheel	✓	✓	✓	
Wei et al. (15)	Ethanol production	✓			
Weiss et al. (149)	Bio-based energy, fuels, materials			✓	
Werpy et al. (39)	Products from biomass	✓	✓		✓
Wright and Brown (26)	Optimal size of biorefineries	✓	✓		
Wright et al. (150)	Biochemical vs. thermochemical		✓		

Technical evaluations are useful for validation of the assumptions used in the process models and to help identify the main advantages and disadvantages of the various routes but it was very difficult to compare and evaluate the best option. The comparison was most often subjective, based on the researchers experience and knowledge about which option was the most practical or preferred. This was not consistent or repeatable.

8.2.2 TECHNO-ECONOMIC EVALUATION

In techno-economic evaluations both the technical and economic performance of the processes are considered. This was the most common form of biorefinery evaluation and the majority of the studies focused on ethanol production as research on bioethanol is more advanced than some of the other biofuels production technologies (23). In general the techno-economic evaluations involved detailed process models to be constructed, often using simulation software such as Aspen, to generate process and economic data. The data was then evaluated in order to make some judgements about the processes studied. The modelling technique for this thesis is defined in Chapter 5 but an evaluation technique was required to evaluate the large quantity of results produced for the 27 concepts. It was interesting to review the literature in order to see how other researchers are using the data generated in these models.

One example of the techno-economic evaluations found in the literature was the work by Huang et al. (24). Huang's paper consists of an evaluation of the impact of five different biomass species on the process and economic performance of a bioethanol plant. A single process model was used for ethanol production, based on the National Renewable Energy Laboratory USA (NREL) bioethanol plant model (137) and then the feedstock composition was varied to judge the impact on ethanol yield and costs. In this work Huang also evaluates the impact of delivered feedstock cost for each of the five feedstocks on the overall plant size. The delivered feedstock is highly dependent on the location and availability of biomass so can have a large influence on economic performance. For each of the different scenarios a consistent methodology was used in terms of modelling and cost calculation. Due to the defined methodology it was possible to generate results for a number of variations in a clear and consistent way. This also meant that simple comparisons could be made between the scenarios, as a consistent method had been used in results generation. Although the methods applied to generate the results were consistent, Huang et al. evaluate each of the economic and processing criteria in isolation. This makes it hard to gauge the optimum result considering all criteria; i.e. which feedstock at which

scale. The consistent methodology for generation of results was similar to this project but a more robust and less subjective methodology was required for the evaluation of the results.

As mentioned previously, the majority of the techno-economic evaluations in the literature focused on ethanol. The work by Hamelinck et al. (75) was chosen for review because of the scope of the evaluation. They evaluated a wide range of processing options for the short, medium and long term production of ethanol. The most promising technologies for each of these stages in development were identified by a team of experts. The short term configuration consisted of processes that were already commercially available or at the pilot stage, the medium term was either at the pilot stage or promising lab stage and the long term included theoretical possibilities. The team made the choice based on the technical performance, availability of the technology and the judgement of the decision team; they did not use a defined methodology. The chosen configurations were modelled and the results used for the economic estimations. Hamelinck at al. did not identify the most promising option overall but the work does illustrate the improvements in performance as the technologies mature and gives a projection for future plants. There was no defined methodology for the evaluation of the options and it was up to the reader to make a judgement based on the information available in the report. Their work highlights the requirement for a defined evaluation technique.

One paper that did not focus on ethanol production was that by Larson et al. (118) which focused on other biofuels. In this paper gasification based systems were evaluated using a consistent design, simulation and analysis framework. Larson's work looks at alternative designs for producing fuels and power to evaluate future large scale facilities for gasification based systems producing FT fuels, DME and hydrogen from switchgrass. They directly compared 5 different plants at the same input scale. For the gasification and gas clean up plant (which was the same for all 5 scenarios) an evaluation was made by the writer and a judgement made of the optimum technology. The gasifier chosen was a pressurised oxygen blown fluidised bed reactor. In the paper a summary was given of the mass and energy balance results for all 5 process designs and the capital cost was calculated. Larson et al. (118) mention some of the things to take into account in a comparison such as consistent assumptions regarding installation factors, plant factors and expressing all costs in consistent units. They do not make an identification of the best option from those considered, it is up to the reader to sort through the results and make their own decision. Larson et al. generated the information but did not fully evaluate in order to find the best option. It is difficult for the reader to digest all of the produced data

and to take into account all of the different variables. For this thesis a more repeatable method is required plus the ability to handle the data generated.

Most other techno-economic studies were typically carried out on up to 10 different biorefinery concepts, but usually less than 5. The problem with these studies was that it was difficult to quickly re-evaluate scenarios or to include more schemes without requiring a lot of time and effort. These were useful as they provide validation data against which to compare modelled processes, and give an indication of the results to expect. The other issue with techno economic comparisons was that it was difficult to compare different studies. This was due to the fact that the studies will often use different assumptions, scale, year, conversion efficiencies etc. In the paper by Kazi et al. (23) they do attempt to compare results of their bioethanol production models to previous studies, and they found the results to be considerably different. They compared ethanol price from previous studies as a function of feedstock price (23). They state the differences were due to the differing assumptions used in the studies to generate the data. This is a problem that occurs when trying to compare different studies to each other, even the same processes, just because of the assumptions made. There was the need for a fully transparent, repeatable methodology so that the user can confidently make consistent comparisons. The ideal scenario would be the comparison of all the possible options using one system, taking results from the same knowledge base.

Another problem identified in these studies was representation of data. As the number of options increased, or the number of criteria evaluated increased, representing the result in a user friendly format becomes more difficult. It was often impossible to review all data easily in one chart or table, making it even more difficult to identify the best option.

8.2.3 TECHNO-ECONOMIC-ENVIRONMENT EVALUATION

A limited number of techno-economic-environment evaluations have been found (148, 162). Most focus on Fischer-Tropsch (FT) based biorefineries for the production of hydrocarbons. The techno-economic-environment studies illustrate the benefits of including environmental results in the evaluation to highlight the environmental benefits of a bio-based economy. It was surprising that more evaluations did not include environmental criteria, as the environmental benefit of bio-based plants is one of the main drivers for government led development.

One of the most comprehensive techno-economic-environmental evaluations was by Vliet et al. (148). They carried out a “well-to-wheel” analysis of FT diesel production in terms of

carbon, energy and cost. The aim of the research was to make a comprehensive study of the potential for FT diesel as a replacement for conventional diesel. They evaluated 14 different FT fuel production plants in complete biorefinery chains from field to user. The plants were fed with biomass, natural gas, coal or a combination of these. This made it possible to view the real benefits or disadvantages of the bio-based route in comparison to the conventional route and helps identify areas for future focussed improvement. As well as an economic and technical evaluation the environmental performance was assessed in terms of CO_2 emissions/km. The results were displayed in a series of charts and tables. There was no defined methodology for the evaluation. Vliet et al. concluded that it was environmentally beneficial to use FT diesel but emphasise the high level of uncertainty in the results. The benefit of this well-to-wheel type evaluation was that the same modelling methodology was applied to each technology combination. A disadvantage of this work was that a defined methodology was not applied to the evaluation and that each of the criteria was evaluated separately. The economic, process and environmental data were not used in conjunction to give an overall evaluation and they do not identify the best option from those studied. It was possible to identify the best option in terms of a particular variable, but difficult to get an overview. This was difficult because of the amount of information generated and it is hard for the user to combine and visualise all of the results from the analysis in order to identify the most promising route.

8.2.4 TECHNO-ECONOMIC-MARKET EVALUATION

The literature found on technical, economic and market evaluation focussed on the products of a biorefinery, rather than the processing plant itself (38, 39). One such piece of research was carried out by Werpy et al. (39). This focussed on the evaluation of the best products to manufacture in a biorefinery. In this research an effort had been made to evaluate and identify the best options using a defined methodology. The work evaluated building block chemicals which can be derived from sugars via biological and chemical conversions. Werpy et al. (39) identify the top 12 candidates from over 300 different options. First attempts to screen the identified options failed to provide sufficient differentiation amongst the options so a different approach had to be taken. An iterative review process, based on methods employed in the petrochemical industry was used in order to sort and rank the options. This was a method based on chemical data, known market data, properties, performance and the expert knowledge of the evaluation team (39). The fact that the first attempts failed illustrates how difficult it is to create a systematic evaluation approach but the finished methodology illustrates the benefits of a

defined evaluation structure. It enables the decision maker to quickly sort through a large number of options to result in the identification of the most promising. The structure ensures that the results are consistent and it is easy for the reader to understand the logic behind the end results. Because a number of the judgements in the report were made based on the opinion and knowledge of the evaluation team is could be argued that that the method was not as robust or repeatable as a method based on defined rules and relationships.

The paper by Holladay et al. (38) focused on products from lignin and identified more than 50 opportunities on the first screening. The potential uses for lignin were compiled and then evaluated in a similar structure to the work by Werpy et al. (39) based on technical difficulty, market and market risk, the use of the products as potential chemical building blocks and the condition of the lignin (pure or mixture). They attempted to identify the top 10 best opportunities but found this very difficult because of the uncertainty involved in the options and the level of complexity. Instead the opportunities were classified into near, medium of long term opportunities with the main barriers to development identified. Holladay et al. (38) investigated how these products fit into chemical or fuel markets. They evaluated the current available technology for use of the products and the likely acceptance of these products into the market place (known or unknown market) and the degree of difficulty to develop these products. The market was evaluated in terms of market size, expected market value and the market risk. Investigating from a technical and market perspective is useful to identify specific challenges or opportunities and is especially useful for eliminating products which look attractive financially but have no viable market. Some economic data was also included in the study, but the main focus was on the technical and market challenges. They identify the need for a sophisticated techno-economic analysis for evaluation the many different combinations and configurations possible. This technical analysis can be used to make judgements about the best route for the lignin, but this will vary depending on the processes employed in the biorefinery to extract the lignin. The work highlights the difficulties in making an assessment of the best option; illustrating the wide scope of information that needs to be included in evaluations. It also highlights the need for a defined methodology as it is easy for the reader to become lost in the information.

8.2.5 TECHNO-ENVIRONMENTAL EVALUATION

No literature was found that looked purely at the technical and environmental aspects of the biorefinery plants.

8.2.6 TECHNO-MARKET EVALUATION

The technical and market evaluations were found to focus on biorefinery products (40, 41). These were very detailed evaluations, but none made an effort to identify the most promising products. No technical and market evaluations of complete biorefinery plants were found in the literature.

One of the techno-market evaluations was by Corma et al. (41). This detailed technical review describes the chemical routes for the transformation of biomass into chemicals. Corma et al. (41) focused on environmentally friendly process routes that can substitute fossil based routes. As well as the chemical production routes, the application of the product and the market volume was described. Their work contained an extensive evaluation of the possibilities but did not identify the most promising; although they do state that the chosen products for a biorefinery will depend on the feedstock, processing cost, current market volume and price and the potential for creating new market opportunities. Although this paper was primarily a technical review, information about the current market situation for the chemical products was included where available. No attempt was made by Corma et al. to identify the most promising option.

A similar technical evaluation to that carried out by Corma et al. (41) was found in the report by Huber et al. (40) for the synthesis of transportation fuels from biomass. This work evaluated current methods and future possibilities for obtaining fuels from biomass. Huber discussed the chemistry involved in these processes, engineering solutions and the challenges to be overcome. Huber concluded that the optimal type of biomass for biofuels production depends on regional issues such as soil quality, precipitation and climate. The limiting factor was that low cost processing technologies that efficiently convert biomass into fuels do not yet exist. Cost has to be lowered and technologies have to be demonstrated on a commercial scale. This paper evaluated the options in turn but does not make an effort to identify the optimum products, as this is specific to the type of feedstock utilised in the biorefinery plant. These types of evaluation are more descriptive and provide some useful background information on which to build a more detailed assessment.

The work by Huber and Corma both state that the products are highly dependent on the feedstock, processing cost and other factors. This highlights the requirement for a flexible methodology to enable the user to generate and evaluate various biorefinery configurations, in order to identify the optimum product portfolio for a particular feedstock.

8.2.7 ECONOMIC-ENVIRONMENT EVALUATION

There was little work found in the literature combining economic and environmental evaluation of biorefineries (22, 147). This was surprising as the supposed environmental benefits of biorefineries are one of the main driving forces behind the development of these plants. The environmental performance of the biorefinery plants is a very important aspect but is only included in relatively few biorefinery evaluations.

One of the only pieces of literature found on the economic and environmental evaluation of biorefineries was the work by Sendich and Dale (147). They created a flexible modelling tool named the Biorefinery and farm Integrated Tool (BFIT). The modelling methodology differs from this thesis in that it included the biomass production and farm systems. The method allowed the basic environmental and economic analysis of biomass production, processing and bioenergy production across various regions of the United States. In this paper Sendich used BFIT to simulate various ethanol production scenarios, with six different farm management strategies in nine US locations. The tool was created in order to analyse both the economic and environmental impact of cellulosic biofuel systems. In the same way as the modelling methodology created for this thesis the tool is flexible and other scenarios can easily be inserted. Sendich and Dale's system make it easier to carry out multiple analyses and because a defined methodology is used in the modelling it is possible to carry out direct comparison. It is possible to carry out direct comparison of a small number of configurations, but it becomes more difficult as the number of scenarios increases. In this work they do not have a defined methodology for comparison or ranking of the options. This was a disadvantage of the system described. It was hoped that the work for this project would help provide such a methodology.

8.2.8 ENVIRONMENTAL EVALUATION

The environmental performance of biorefineries is one of the main driving forces behind government development of bio-based industry. As stated by Uihlein et al. (10) biorefineries are meant to contribute to a more sustainable future. A large number of environmental assessments were found in the literature (10, 139, 140, 143, 149).

One example of environmental evaluation of biorefineries was found in the paper by Uihlein et al. (10). This work was chosen out of the selection because the product portfolio included products other than ethanol and a defined methodology was used in the evaluation. Their work was based around a biorefinery fed with straw followed by hydrolysis, xylose to xylite and cellulose to ethanol, with lignin used as a binder. In this

paper six different variants of the same overall configuration were analysed: the standard configuration, optimised acid recovery, optimised heat recovery and optimised acid recovery and heat recovery combined, lignin for heat, lignin for electricity. From the results the optimal variant was identified in terms of environmental performance. For all variants of the biorefinery system analysed, the environmental performance in some impact categories was worse compared to the fossil counterparts, while advantages could be seen in other categories. Thus, the results do not support a clear-cut decision in favour of or against biorefineries. The comparison comprises of a summation of the environmental impacts for each variant. The same method is applied to each of the configurations to enable a comparison to be made between the options. This simple summation method for evaluation and ranking of variants is ideal for situations where the units of measurement are the same. It becomes problematic if trying to combine economic, environmental or other measures with differing units.

The environmental performance of these plants is of interest to researchers and policy makers, but industrial stake-holders are more interested in the financial benefits. Therefore an environmental evaluation by itself is of limited value. It is clear that the environmental performance alone cannot be used to identify the most promising biorefinery. When making an evaluation many factors should be considered including environmental performance. A more robust and inclusive methodology is required than that used by UIhlein (10) to compare criteria with potentially different units.

8.2.9 ECONOMIC EVALUATION

Most of the biorefinery evaluations were techno-economic, and only one piece of work was found that focussed on just the economics (145). This was the paper by Wright et al. (150) that compared the economics of five different biorefinery process schemes. In this paper Wright directly compared biochemical and thermochemical routes in terms of operating and capital costs. The five routes included were a starch-based (grain) ethanol plant (first generation biorefinery), LCF to ethanol, biomass gasification to produce hydrogen, methanol and FT liquids. The economic data was collected from literature and adjusted to account for differences in scale, currency and year. Wright's work highlights some of the problems when making comparisons of biorefineries, such as scale, technology status and comparing on the same basis. The work demonstrates the importance of the costs, and how the economics and therefore the products, will change as feedstock costs fluctuate. They show by representing the results graphically and in tables that based on current technology and by looking at capital and operating costs, that neither biochemical

nor thermochemical have the clear advantage in terms of capital or operating cost for production of biofuels (150). Wright states that both have the opportunity to compete against grain ethanol as corn prices continue to rise. In order to compare the five options the capital cost, biomass cost, operation and management cost and the income from the products are displayed as a function of operating cost ($/gallon of gasoline equivalent). This is adequate for the comparison of economic criteria for a small number of configurations, but becomes more difficult if criteria to be included in the evaluation have non-monetary values. The work by Wright (150) demonstrates that we need to look at more than just the cost criteria when carrying out evaluations in order to distinguish between the most promising options.

8.2.10 ECONOMIC-MARKET EVALUATION

Only one evaluation was found that combined an economic and market evaluation of biorefineries. This was the work by Lynd et al. (4). The evaluation aimed to identify the advantages of producing ethanol in a biorefinery with a varied product portfolio, rather than a single product facility. In this paper Lynd et al. (4) consider succinic acid as the high value co-product to be manufactured in conjunction with ethanol. In these biorefineries the lignin is used to provide heat and power, and meets all of the energy needs with some extra electricity for export to the grid. Four different scenarios were investigated; ethanol and power, ethanol, succinic acid and power in the near term and the advanced technology case. The market investigation included in this work concludes that there are few organic chemical or polymers with markets large enough to sustain a biorefinery plant as the primary product. To evaluate the scenarios Lynd (4) used equations to calculate various economic measures. The same equations were used for all scenarios ensuring consistency in the comparisons. The results for each criterion are displayed graphically so it was clear to the reader the scenarios that perform well, but at no point do the authors state which the best option is, but they do conclude that integrated production of ethanol and other added value products is beneficial in financial terms.

8.2.11 MARKET EVALUATION

No work was found that evaluated biorefineries in terms of the markets available for the biorefinery products, or the potential impact that the introduction of these products might have on the market. In addition no work was found on the impact on price that the introduction of biorefinery products may have. This is a very important issue, if a biorefinery produces a high value product with only a tiny market, it may not be feasible.

8.2.12 TECHNO-ECONOMIC-ENVIRONMENT-MARKET EVALUATION

Only one report was found that took into account technical, economic, environmental and market performance of biorefineries. This was the report written by Black and Veatch (25) on behalf of the National Non Food Crop Centre (NNFCC). This report contained the most comprehensive evaluation of biorefineries found in the literature, but a defined and consistent methodology was not used. The work consisted of a feasibility study for a lignocellulosic ethanol plant located in the UK. Black and Veatch carried out an extensive evaluation of each configuration considered; biochemical, thermochemical and hybrid configurations. Each of these was considered separately, with no defined comparison methodology applied. In this study market scenarios were also included in the evaluation. The crude oil and ethanol market situations were investigated and also the best option for lignin. Black and Veatch identify the best option in terms of return on investment as selling a fraction of the lignin to alternative markets and utilising a fraction for heat and power. It was difficult for the reader to compare the different configurations because of the large amount of information generated. They considered a large number of criteria in the evaluation, but they did not consider more than one criterion at any time. Even after consideration of all of the factors Black and Veatch state that it is difficult to identify the preferred technology.

8.2.13 SOCIO-ECONOMIC EVALUATION

No work was found that evaluated the socio-economic performance of biorefinery plants. Nor was any work found that combined socio-economic performance with any other criteria.

8.3 SUITABILITY FOR THIS PROJECT

From the literature review of biorefinery evaluations it became clear that a different and more methodical approach was required in order to evaluate and rank the biorefinery concepts for this thesis. There were a number of problems with the evaluation methods found in the literature which made them unsuitable for this project.

No two papers evaluated biorefinery processes, products or complete plants in the same way. The methods used for evaluation were often very inconsistent, with very few papers having a defined methodology for evaluation. Some of the work, such as that by Huang (24) and Vliet (148) had a comprehensive and defined methodology for modelling and data generation, but no such method for evaluation and comparison of this data. Most evaluations consisted of a series of tables and charts. This was acceptable where a small

number of options were to be considered but data handling and representation becomes a problem as the number of configurations or criteria increases. It was not possible to assess all the data at once and the decisions about the most promising option were often based on the opinion and knowledge of the researcher. A drawback of this is that it is quite easy to overlook an important aspect that should be taken into consideration. Basing decisions on opinion also leads to inconsistencies and it means that the evaluation cannot be repeated by another group of researchers. The ability to repeat evaluations using the chosen methodology was a requirement for this thesis.

In the literature very few cases were found that considered technical, environmental, socio-economic and/or market criteria. Most studies focussed on techno-economic evaluation, neglecting other important criteria such as the environmental performance. It was surprising that more evaluations did not include any environmental criteria, as the alleged environmental performance of these processes is one of the main driving forces for biorefinery development. The papers that did include more criteria often evaluated the process or product one criteria at a time, for example, the cost performance or the environmental performance. No work was found that made it possible to evaluate all or a selected number of the criteria in the overall evaluation in order to identify the best option in terms of cost, environment or the best option in terms of all criteria. No evaluations were found that made it possible for the user to set and also change the objective of the evaluation.

As more criteria or more options were included in the evaluations, data handling became an issue. In many of the papers the large amount of data was represented by a series of charts or tables. It was difficult to review all of the data at once, or to isolate certain areas without having to sort through numerous sets of data. This was often confusing due to the large amount of data to be taken into consideration. No evaluations were found that used improved methods for representation of the results. In general, the biorefinery evaluations compared up to a maximum of 10 different options and as the number of options increased, the evaluations became more complex and involved. For this thesis there were 27 concepts, but the evaluation methodology chosen was not to be limited by this number. It had to be highly flexible and capable of evaluating many options.

None of the literature established a defined method for evaluation apart from the work of Werpy et al. (39) and Uihlein (10). The work of Werpy et al. (39) work focussed on products from biomass rather than complete plants, but it illustrated the benefits of a defined methodology. The methodology allowed Werpy and co-workers to sort and rank

over 300 different options in order to identify the top 12 building block chemicals from biomass. It allowed the decision makers to quickly sort through all the options in a defined and consistent way with a clear logic for the decisions. This method was based in some part on the knowledge and opinion of the decision team, as well as more qualitative criteria. This makes it unsuitable for this project where a more robust, measurable and transferable method was required. A methodology was required that would allow the evaluation to be repeated, independent of the knowledge of the researcher using the system. The advantage of a defined methodology based on measurable performance is that the same structure is applied to all options in the evaluation.

The work of Uihlein et al. (10) focussed on the environmental performance of a number of different biorefinery configurations. The environmental results were combined to give a single environmental "score" for each of the options. This made it easier for the user to identify the most promising option. The logic behind the ranking is clear, and it would be easy for someone to follow the methodology to apply it to other biorefinery configurations. Due to the fact it only considers environmental criteria, the methodology would have to be expanded for application to this thesis, but it highlights the benefits of combining results to give each option a single score in order to rank them.

There have been studies to identify the optimum scale (24, 150), the best feedstock for ethanol production (145), best environmental performance (10) and the most profitable (118) but none that look at all of these criteria or more for a large number of biorefineries. This type of overview is needed to evaluate the wider ranging possibilities and impacts of biorefineries. In addition many of the studies focus on ethanol production but many other products from biomass exist, as identified by Werpy (39), Holladay (38), Corma (41) and Huber (40). Evaluation of many biorefinery plants, not only focussing on ethanol, is required in order to identify the optimum product portfolio.

From the review of biorefinery evaluations it became clear that nobody had yet developed a consistent and flexible evaluation method that properly considered all criteria. A flexible methodology for the ranking of biorefinery process chains according to objectives set by the user had not yet been created. For these reasons, alternative evaluation methods were researched, that would meet the requirements described in Section 8.1. The type of evaluation most suited to the objectives of this thesis is called multi-criteria decision analysis (MCDA) and is described further in Chapter 9.

9 BIOREFINERY EVALUATION BY MULTI-CRITERIA DECISION ANALYSIS (MCDA)

A more substantial and inclusive evaluation technique than the methods reviewed in Chapter 8 was required to assess the biorefinery concepts against a wide range of criteria and from a number of different viewpoints. The comprehensive and structured evaluation techniques offered by multi-criteria analysis were investigated for application to this evaluation task, in order to meet the specification defined in Section 8.1.

The chapter begins in Section 9.1 with an introduction to MCDA followed by a review of the main techniques. In Section 9.2 there is a review of MCDA applications in the literature. In Section 9.3 the application of MCDA to this project is described including the choice of software, criteria (Section 9.3.1), the use of the modelling results (Section 9.3.2) and the choice of weighting to set the objective of the analyses (Section 9.3.3).

9.1 MCDA INTRODUCTION

Multi-criteria decision analysis (MCDA) methods offer a number of different techniques for making decisions by comparing a number of options against a list of criteria (151).In most real decision scenarios, basing the decision on only a single criterion is often insufficient (155) and MCDA methods can give better results than the sum of single criteria analysis (154). In many cases the ideal solution to a problem consists of a compromise between the criteria giving a satisfactory performance in all areas (157).There are a number of different acronyms for multi-criteria decision analysis (MCDA) such as multi-objective decision making (MODM), multi-attribute decision making (MADM) and multi-criteria decision making (159). These techniques offer both an approach and a set of defined techniques (153) with the goal of providing an overall ranking of the options.

The main role and benefit of MCDA techniques is that they help deal with the difficulties human decision makers have in handling large amounts of information in a consistent way (153). These methods provide a formal defined methodology for the systematic evaluation of complex decisions (152). Multi criteria analysis may be used to help identify the single preferred option, to rank options or to shortlist options for further analysis (153) which makes MCDA methods a solution to the problem of identifying the most promising biorefineries from differing points of view. MCDA provides a technique to measure the extent to which the biorefinery concepts achieve the desired objectives.

MCDA can be used in order to (153):

- Give the decision maker a view of the best way forward.
- Identify the areas of greater and lesser opportunity.
- Prioritise the options.
- Clarify the differences between the options.
- Indicate the best allocation of resources to achieve the goals.
- Facilitate the generation of new and improved options.
- Or any combination of the above.

A very extensive guide and manual for multi-criteria decision techniques has been written by Dodgson et al. (153) to aid government officials make the best use of multi criteria analysis for policy and other decisions. This manual contains a detailed description of various MCDA methods and provides excellent descriptions of the MCDA techniques available.

MCDA most commonly applies a numerical analysis to the options using a scoring and weighting system (153). Highway investment decisions in the UK have for many years used multi-criteria techniques that take account of both monetary and qualitative (e.g. social, environment) impacts (153). MCDA methods help improve understanding of the problem and the potential solutions, and force the decision makers to evaluate all options carefully (159). The methods are consistent and methodological so that scenarios can readily be re-evaluated as new information becomes available.

The main advantages of MCDA techniques as described by Dodgson et al. in the extensive MCDA manual (153) are:

- The techniques are open and explicit.
- The choice of objective and criteria is open to analysis and change if they are felt to inappropriate.
- Scores and weights are explicit.
- The results and analysis can provide a means of communication about decisions between the decision groups involved.
- The scores and weights can be used to provide audit trail.
- The methods avoid intuitive solutions (157).

9.1.1 REVIEW OF THE MAIN MULTI-CRITERIA TECHNIQUES

There are a number of different multi-criteria analysis techniques used and described in the literature:

- Cost effectiveness analysis (CEA).
- Cost benefit analysis (CBA).
- Value measurement models.
- Analytical hierarchy process (AHP).
- Goal, aspiration or reference level models (GP).
- Outranking models.

These analysis techniques are briefly reviewed in the following section. The methodologies all try to overcome the problem of conflicting criteria, incomparable units and the selection or ranking of alternatives (159).

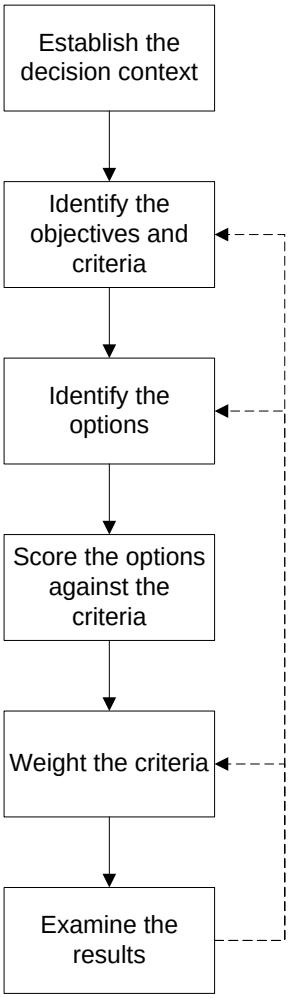

Figure 9.1 – MCDA flow diagram

All of these methods tend to follow the same structure, as illustrated in Figure 9.1. This diagram highlights the key stages in MCDA and illustrates that MCDA is an iterative

process; it is usually necessary to cycle back through the stages as new insights develop or new data become available.

In relation to Figure 9.1, for this thesis the decision context is to identify the most promising biorefinery concepts from a number of different viewpoints. The criteria were chosen from the information available to include cost, plant, environmental and socio-economic performance in order to comprehensively evaluate the biorefinery concept. A further discussion of the MCDA technique applied to this project, including the choice of criteria and weighting is given in Section 9.3.

9.1.1.1 COST EFFECTIVENESS ANALYSIS (CEA)

Cost effectiveness analysis (CEA) aims to find the least cost way of achieving the objective by comparing the costs of the alternative options (153). All of the criteria included are evaluated on a cost basis. CEA is the one of the most common methods of multi criteria analysis used by the UK government (153). A disadvantage of this method is a lack of transparency as it is not initially clear to the user how the costs have been calculated for the non-monetary criteria (6). This method is not suitable for this project as a number of the criteria, such as environmental impact, cannot easily be converted into a monetary value and if so are often subjective and open to greater uncertainty and debate. The method chosen for this thesis had to be transparent to the project partners and CEA makes it difficult to achieve this.

9.1.1.2 COST BENEFIT ANALYSIS (CBA)

Cost-benefit analysis assigns a value in monetary terms to the expected impacts and benefits of the options (153). The valuation of the benefits is based on an economic theory based on willingness to pay or to accept (153).These benefits are not easy to calculate, especially if they refer to environmental performance, human health or biodiversity (157). The calculated cost-benefits are then used to make an assessment of the options. The cost benefit analysis method is widely used in transport and health and safety decisions (153). An advantage of this method is that all benefits and losses are judged in terms of a single familiar measurement (i.e. money) (153). A disadvantage is that it is very difficult to assign all gains and losses a financial value, which makes these methods less flexible and comprehensive than others (153). In practice it is not realistic to value all costs and benefits in this way (153). Similar to the CEA method, it is not suitable for this project as a number of the criteria such as environmental impact cannot easily be converted into a monetary value or benefit.

9.1.1.3 VALUE MEASUREMENT METHODS

Most MCDA approaches for energy allocation decisions use value measurement methods in which the values and weights for each option are combined into a single overall value or score (153). This method is also known as the linear additive model, multi-attribute value theory (MAVT) (155) or weighted sum method (WSM). Each criterion against which the options are to be judged is assigned a weight that represents their relative importance in the whole analysis. The score for each criteria is then multiplied by the weight to give the weighted score. The weighted scores are then added together to obtain the overall score for that option (153). The option with the highest overall score is the most preferred. This is the most commonly used MCDA approach (153,159) with the WSM method the most commonly used for sustainable energy decisions (154). The advantage of this approach is that it is simple and understandable (155) and it is relatively easy for the user to understand how the final score has been obtained for each option. This method was judged to be suitable for this thesis (see Section 9.3).

9.1.1.4 AHP – ANALYTICAL HIERARCHY PROCESS

This method is a development of the value measurement methods described in the previous section and uses procedures for deriving weights and scores, based on a pairwise comparison between criteria and options (153, 154, 155). Decision makers are asked to compare the importance of two criteria at a time, judging which is more important using a comparison scale (154) as shown in Table 9.1. From this pairwise comparison of criteria the weights are derived. Following the derivation of the weights by pairwise comparison, there follows pairwise comparison of each option against each criterion (153). The procedure for carrying out the pairwise comparison of the options and for calculating the overall rankings are complex, so it is usually carried out by specially designed computer programs (155). As for the linear additive approach, single scores are generated for each of the alternatives (155) based on the overall results of the pairwise comparison approach.

Table 9.1 – AHP comparison scale (155)

Scale	
1	Equally preferred
3	Weak preference
5	Strong preference
7	Very strong or demonstrated preference
9	Extreme importance
2, 4, 6, 8	Intermediate values

Generally non-specialists find the pairwise form of data input straightforward and convenient (153, 155). This method also allows the comparison of both quantitative and

qualitative criteria (155). The disadvantage of this method is that it can be time consuming if a large number of alternatives are to be considered (155) and some argue that it is inconsistent (153) because it is not possible to check the consistency of the user's preferences (154). Due to the fact that it is time consuming for a large number of alternatives this method is not suitable for application to this project. Furthermore introducing new options may change the relative ranking of the other options, so the whole pairwise comparison exercise must be repeated (153). This method does not provide the level of flexibility required for this thesis.

9.1.1.5 GOAL, ASPIRATION AND REFERENCE LEVEL MODELS

When using goal, aspiration and reference level models the user attempts to determine the options that are closest to achieving the determined goal or aspiration level (154, 155). The abbreviation GP (goal programming) is used as a common abbreviation for these methods (155). This approach is often used in the initial screening of options, to eliminate unsuitable alternatives quickly and efficiently (155). Mathematically the aim is to find the option whose variables have the smallest deviation from the ideal (155).

An example of software using this GP methodology is TOPSIS (159) which stands for Technique for Order Preference by Similarity to Ideal Solution. It is based on the concept that the best option is the one that has the best values for all criteria, whereas the worst option has the lowest values for all criteria (154). The best solution is that with the highest so called relative closeness to the ideal situation.

A disadvantage of this method is that the criteria need to be on a defined and measurable scale, which means that they are not capable of handling qualitative criteria (155). As a consequence GP must be combined with some other analysis e.g. if qualitative values are to be included (155). Due to the complexity of this method, it was not suitable for application to this project as it would be very difficult to represent the deviations from the ideal scenario, as it is not yet known what the ideal scenario is.

9.1.1.6 OUTRANKING MODELS

Outranking methods compare either criteria or results and then rank one above or below the other. Ultimately the method eliminates options that are "poor performers" (153). Outranking methods eliminate alternatives by also using weighting to give more influence to some criteria (153). An option is said to be preferred if is outperforms the other on enough criteria of significant importance (reflected by the criteria weighting) (153). All

options are then assessed as to the extent to which they sufficiently outrank the others (153).

A number of procedures have been developed to carry out the outranking analysis such as ELECTRE (153) or PROMETHEE (159). These models aim to reduce the complexity of the outranking principle (159) and make the representation of results easier to understand for decision makers (155). ELECTRE stands for the elimination and choice translating reality and the method aims to identify options that are preferred for most of the criteria (155). Alternatives that perform very badly for any of the criteria are not chosen, even if they perform well for all other criteria, and it makes use of strict preference thresholds (155). ELECTRE methods are sometimes unable to identify the preferred alternative in which case a list of leading alternatives is generated (154). It has been stated that this method is the best for initial screening processes to categorise suitable and unsuitable options (155).

In PROMETHEE, which stands for preference ranking organisation method for enrichment evaluation, a pairwise comparison of the alternatives is performed to give each criterion a preference function. The preference functions are used to measure the alternatives for each criterion (154). Based on these functions an index for ranking of *a* over *b* is determined and used to give a ranking of the alternatives (155). Within the literature it has been stated that PROMETHEE has a more transparent calculation method that users find easier to understand than ELECTRE (154, 155).

An advantage of the outranking method is that it stimulates debate among decision makers if options are eliminated that perform badly for only one criterion (153). This may encourage the development of better options (153) and provides insight into the structure of the problem (155). A disadvantage of this method is that it is possible to find two options that are difficult to compare (153). The main concern with this method is the definition of what constitutes outranking within the options and how the threshold parameters are set (153). These methods are most often used for initial screening and not for the final selection of alternatives (155). For this project this method is not suitable as it is not easy to use where there are a large number of options and the logic is not transparent. The pairwise type method means that if more options are included the whole pairwise evaluation must be repeated. This method does not provide the flexibility required for this thesis.

9.2 REVIEW OF MCDA APPLIED IN THE LITERATURE

No literature was found about the application of MCDA techniques to the identification of the most promising biorefineries. MCDA methods have been used for making choices about renewable energy provision (155, 159, 156) and energy planning (157, 158). MCDA methods are used because energy planning problems are complex with multiple decision makers and multiple criteria (155).

The paper by Diakoulaki and Karangelis (157) illustrates the application of MCDA methods to an energy planning problem. This paper was chosen for review because it includes the use of two different MCDA methods to a problem with similar objectives to this thesis; to identify the best option considering a variety of criteria. Four different options for the expansion of the Greek electricity provision were evaluated in terms of economic, technical and environmental performance. The four options included the current provision scenario, a large public corporation providing electricity, a climate change abatement scenario and an unsteady scenario assuming high electricity demand and unfavourable political conditions. These four options were evaluated using the PROMETHEE outranking method and CBA techniques. Using the two completely different evaluation techniques the same conclusion was reached. They identify the climate change scenario as the most promising. Using both methods enables the checking of consistency of results and more confidence in the final results. Diakoulaki's work demonstrates the successful application of MCDA techniques to a problem with similar objectives to this thesis.

Pohekar and Ramachandran (159) have reviewed the application of multi-criteria techniques to sustainable energy planning and state that multi-criteria techniques provide a solution to evaluating alternatives with conflicting and multiple objectives. In their paper more than 90 pieces of work are reviewed, with identification of the most popular MCDA methods for energy planning. Sustainable energy planning has similar objectives to the evaluation required for this project; the options need to be evaluated taking into account a number of considerations such as cost, environment and social issues. The need to include environmental and social considerations in energy planning was one of the main reasons for the increasing use of multi-criteria techniques (159) and highlights its applicability to this thesis for identifying the most promising biorefineries. Their work provides useful background information about the different techniques applied to energy planning problems and identifies AHP as the most popular technique for energy planning, followed by outranking techniques using methods such as ELECTRE and PROMETHEE (159).

The paper by Elghali et al. (6) supports the use of MCDA for the development of a methodology for the assessment of bioenergy systems. Elghali et al. explore how MCDA processes are able to integrate the interests and concerns of a diverse group of decision makers. They identify the lack of a "coherent cross-sector strategy for bioenergy development and deployment." The criteria included in their work were very similar to the criteria under consideration within this project; economic viability, environmental performance and social acceptability. Their paper describes an approach to assessing the bioenergy systems which has many similar characteristics to the method required for this project. The approach chosen by Elghali and for this thesis had to manage the conflicting criteria in a transparent and fair way. Their aim was to apply the methodology to small, medium and large heat and/or power plants and to the transport sector. Their work does not give the final methodology or results, but describes the background behind the decision about the methodology, detailing the elements that had to be taken into consideration. Decision conferencing is mentioned as a method for assessing decision maker's weightings. An attempt was made to look at the views of the partners for this thesis (see Section 9.3.1.1) but the views were not different enough to merit any further analysis. A systematic approach was taken to the weightings in this thesis in order to generate some useful and understandable results (see Section 9.3.3).

Although most applications of MCDA in chemical engineering scenarios have been to energy planning, in the paper by Cziner et al. (160) the MCDA method is applied to process integration. The aim of their work was to assess the potential of MCDA methods to aid process integration. The criteria for optimum operation include safety, cost, and environmental measure, which cannot be measured and compared using typical evaluation methods. In their paper they use the AHP as it fitted with the problem structure. They chose this method as AHP provides a powerful and flexible methodology for making decisions when both qualitative and quantitative factors have to be considered. In this paper the application of AHP to the case study of a calcinations kiln is described in detail. The decision makers work through the criteria to build a hierarchy of the criteria to be considered of more importance. The options were the existing configuration, plus two new options for increasing the production rate. All three options were compared using a number of different criteria including investment cost, emissions and safety measures. The criteria were compared in pairs in order to determine the weighting. The three options were modelled to provide the "scores" for the comparison. The options were then ranked based on the weightings and values. One option was identified as the most promising proving the

successful application of MCDA techniques to the problem of process integration and the solution of a problem under uncertainty and with conflicting criteria.

9.3 MCDA APPLICATION TO THIS PROJECT – HIVIEW

It was hoped at the beginning of the project that a single comprehensive modelling and evaluation system could be developed but decoupling the modelling and evaluation means that the methodology is more robust and provides added flexibility (69). It would be possible to create the MCDA analysis within Excel, by writing the relevant algorithms, but dedicated MCDA software provides much more potential for analysis as well as a proven framework for inputting data. There are a large number of inbuilt tools in dedicated MCDA software that allow greater insight into the results and provide inbuilt sensitivity analysis. The sensitivity analysis function makes visible the effect on the results of adjusting the scores or weights. A disadvantage is that the results from the modelling have to be manually input into the software, but once this is done there is the potential for a large number of analyses.

MCDA software is a useful aid for decision makers as it provides a way to handle the large amount of data required and to ensure that the calculations are consistent. The software packages provide a way of carrying out a large number of analyses rapidly. Some software also aids the decision makers in the choice of weighting. For AHP methods this process is complex but is simplified by the use of software. There are a number of MCDA software packages available including Hiview, Macbeth, Visa, Desysion Desktop and Logical Decisions Package (153).

Using a software program to carry out the MCDA has a number of advantages:

- Easy amendment of input data (including sensitivity testing) (153)
- Attractive and informative presentation of outputs (153).
- Flexible
- Improved data handling

The software chosen for the appraisal and evaluation of biorefinery concepts for this thesis was Hiview 3 by Catalyze. Hiview is a well established piece of software developed by the London School of Economics (LSE) and sold under license by Catalyze. It is used to support the case studies described in the very extensive multi-criteria analysis manual by Dodgson et al (153) and is used by UK government (153). Hiview uses a linear additive type model to evaluate the different options against the chosen criteria. Using this type of method simplifies the weighting procedure.

Hiview was chosen for a number of reasons. The system is user friendly and it is simple and quick to carry out a new analysis. The results and logic are clear to the user and the inbuilt tools allow insight into the main conflicts between options. It is easy to identify the strengths and weaknesses of the biorefinery plants and it is very quick and easy to repeat analysis. The results are clearly presented and the data input is intuitive.

Within Hiview the criteria are displayed in the form of a tree diagram. At the top of the tree is the root node, which acts as the focus for the final decision– in this case, what is the most promising biorefinery? The root node branches into the criteria, which represent the main trade-offs facing the decision makers (151).

The results of the Hiview MCDA analysis was a set of biorefinery concepts ranked according to the inputs. Hiview 3 has many tools for analysing the MCDA model and enables the decision makers to compare all results and criteria. New insights are fed back into the model, which develops with the project. Using Hiview the steps in the MCDA analysis were followed as illustrated in Figure 9.1.

According to the MCDA flow diagram the first step is to establish the decision context. For this project this is the identification of the most promising biorefineries. The second step is to identify the objectives and criteria. The objectives are set by the choice of weighting (described in section 9.3.3) and vary between analyses. The choice of criteria is vital and is described in section 9.3.1. Following this according to the diagram is the identification of the options. This has already been defined as the 27 complete biorefinery concepts (section 5.4). The scores for the options were generated in the modelling step (Chapter 5 and 6) to give economic, process performance, environmental and socio-economic data. This data forms the scores in Hiview (Section 9.3.2). Finally the weighting is applied to the chosen criteria and the results examined (Chapter 10). In the following sections the application of MCDA and Hiview to this project is described in more detail.

9.3.1 CRITERIA CHOICE

Choosing the correct criteria was one of the most important decisions to make for the success and validity of the MCDA analysis. The criteria had to be considered carefully to ensure that all aspects of the biorefineries were included, as the criteria are the measures of performance by which the options were judged (153). The number of criteria to be included was also carefully considered as it is not always the case that the more criteria included, the better the results obtained (154). An excessive number of criteria leads to

extra analytical effort in assessing the data and can make communication of the results more difficult (153).

The criteria had to be relevant to the objective of the analysis and also measureable (154). The question kept in mind when choosing criteria was ‘Is it possible in practice to measure or judge how well an option performs on these criteria’ as stated by Dodgson et al. in their MCDA manual (153). The criteria had to be complete and not double counted since double-counted criteria are given a higher weighting in the final overall decision than they should receive (153) and potentially change the end result.

9.3.1.1 BIOSYNERGY INDUSTRIAL ADVISORY BOARD CRITERIA CHOICE

Within Biosynergy there was an Industrial Advisory Board (IAB) consisting of expert advisors from industry. This group represented the views of industrial stakeholders so they were requested to generate a list of criteria by which the biorefineries could be judged. It was also requested that the criteria be given a weighting, to indicate their perceived importance in the assessment. The members of the Board had no detailed knowledge of the models being created as part of WP6 and they were asked to make judgements from an industrial viewpoint. They did not know whether it would be possible to include the criteria identified as part of the final MCDA. This exercise was carried out at a relatively early stage of the project, before the final evaluation methodologies had been defined. The criteria chosen by the IAB are shown in Table 9.2.

The IAB generated a large list of criteria. Some of these were double counted, for example profitability and value of co-products are not independent so only one of these could be included in any analysis. From this list it became clear that from an industrial viewpoint the availability of a market is of great importance, as market criteria appear a number of times in the list.

Table 9.2 – IAB criteria

External issues	
Current market situation features	Existence of market leading companies
	Maturity of technologies
	Barriers to technology development
	Legal issues
	Difficulties
Short-medium term market situation	Potential change
	Expectatives (sic)
	Size/ Disturbs of market
Main players	Potential competitors
	Ability to take risks
Competitive sectors	Competitors market share
	Benchmark of current technologies
Complementary sectors	Synergies
	Potential market
Raw material market	Breadth/Availability
	Synergies/Secure & Continuous supply
	Costs
	Fulfilment of traceability criteria
	Competition for raw material sources
Applicability of selected products	Known and demonstrated applications
	Potential market
	Synergies
Support to developing technologies	Existence of incentives
	Incentives for financing
	Acceptance by the market, manufacturers and consumers
Internal issues	
Process/ Technology	Robustness of the technology
	Flexibility of raw material and products
	Yield to main products
	Value of coproducts
	High yield to coproducts (1)
	Low yield to subproducts (2)
	Profitability
	% GHG Emissions saving
	Other sustainability issues

(1) Coproduct means 'high added value products'
(2) Subproduct means 'residue'

Some of the criteria chosen by the IAB were omitted in the final selection for a number of reasons, detailed below:

- Flexibility of raw materials – Within Biosynergy only two feedstocks were considered; wheat straw and softwood. It may be of interest to include more feedstocks in further studies.
- Potential change to the market situation in the short to medium term – No market data was generated as part of the modelling process, so it could not be included in the evaluation. It is highly recommended to include a market assessment in any further work.
- Difficulties – It was not understood what was meant by difficulties. This is totally subjective and not measureable.

- Legal issues – Again are hard to quantify and judge.
- Competitors market share – As for previous market criteria, no data available in current study.
- Synergies/secure and continuous supply – This would very much depend on the chosen location of the plant. It was not possible to judge at this stage in the analysis as the evaluation looked at generalised results for a country, not a specific location.
- Competition of raw material resources – This was partially covered in the socio economic factors.
- Fulfilment of traceability criteria – This was outside the scope of this project but may be added to the methodology at a later stage.
- Expectatives (sic) – It was not understood what was meant by this criteria.

9.3.1.2 FINAL CRITERIA

Data was generated in the modelling step on process efficiency, process economics, environmental impact and socio-economic impact (see Chapter 5). The criteria chosen for this project had to include these aspects of the modelling to carry out a full and fair analysis and comparison. Looking at the modelling results available, the views of the IAB and the structure of MCDA analysis the final choice for the criteria was made. The topics of efficiency, cost, environment and socio-economics neatly represented the main groups of criteria for this analysis. Any criteria below these are called the sub-criteria. Grouping the criteria in this way makes the weighing process simpler and easier to understand.

The final Hiview tree diagram is shown in Figure 9.2.The criteria chosen were:

- Profit/loss
- Energy conversion efficiency
- Environmental performance
- Socio-economic performance

A market criterion was not included in the MCDA analysis despite being identified as important by the IAB. Within Biosynergy no detailed market information or models were available for inclusion in the evaluation. It may have been possible to create a simplified market assessment but it was judged to be detrimental to the high level of detail included in the other models. The less precise the data inputs to any decision support procedure the less precise and reliable are the outputs it generates (153) hence a market criteria has been omitted to ensure the accuracy of the results produced.

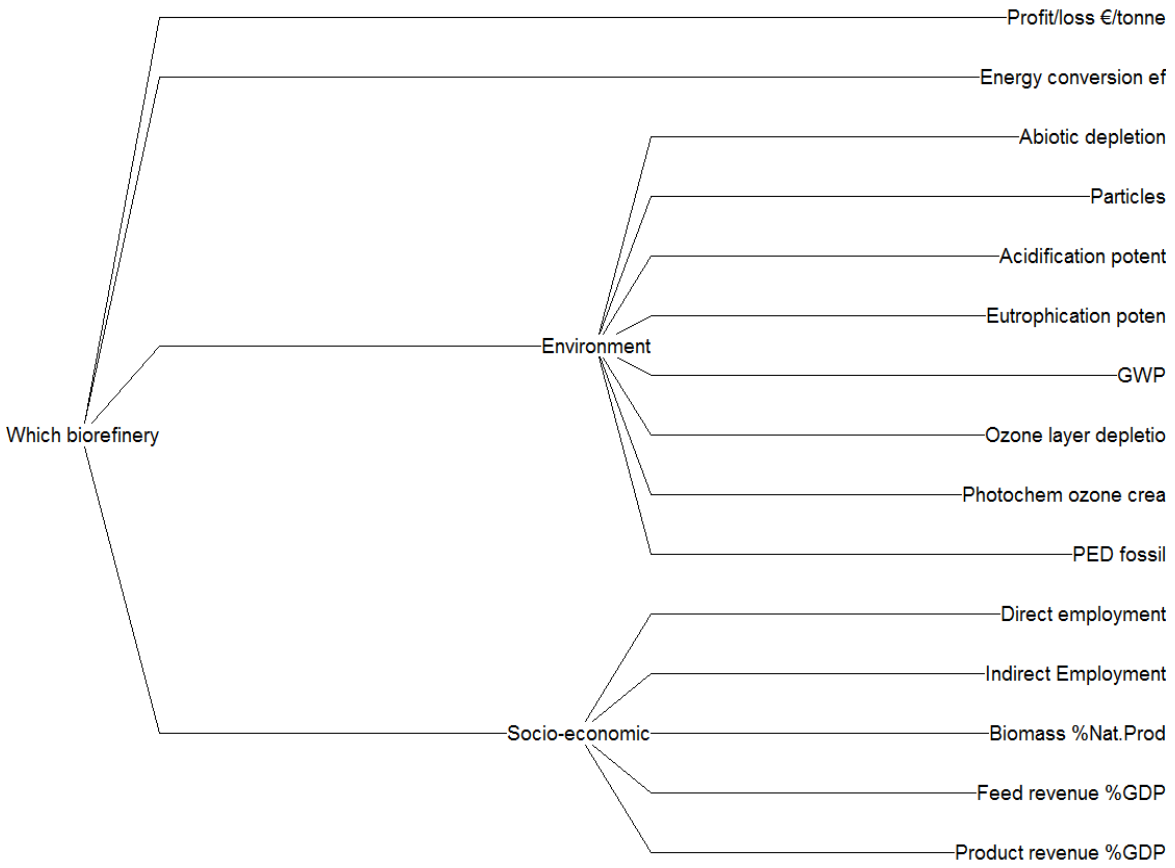

Figure 9.2 – MCDA tree diagram

Profit/loss

As part of the modelling step many economic factors were estimated, such as fixed capital investment, operational cost, income, production cost and profit/loss (see Section 5.6 for more details). Economic criteria were essential in the biorefinery evaluation as this is often of most interest to stakeholders. When choosing criteria they had to be independent and not double-counted. For these reasons the value of profit/loss was chosen to represent the economic performance. The calculation for profit/loss included many of the other economic values. It is calculated from the product income and the production cost, which includes the TFCI, an estimate of capital repayments and the operational cost. The profit/loss value therefore represents the overall economic performance of the biorefinery concept.

Energy conversion efficiency

Another criteria was required to represent the overall process performance or efficiency of the biorefinery concept. A measure was needed to represent the efficiency of conversion of the biomass into useful products/energy.

The energy conversion efficiency was used because it was not possible to represent all of the biorefinery products in mass terms. A number of the concepts generated electricity or

heat as products; these are not easily represented in mass terms but had to be included in any efficiency measure, as they are products of the plant. Therefore the energy content of the biomass and products were used to measure the efficiency of conversion of biomass into products. The higher the value the more effectively the biomass has been converted to products (see Section 10.2.1.6 for more details).

Environmental

The environmental criteria were included to evaluate the options in terms of the environmental performance and to include the results of the environmental model. There were a number of sub-criteria under this heading based in the results of the model created by JR (for more details see Section 5.7). There were 8 impacts included as the environmental sub-criteria. These were:

- Particles
- Abiotic depletion
- Acidification potential
- Eutrophication potential
- Global warming potential
- Ozone layer depletion
- Photochemical ozone creation
- Primary energy demand (fossil)

Socio-economic

The socio-economic criteria were included to evaluate the biorefineries utilising the results of the socio-economic model. A number of different socio-economic impacts were evaluated as part of the socio-economic model, and these formed the sub-criteria (see Section 5.8 for more details). Not all of the impacts in the model were included in the MCDA to avoid double counting of results. The full list of impacts included in the socio-economic model and those included in the MCDA are listed in Table 3.

Table 3 – Full list of socio-economic impacts (161)

Employment assessment for biorefinery plant	Included in MCDA
Direct employment (man years)	Yes
Induced employment (man years)	Yes

1 man year equivalent to 8760 man hours

Agricultural and land assessment for biorefinery plant	
Biomass consumption as % of national production	Yes
Land required for biomass supply (ha)	No
Land required for straw supply as % of regional agricultural land	No
Land required for straw supply as % of national agricultural land	No

Trade assessment for biorefinery plant	
Revenue from traded feedstock (euro pa)	No
Revenue from traded feedstock as % of agricultural GDP	Yes
Revenue from biorefinery products (euro pa)	No
Revenue from biorefinery products as % of national GDP (%)	Yes

9.3.2 USE OF MODELLING RESULTS IN HIVIEW

The results from the process, environmental and socioeconomic models formed the input, or scores, for the MCDA analysis. The MCDA software uses these scores and the weightings to make a judgement of the most promising biorefinery concepts.

Hiview converts the input scores to a value scale. In this case a relative scale was used with the input scores from the modelling automatically converted to a scale from 0 to 100. This is the default option and the easiest to use (151). A score of 0 does not mean no value, it just means the least preferred. The results were input for each of the 27 biorefinery concepts.

9.3.3 WEIGHTING CHOICE

The final step once the scores had been entered in Hiview was the weighting. This assigns a value to the each criterion or group of sub-criteria according to their perceived importance for that analysis. The weighting sets the objective of the analysis.

When choosing the weighting for the criteria, the question asked is "which of these criteria is the most important". Each of the criteria is weighted separately, with the most important criterion given the highest weighting. All other criteria are ranked relative to the most important. For example, if the most important criterion is ranked at 100 and the next criterion is ranked at 50, it is classed as only half as important as the most important criterion (151).

An exercise was carried out to gauge the viewpoints of different groups within the project about their views regarding criteria that should be used to judge the biorefineries (see section 9.3.1) and also the relative weights that these criteria should be assigned. The Industrial Advisory Board was one of the groups asked to make a judgement. The list of

criteria they thought should be included in biorefinery evaluation is given above in Table 9.2. They also judged the relative weights of these criteria.

Another group that were asked to make a judgement about criteria weightings were the co-ordinators of the individual work packages. A list of criteria derived by the IAB was supplied to the WP leaders based on the judgements made by the IAB, removing categories that were double counted to leave the main headings of process cost, process efficiency, environmental impact and socio-economic impact. The WP leaders were then asked to rank the importance of these criteria by giving them a value out of 100%.

Table 9.4 – Weightings from Biosynergy Groups

	Profit/loss	**Conversion efficiency**	**Socio-economic**	**Environment**
IAB	27.6%	24.8%	22.8%	24.8%
WP leaders	27%	25.8%	27.7%	19.4%
Equal weighting	25%	25%	25%	25%

When looking at the weightings chosen by the groups it became clear that they did not differ from the application of equal weighting to each of the criteria (see Table 9.4). For this reason the decision was made not to include the slightly different IAB and WP leader weightings in the finished analysis, as the weighting and overall results from using these weightings were so similar to that of an equal weighting.

Due to the speed at which it was possible to generate evaluation results (once all the scores have been input) a number of different weightings were tested. It takes less than a minute to generate results once a new weighting is applied. The weightings were chosen based on a judgement of the main interests of the Biosynergy Consortium and take into account a number of different viewpoints. The weightings applied are shown in Table 9.5.

Table 9.5 – Weightings applied in MCDA analysis

	Profit/loss	**Conversion efficiency**	**Socio-economic**	**Environment**
Equal	25%	25%	25%	25%
Techno-economic	50%	50%	~	~
Enviro-socio	~	~	50%	50%
Profit/loss bias	49%	17%	17%	17%
Efficiency bias	17%	49%	17%	17%
Socio-economic bias	17%	17%	49%	17%
Environment bias	17%	17%	17%	49%

Once the scores and weights have been input the analysis is run to generate the results. The result is the biorefineries ranked according to the objectives set by the weighting. The results of the MCDA analysis can be found in Section 10.4.

10 RESULTS AND DISCUSSION

This chapter presents and discusses the results of the thesis. The results of this project are twofold. As well as the identification of the most promising biorefineries from the 27 studied, a robust and comprehensive methodology was created which allows the generation and evaluation of around 3000 process configurations in 5 European locations.

The creation of a comprehensive and flexible process synthesis methodology is described in Section 10.1 followed in Section 10.2 by the results derived from the modelling of the 27 concepts. In Section 10.3 the results of a sensitivity analysis are presented and discussed. For the sensitivity a number of variables such as the scale, feedstock price and TFCI were adjusted to judge the impact on the profit/loss of the biorefinery concepts. The results of the modelling were used to carry out an MCDA evaluation described in Section 10.4; the result of which was the identification of the most promising biorefineries. Finally the limitations of the methodology and results are discussed in Section 10.5.

The 27 concept biorefineries (see Table 10.1 below) were evaluated on the basis of 500,000 tonnes of biomass per year (dry basis). This excludes any biomass required for heat and power provision. Such a relatively large scale was chosen and agreed by the project partners for the evaluation because it is envisaged that the markets for the transport fuels produced are very large (136). Such a large scale would also mean reduced specific costs and heat integration is easier, although these benefits may be outweighed by the additional transport costs for biomass. It is possible using the methodology to assess any scale of interest although the accuracy becomes more questionable as the deviation from 500,000tpa increases.

Five countries were chosen for modelling the socio-economics and cost; Spain, UK, Germany, Poland and the Netherlands and this choice is built into the model. The overall MCDA results are given for all five countries (see Section 10.4.1). For the detailed evaluation and MCDA work the decision was made to focus on Spain due to the interest and close links of the Biosynergy Project to the work carried out by ABNT in Spain. An evaluation of all 27 concepts in all 5 countries was not sensible within the context of this thesis.

Table 10.1 – Full list of all concepts considered

	Feed	Pretreatment	C5	C6	Lignin
0	Straw	Mechanical/alkaline fractionation	Furfural	Ethanol	Bio-oil phenolic fractionation
1	Straw	Steam explosion	Furfural	Ethanol	Bio-oil phenolic fractionation
2	Softwood	Steam explosion	Furfural	Ethanol	Bio-oil phenolic fractionation
3	Straw	Gasification	Syngas to ethanol/ mixed alcohols		
4	Straw	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
5	Straw	Steam explosion	Ethanol	Ethanol	Gasification to ethanol
6	Straw	AVIDEL	Surfactants	Ethanol	Bio-oil phenolic fractionation
7	Straw	Organosolv	Ethanol	Ethanol	Bio-oil phenolic fractionation
8	Softwood	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
9	Straw	Steam explosion	Furfural	Ethanol	Pyrolysis to bio-oil
10	Straw	Steam explosion	ABE	Ethanol	Bio-oil phenolic fractionation
11	Straw	Mechanical/alkaline fractionation	ABE fermentation	Ethanol	Dry lignin product
12	Straw	Mechanical/alkaline fractionation	ABE fermentation		Dry lignin product
13	Straw	Mechanical/alkaline fractionation	Furfural	Ethanol	Dry lignin product
14	Straw	Aquathermolysis + further processes	Bio-oil phenolic fractionation, furfural		
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
16	Straw	Steam explosion	ABE fermentation		Dry lignin product
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
18	Straw	Organosolv	Surfactants	Ethanol	Dry lignin product
19	Straw	Organosolv	Surfactants	FDCA	Dry lignin product
20	Straw	AVIDEL	Furfural	FDCA	Dry lignin product
21	Straw	Fast pyrolysis	Bio-oil for heat and power		
22	Softwood	Gasification	Fischer-Tropsch synthesis to hydrocarbons		
23	Straw	Fast pyrolysis	Bio-oil gasification → alcohol synthesis		
24	Straw	Mechanical/alkaline fractionation	Ethanol		Dry lignin product
25	Straw	Steam explosion	Ethanol, stillage to animal feed		Lignin combusted
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

10.1 THE PROCESS SYNTHESIS METHODOLOGY

After reviewing available process synthesis techniques (see Section 4.2) a hybrid approach was chosen for this project. The approach was based on the principles of expert systems combined with heuristics and integrated in a traditional process design approach. A simple expert system was created in which heuristics or rules defined the connection of processing modules. The approach involved the creation of a user interface which allowed the generation of user defined biorefinery concepts. The creation of the complete biorefinery concept involves a series of decisions by the user beginning with the scale, feedstock and

plant location. The user chooses the pretreatment and subsequent steps until a complete biorefinery is defined. This method allowed greater flexibility in the finished system and it is easy to examine the reasoning process behind the linking of the process modules.

No work was found in the literature that allowed the user to freely generate and evaluate biorefinery process chains including such a wide range of process steps and process chains. There were very few studies that took into account a wide range of criteria when carrying out biorefinery evaluations (see Section 8.2) and none were found that allowed criteria for evaluation to be included or excluded at the discretion of the user. A gap in the research knowledge was thus identified and this thesis is believed to represent an important breakthrough in the application of process synthesis, process modelling and decision support systems to the field of biorefineries.

The use of a defined methodology has a number of benefits. The methodology provides a flexible tool for the evaluation of many biorefinery configurations, not limited to the 27 studied for this thesis and every effort was made to make the model user friendly. The modular structure means that additional feedstocks or processes can be added easily, without having to re-work the whole model providing a tool that may continue to be used in the future.

The methodology protects against bias in the evaluations, as the same method is applied to all technologies. The defined methodology provides a consistent approach as all evaluations follow the same procedures, with no possibility of influence from the user. This means that the system allows a fair and consistent evaluation of the Biosynergy project within the limitations of the data provided. There was the possibility for bias in the provision of data for building of the module models. This was due to the project partners invested interest in particular process technologies and lack of process engineering expertise in specifying design and costing processes.

The models and results bring together the information and data from across the Biosynergy Project. Data was collected successfully from 17 different project partners in order to create the process model and accurately represent the project. The module models were validated by the project partners and also by comparison to literature results if available. A total of 32 different process modules were created and linked together. These modules and the model as a whole provide a long lasting record of the Biosynergy project and the completed methodology provides an important tool for the project partners after

completion of the project. The completed model can be found on the attached CD (Appendix 5).

10.1.1 UNCERTAINTY IN MODULES AND THE PROCESS MODEL

The module models contain several sources of uncertainty relating to performance, design and costs. As the project progressed and other work packages developed new processes, there was uncertainty in the optimised performance of the individual processes, the translation of laboratory results and procedures into working fully engineered processes, the prediction of the performance and design of the scaled up processes, and the estimation of capital and other costs. The approach taken was to accept the data provided by the partners and only resort to literature in the absence of relevant data. Where possible data provided by the partners was compared to published data and agreed adjustments made when relevant.

Having the module models based on experimental results from partners was a positive that ensured that the models truly represented the process, but it also had its disadvantages. Any experimentally determined data is subject to error due to precision errors, errors of measurement and errors of method (55). Hence any models based on experimental data also contain the same errors and are limited in accuracy. The information may not represent the optimal case, as the results of a large scale plant may differ greatly from the results achieved experimentally. Although partners were requested to supply anticipated performance data, there is no way of accurately realising the final performance of these technologies at a commercial scale. The level of error can only be estimated as it is near impossible to measure it (55).

Some of the individual modules contained a higher level of uncertainty than others and this varied based on the source, status of the technology and quality of the data. An estimate of the uncertainty in terms of performance and cost was made (see Table 10.2). A star system was used with five stars indicating a high level of uncertainty and one star a low level. Within this table the development status of these processes is listed, as this also has an impact on the uncertainty of the data and results. For example, models created using data supplied by ABNT were based on operational demonstration or commercial scale plant; therefore the level of uncertainty in data is lower. For more innovative processes like aquathermolysis or xylonic acid production, the models were based on projected laboratory scale data, which is less certain. The degree of uncertainty cannot be predicted but module performance may be affected by up to 50% and capital costs by up to a factor of three. The

uncertainty of different biorefinery concepts will vary depending on the status of the technologies included but it has been estimated that on average the models contain an uncertainty factor of ±40%.

Table 10.2- Estimated performance and cost uncertainty per module

Module	Performance uncertainty	Cost uncertainty	Development stage	Data source
RSH	*	**	Commercial	Toft (89)
Steam explosion	**	**	Demonstration	ABNT, Aden (137)
Fractionation	**	**	Demonstration	ABNT, Li (95), Nguyen (94)
AVIDEL	**	***	Pilot	ARD
Organosolv	**	***	Laboratory	ECN
Mechanical/alkaline fractionation	****	****	Laboratory	A&F
Concentrated HCl	****	****	Laboratory	Bioref
Aquathermolysis	****	*****	Laboratory	ECN
Fluidised bed gasification and gas clean up	*	**	Commercial	ABNT, ECN, Phillips (120, 121), Dutta (122), Boerrigter (114)
Fluidised bed gasification, Fischer-Tropsch synthesis	***	***	Demonstration	Kreutz (116), Bechtel (117)
Mixed alcohol synthesis	**	***	Pilot	ABNT, Philips (120, 121)
Mixed alcohol distillation	**	***	Pilot	ABNT
C5 to ethanol	**	***	Demonstration	ABNT, IFP, Aden (137)
C5 to ABE	***	***	Laboratory	IFP
C5 to furfural	**	**	Pilot	TUD
C5 to surfactants	*	***	Pilot	ARD
C5 to xylonic	*****	*****	Laboratory	VTT
C6 to ethanol	*	**	Commercial	ABNT, Sassner (145), Aden (137)
C6 to ABE	**	***	Laboratory	IFP
C6 to FDCA	****	*****	Laboratory	Bioref
Ethanol distillation	*	*	Commercial	ABNT, IFP
Fast pyrolysis	*	*	Demonstration	Aston (AVB), ECN
Lignin drying	*	**	Demonstration	Toft (89)
Stillage drying	*	**	Commercial	ABNT
Bio-oil fractionation	** (ex *****)	****	Laboratory	BTG
Bio-oil gasification	**	**	Laboratory	ECN, Drift (136)
Heat and power from biomass	***	***	Demonstration	JR, ABNT, Aden (137)
Heat from biomass	*	**	Demonstration	JR, ABNT, Aden (137)
Heat and power from non-renewables	*	*	Commercial	JR, ABNT, Toft (89)
Wastewater treatment	* to ***	* to ***	Commercial	Aden (137)

Where possible the project partners provided capital cost estimates or an equipment list on which the cost estimates were based. If the equipment list was generated by inexperienced scientists rather than experienced chemical engineers pieces of equipment may have been omitted, leading to underestimates of the cost. Equipment specification may have been incomplete, due to the level and status of the research. Furthermore, cost estimation factors were used to make an estimate of the fixed capital investment (see Section 5.6). There is

inbuilt uncertainty in the use of these factors as they are based on generalised assumptions and may not be wholly applicable to biorefineries.

10.2 CONCEPT MODELLING RESULTS,

The process model described in Chapters 5 and 6 was used to generate results for the concepts listed in Table 10.1. These models generated large amounts of information to be used in the evaluation step for the identification of the most promising biorefineries.

10.2.1 PROCESS MODEL RESULTS

In Table 10.3 the economic and efficiency results are shown for each of the 27 concepts. The results are based on biorefineries processing 500,000tpa dry biomass input, heat and power provided by biomass and process residues, located in Spain. Any surplus electricity produced in the heat and power plant is exported to the grid to generate extra income. All costs are calculated in €2009.

Table 10.3 – All concepts (Spain), process modelling results

	Total fixed capital investment	Operational cost	Production cost	Product income	Profit/loss	Conversion efficiency
	€M	€M/annum	€M/annum	€M/annum	€M/annum	%
0	323	84.0	143	83	-60.0	35%
1	454	71.5	152	92	-59.6	41%
2	485	87.5	174	99	-74.4	41%
3	474	35.3	117	81	-35.9	37%
4	366	75.6	141	64	-77.3	24%
5	494	118.4	208	97	-110.7	45%
6	316	124.4	184	143	-41.2	43%
7	387	89.9	160	81	-79.2	27%
8	376	99.4	168	67	-100.9	25%
9	448	71.1	150	93	-57.1	46%
10	489	122.7	211	101	-110.7	33%
11	288	120.4	175	104	-71.1	49%
12	382	130.3	202	120	-81.0	51%
13	293	83.6	137	104	-33.1	49%
14	285	31.0	81	50	-30.9	20%
15	121	28.6	50	60	9.3	73%
16	611	122.7	232	121	-111.1	53%
17	456	79.8	161	178	16.8	59%
18	357	114.4	181	173	-7.5	50%
19	581	132.1	237	242	5.2	21%
20	450	79.6	160	152	-7.2	31%
21	288	28.9	79	43	-35.7	65%
22	614	57.5	164	77	-86.6	29%
23	699	35.8	155	80	-75.9	20%
24	345	139.0	204	112	-92.1	49%
25	372	123.9	193	108	-84.6	75%
26	358	101.1	167	206	39.4	49%

In each column the best results are highlighted in green and the worst results highlighted in red. This makes it easier for the reader to assess the results at a glance. Due to the uncertainty contained within the models, the three top and bottom performing concepts are highlighted as it cannot definitively be stated which is the best concept and which is the worst. Displaying the results in this way makes it easier to identify concepts that perform particularly well or badly.

Concepts 15 and 21 stand out as having good performance in terms of the variables included in the table. Concepts with consistently poor performance appear to be Concepts 16 and 19. It is interesting to compare the best and worst in this simple analysis with the MCDA results, to see if there is any correlation (see Section 10.4.8). In the following sections an attempt is made to identify why the best and worst concepts perform as they do for each of the variables in Table 10.3.

Much more data is generated by the models than shown in Table 10.3 but as each output file occupies at least 5 pages, these cannot be included for all 27 cases. An example is given in Appendix 4 for Concept 25, the ABNT base case.

10.2.1.1 TOTAL FIXED CAPITAL INVESTMENT (TFCI)

The total fixed capital investment (TFCI) is an estimate of the amount of capital required to supply all equipment and facilities needed to run a process plant (see Section 5.6.1 for more details). For each of the concepts the Total Fixed Capital Investment (TFCI) was estimated.

A further breakdown of the TFCI for the 27 Cases is shown in Figure 10.1. This chart displays the contribution of each module to the overall capital investment. A large proportion of the TFCI for the concepts can be attributed to heat and power plant for the biorefinery (on average 40% of TFCI).

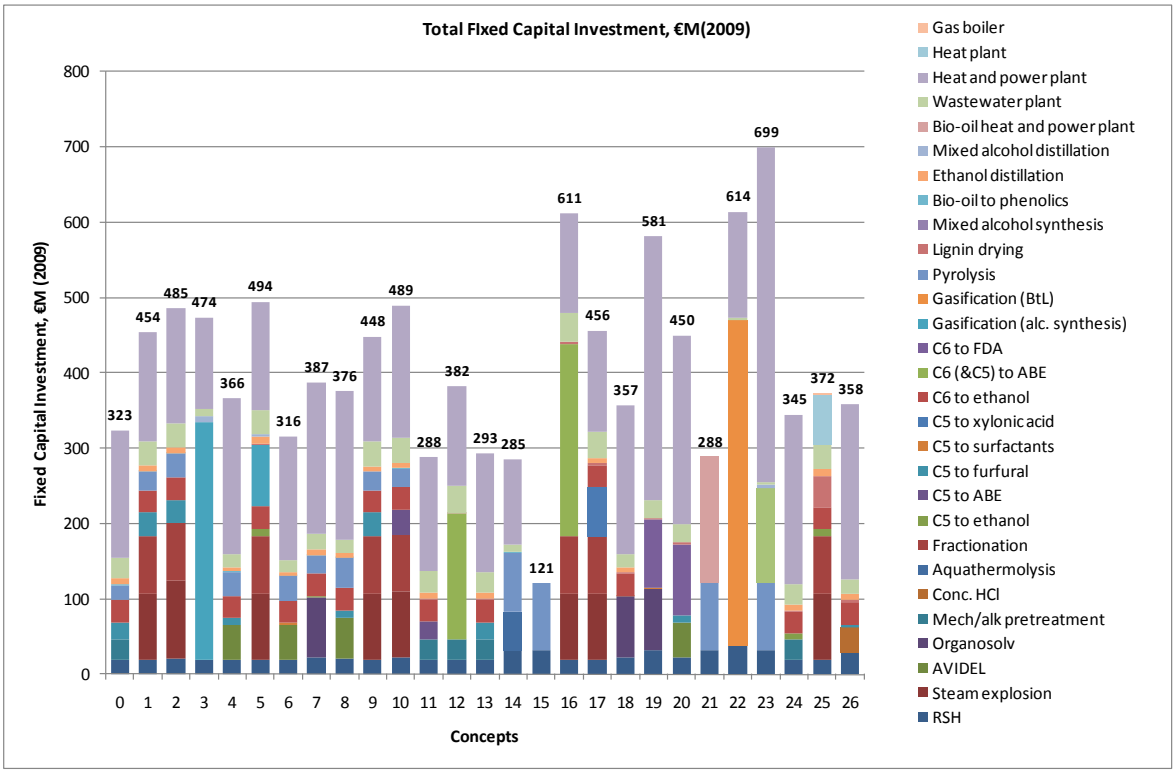

Figure 10.1 – Total fixed capital investment breakdown, €

For the 27 concepts the heat and power was mostly provided by the combustion of process residues to generate steam that was then passed through a turbine to generate electricity. If the concept had high heat and power demand this had two effects; the cost to purchase the heat and power plant increased, and if the existing process residues did not provide enough heat and power, then extra biomass had to be purchased. This in turn adds to the operational and so the production costs (see Figure 10.2). On average feedstock costs account for 40% of operational cost, for those plants requiring additional biomass for heat and power this increases to 50% of the operational cost. Purchasing more biomass has an impact on the socio-economics and feasibility of the plant because if the extra biomass required is too great, the region may not be able to supply the plant at a reasonable cost (due to increased transport costs).

Highest TFCI

Concept 23 – This concept includes a gasification process that generates a large volume of surplus steam. It was assumed in the models that any surplus steam generated be used to generate electricity. Any electricity in excess of that required to operate the biorefinery is then sold to provide extra income. To utilise the waste heat a large heat and power plant is required, which causes the FCI of the heat and power module to be high. In Figure 10.1 this is illustrated as the proportion of the overall cost attributed to heat and power plant

(which includes the electricity generation) is shown. If this excess heat was not utilised for electricity generation, the plant cost would be lower, but so would the income and overall plant efficiency. The impact of heat and power generation is investigated in Section 10.3.5.

Concept 22 – This concept is also expensive in terms of TFCI. The majority of the cost can be attributed to the gasification and biomass to liquid plant. This plant is highly complex and hence expensive.

Concept 16 – The largest proportion of the cost for this plant can be attributed to the ABE conversion steps. There are a large number of steps in ABE production including neutralisation, enzymatic hydrolysis, solids removal etc. The large number of steps and the high volumes involved mean that the cost of the plant is high.

Lowest TFCI

Concept 15 – This concept has the lowest TFCI at €121M and is significantly lower than all other concepts. This concept includes the fast pyrolysis of biomass to produce bio-oil. No complex pretreatment plant is required prior to the fast pyrolysis, apart from drying and comminution of the feed. The heat and power requirement is also low meaning that no expensive heat and power plant is required. Furthermore the bio-oil product does not undergo any further processing, reducing the number of overall processing steps in the biorefinery concept.

Concept 14 –The aquathermolysis process involves a large number of steps, but the equipment consists of standard vessels and reactors with no innovative equipment. There is greater uncertainty over the process performance and cost estimates for this concept as the technologies are still at the lab-scale.

Concept 21 – For the same reasons as Concept 15 this concept has a low fixed capital investment i.e. no pretreatment.

10.2.1.2 OPERATIONAL COST

The operational cost is an estimate of the cost for operating the plant in terms of materials and auxiliary heat/power (if required). It excludes capital related costs and labour but takes into account the cost of feedstock, chemicals and any other materials required for operation. If the process residues did not provide all heat and power requirement then additional fresh biomass had to be purchased increasing the operational costs. For more details see Section 5.6.2. The operational costs for each concept are shown in Figure 10.2.

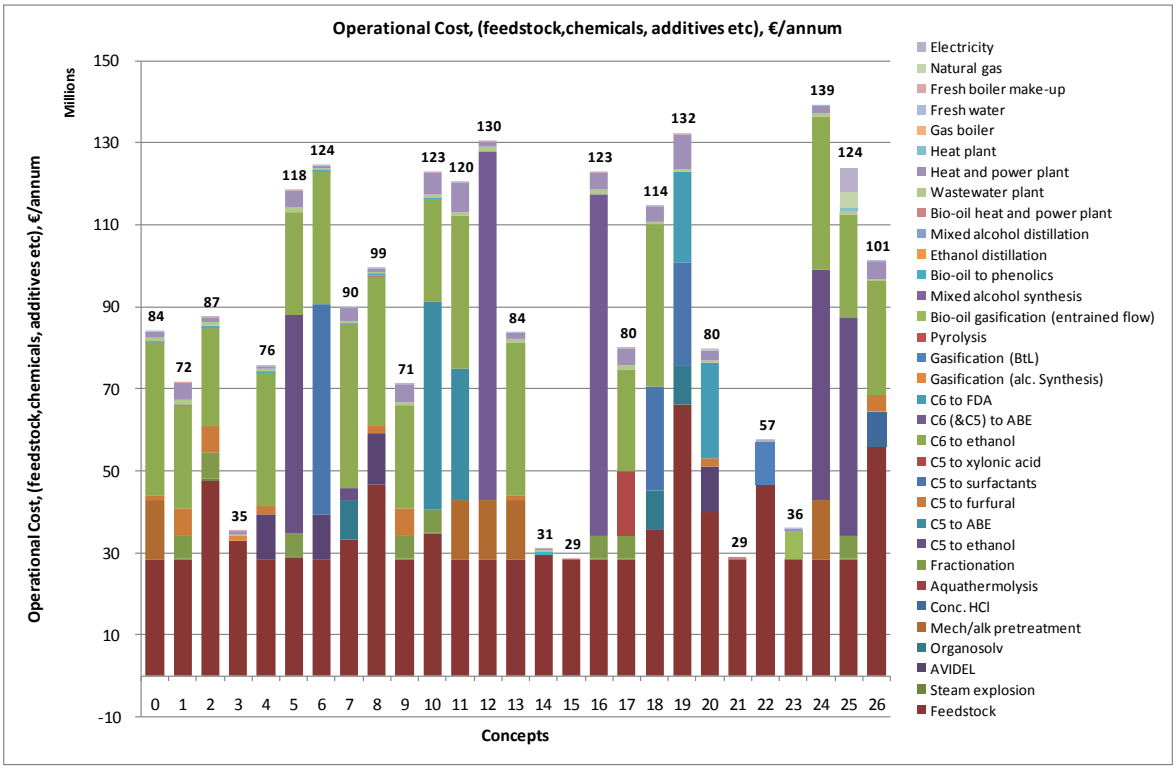

Figure 10.2 – Operational cost, €/annum

Highest operational cost

Concept 24 – In this process the high cost of €139M/annum can be attributed to the enzymes required for ethanol production and the neutralisation chemicals required after the pretreatment step.

Concept 19 – The majority of the operational cost is for the purchase of feedstock. The processes included have very high heat and power demand so as well as the 500,000tpa required for conversion into products, a large amount of biomass is required in order to provide sufficient heat and power to the plant. In addition the conversion processes involved require the purchase of expensive auxiliary chemicals and materials.

Concept 12 – This concept is expensive due to the cost of chemicals and enzymes for the C5 and C6 fermentation to ABE. In addition, the mechanical/alkaline pretreatment is the most expensive pretreatment method in terms of operational cost leading to a high overall operational cost.

Lowest operational cost

Concept 15 – This concept has a low operational cost due to the fact that no expensive chemicals are required in the process. Many of the other concepts require chemicals and other auxiliary materials in order to carry out pretreatment and synthesis steps. The bio-oil

is sold directly so no further chemical processing is required and no costly pretreatment or chemicals are required. The majority of the cost is attributed to the feedstock only. See Figure 10.2.

Concept 21 – As for Concept 15 the fast pyrolysis process does not require any expensive chemicals. The cost is made up of the feedstock only.

Concept 14 –Only limited chemical and auxiliary materials are required for this concept. The process requires mostly water and a small quantity of chemicals for furfural production. There is a high level of uncertainty in this biorefinery concept as the results and assumptions could not be validated with literature due to the innovative nature of the process.

10.2.1.3 PRODUCTION COST

The production cost was calculated based on the operational cost and the TFCI. This included the cost of capital repayments, fixed costs and other miscellaneous costs. The production cost for each concept is shown in Figure 10.3. For more details on the calculation of production cost see Section 5.6.3.

Highest production cost

Concepts 19, 16 and 5 all have high production cost. This is due to the high TFCI of these concepts coupled with high operational costs.

Lowest production cost

Concepts 15, 21 and 14 had the lowest production costs due to the low TFCI and low operational cost. This led to a low production cost.

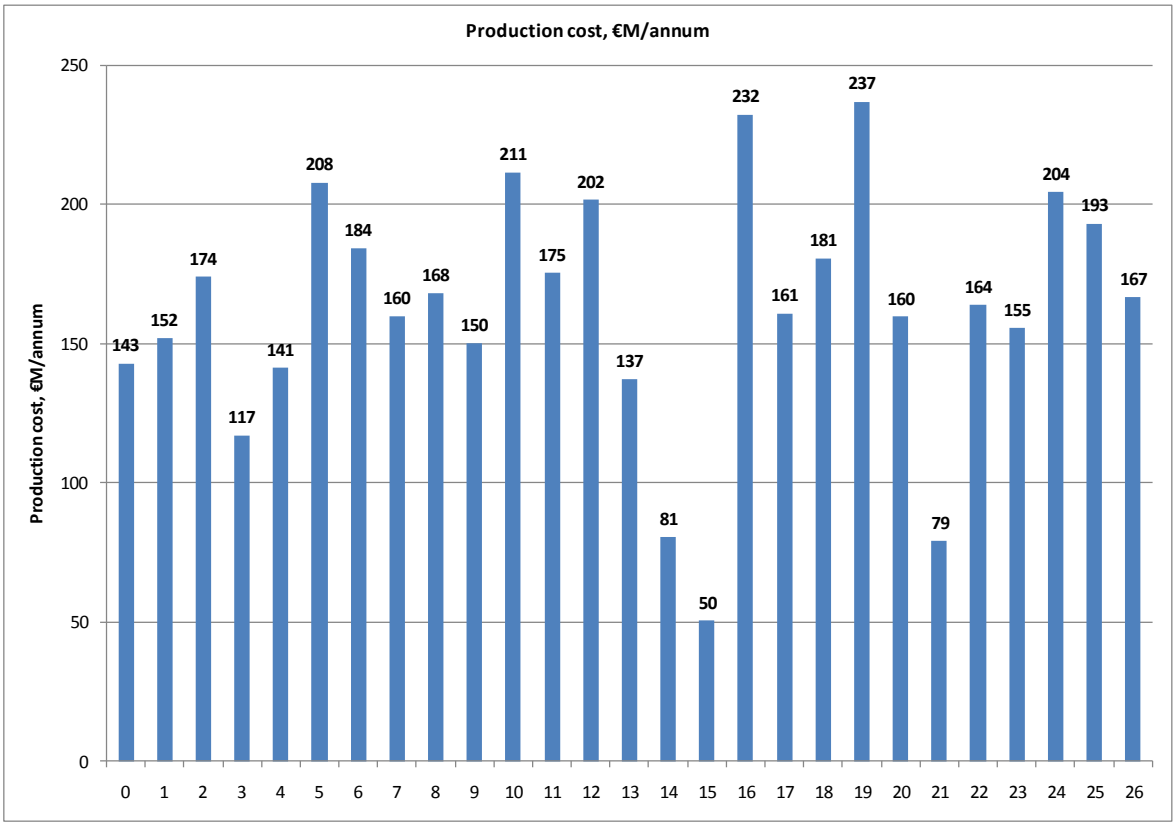

Figure 10.3 – Production cost, €M/annum

10.2.1.4 PRODUCT INCOME

The potential product income was calculated for each of the concepts based on the amount of product manufactured and the assumed product prices. The product prices assumed are shown earlier in Table 5.14. The results for each concept are shown in Figure 10.4.

Highest product income

Concept 19 – Produces surfactants, FDCA and lignin. All of these are relatively expensive specialty products. As well as the high value specialties this concept generates substantial amounts of electricity for sale back to the grid. However, there is uncertainty in the prices assumed for specialty products as they are not yet commercially available. A sensitivity was carried out on the product values in Section 10.3.4 to investigate the impact of product price variation.

Concept 26 – Produces furfural, ethanol and lignin. Lignin constitutes the biggest income from the products in this configuration, although there is greater uncertainty over the value attributed to this product. The value was based on an investigation by ABNT of the required selling price for lignin to make the fractionation process worthwhile (115).

Concept 17 –Produces xylonic acid, ethanol, and lignin. The highest proportion of income is generated by the sale of xylonic acid. This illustrates the economic benefit of producing high value specialties alongside lower value commodity chemicals.

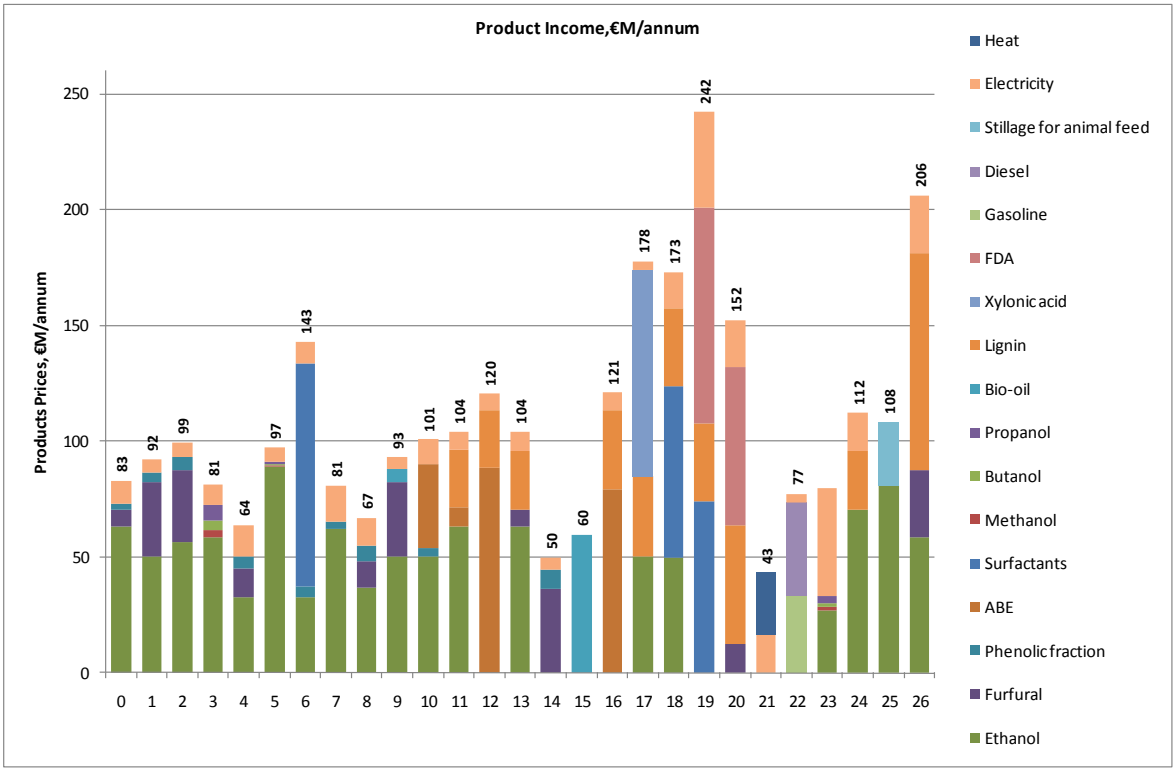

Figure 10.4 – Product income, €M/annum

Lowest product income

Concept 21 – Generates heat and power for integration into a petrochemical refinery. This indicates that only a poor income is received for transforming the biomass into bio-oil and then into heat and power for use in a conventional petrochemical refinery. The results from this concept raise the question of whether the extra processing before heat and power generation is valuable.

Concept 14 – Produces bio-oil phenolics and furfural (aquathermolysis concept). The conversion of biomass into products in this concepts is low, hence the low income. The level of uncertainty is high due to the innovative process and the lack of operational data.

10.2.1.5 PROFIT/LOSS

The profit/loss is calculated using the product income and the production cost (see Section 5.6.4). This gives an indication of whether the biorefinery concept is likely to be profitable or not. The profit/loss for each concept is shown in Figure 10.5.

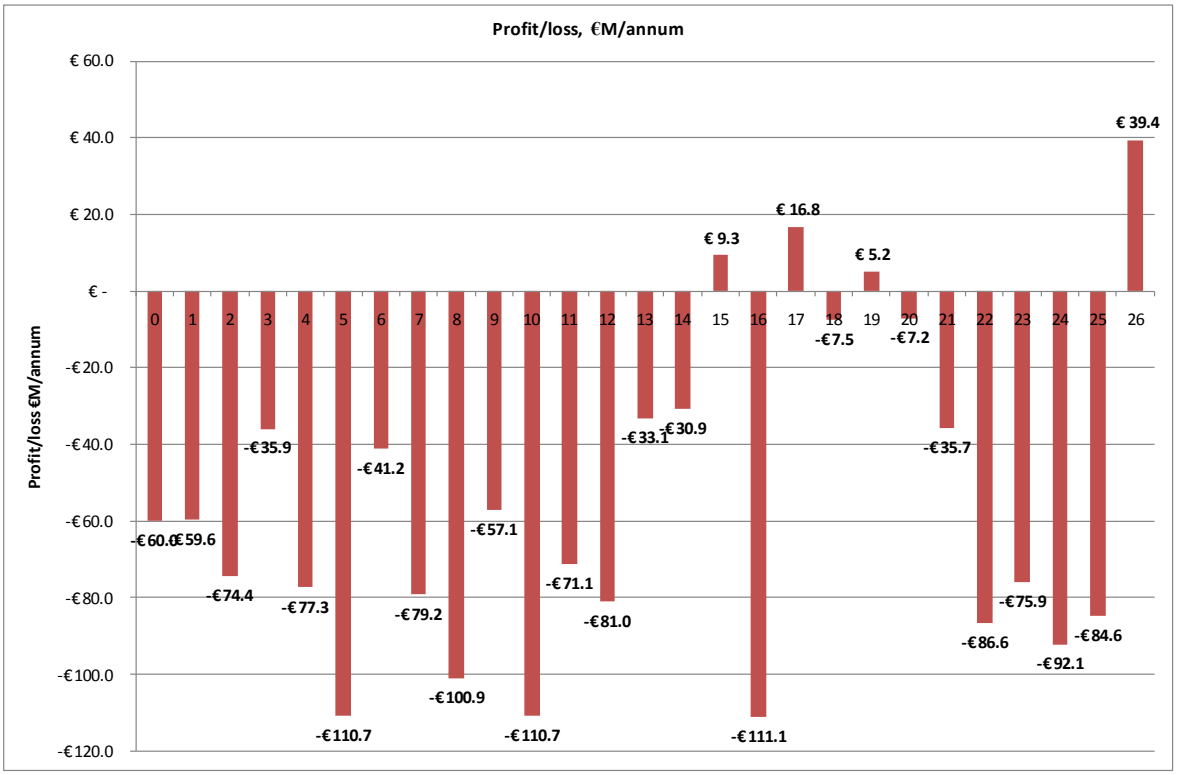

Figure 10.5 – Profit/loss, €M/annum

Unfortunately the vast majority of the concepts are not profitable, which means that they are likely to be disregarded by industrial stakeholders unless there are financial support mechanisms in the form of tax relief or other incentives. Only 4 out of the 27 concepts are projected to make a profit, based on the estimations made in this model. These are Concepts 26, 17, 15 and 19. The result of negative profitability for many of biorefinery concepts was not unexpected. In the report by Boerrigter (162) it was also found that none of the gasification routes to synthetic natural gas (SNG) or Fischer-Tropsch fuels were economically feasible. This indicates that any biorefinery complex would require incentives to make them feasible or significant improvements in capital and operating costs or efficiency. The ideal biorefinery concept would couple low investment and operational costs with high product income. In the long term, as fossil based products increase in price, this may help make biorefineries more competitive from a cost point of view.

The most profitable biorefinery is Concept 26. This processes wheat straw, through concentrated HCl pretreatment to furfural, ethanol and dry lignin product. This concept generates one of the highest incomes and coupled with an average production cost generates the highest profit at €39.4M/annum.

The other profitable concepts are 15, 17 and 19. Concept 15 has a relatively low income but also has the lowest production cost. Concept 17 has a high income with an average

production cost and Concept 19 has a high income but also a high production cost. For Concept 19 the production cost is identified as an area for development in order to improve the profitability. Later in this chapter (Section 10.3) a sensitivity analysis is described. This was carried out to assess the improvement to profit/loss by increasing or decreasing the product income. These results can be used to investigate the benefits of improved income.

10.2.1.6 CONVERSION EFFICIENCY

As well as economic performance of the concepts the processing performance was calculated in terms of conversion efficiency. The energy conversion efficiency gives an efficiency value using the energy contained in the products compared to the initial energy input from the biomass feedstock. The higher the value, the more effectively the energy contained within the biomass has been converted to products in the biorefinery. The equation to calculate this:

$$\text{Energy conversion efficiency \%} = \frac{\text{Energy flow rate products (MJ/h)}}{\text{Energy flow rate biomass input (MJ/h)}} \times 100 \qquad [5]$$

The energy conversion efficiency was used instead of the mass conversion efficiency due to the difficulty of representing all products of the biorefinery in mass terms. The majority of the biorefinery concepts also generate electricity as a by-product and one of the biorefinery concepts (Concept 21) generates heat as a product. These cannot easily be expressed in mass terms, hence the use of the energy conversion efficiency. For the products the lower heating value (LHV) is used to calculate the energy contained in the product. The heat and electricity are easily expressed in energy terms. The calculation is made based on the total amount of biomass used by the biorefinery i.e. including any additional biomass required to meet heat and power requirements. This led to lower conversion efficiency for those concepts requiring extra biomass for heat and power. The results are shown in Figure 10.6.

For validation the energy conversion efficiency values (see Table 10.3) were compared to those found in the literature. They compare favourably with the values detailed in Bridgwater's assessment of thermochemical routes (86) which gives efficiency values of between 30 – 50%. For his thesis some of the efficiencies achieved were higher, but this was anticipated due to the high level of uncertainty in those particular models. The models were built based on projected performance, which means that the efficiencies were probably higher than would actually be achieved.

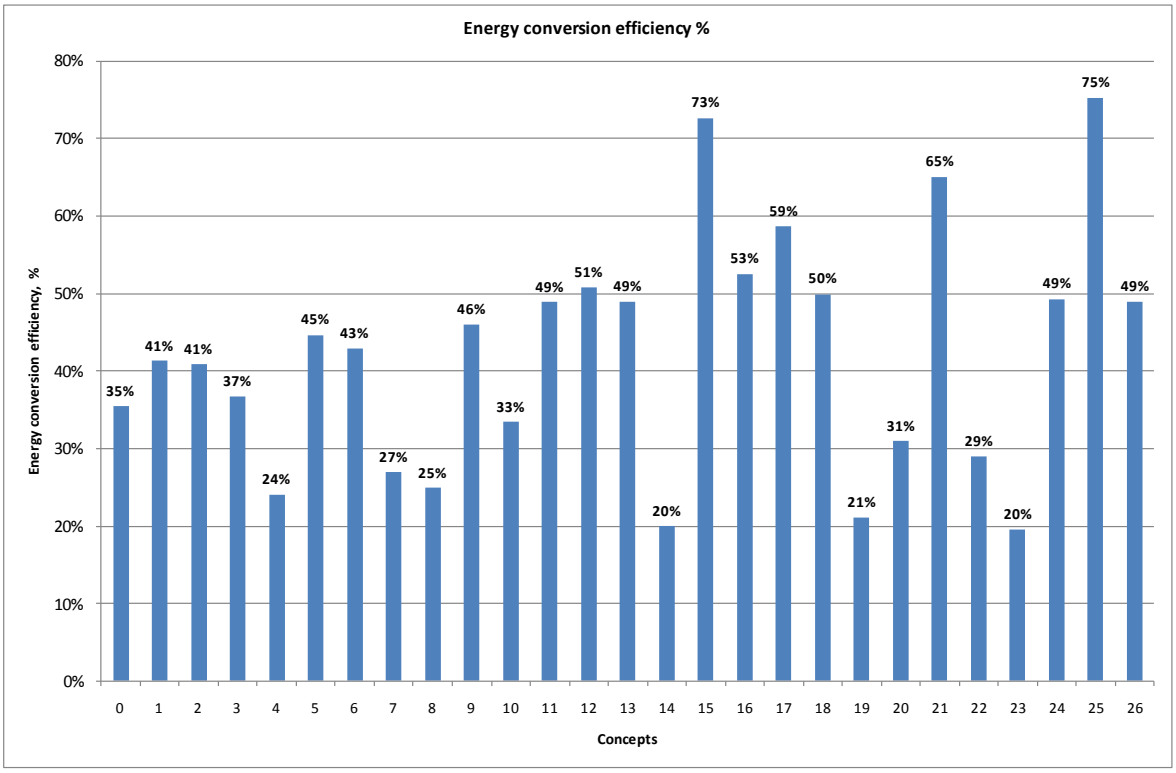

Figure 10.6 – Energy conversion efficiency, %

Highest conversion efficiency

Concept 25 – This concept is the ABNT base case. The reason for the high conversion efficiency is due to the use of the stillage as an animal feed product. The stillage contains all of the lignin and unconverted C5 and C6 components; it is effectively a waste stream. In other concepts these streams are converted into value added products. There is uncertainty about the selling of the stillage as animal feed, especially if genetically modified enzymes are used in the hydrolysis and fermentation process.

Concepts 15 and 21 – Achieve a high yield of bio-oil product which gives high conversion efficiency.

Lowest conversion efficiency

Concept 23 – This process contains fast pyrolysis followed by gasification of the bio-oil. The resulting syngas then undergoes alcohol synthesis. The reason for the low conversion efficiencies is the relatively conservative yields assumed on this unproven arrangement. This concept includes a large amount of processing and with each additional process step more losses occur.

Concept 14 – Aquathermolysis is a new technology still at laboratory scale testing, so conservative estimates were made of the expected yields.

Concept 19 – The reason for the low yield is that a large proportion of the biomass input is used to provide heat and power to the plant. Low yields were achieved by the Organosolv pretreatment, followed by FDCA, surfactants and dry lignin. If the biomass used only for processing into products is considered the energy conversion efficiency increases to 49%.

10.2.2 BIOCHEMICAL VS. THERMOCHEMICAL

It was of interest to compare biochemical processes to thermo-chemical routes to ethanol and other fuels. A comprehensive evaluation was found in relatively few papers in the literature (see Section 8.2). For this evaluation, additional results were generated for the biorefineries shown in Table 10.4 at a scale of 500,000 tpa wheat straw (dry basis).with the plant located in Spain.

Table 10.4 – Biochemical vs. thermochemical concepts

	Feed	Pretreatment	C5	C6	Lignin
Biochem - steam explosion	Straw	Steam explosion	Ethanol	Ethanol	Dry lignin product
Biochem - AVIDEL	Straw	AVIDEL	Ethanol	Ethanol	Dry lignin product
Biochem - Organosolv	Straw	Organosolv	Ethanol	Ethanol	Dry lignin product
Biochem - Mechanical/alkaline	Straw	Mechanical/alkaline fractionation	Ethanol	Ethanol	Dry lignin product
Biochem - Conc. HCl	Straw	Conc. HCl pretreatment	Ethanol	Ethanol	Dry lignin product
ABNT base case	Straw	Steam explosion	Ethanol, stillage to animal feed		Lignin combusted
Thermochem - mixed alcohols	Straw	Gasification	Syngas to ethanol/ mixed alcohols		
Thermochem - hydrocarbons	Straw	Gasification	Fischer-Tropsch synthesis to hydrocarbons		
Thermochem – bio-oil	Straw	Fast pyrolysis	Bio-oil		
Hybrid	Straw	Steam explosion	Ethanol	Ethanol	Gasification to ethanol

For the biochemical routes it was interesting to include different pretreatment methods with the C5 and C6 streams fermented to ethanol and the lignin stream dried and sold as a product. The ABNT base case was included as this represents a plant in operation (albeit at a different scale). For the thermochemical routes three different options were included. The first involved gasification of the biomass followed by mixed alcohol synthesis. A gasification route in which the syngas was converted to hydrocarbon fuels and the hybrid configuration of Concept 5 was included which combined both biochemical and thermochemical production of ethanol.

The economic and efficiency results are shown in Table 10.5. In this table the top (green) and bottom (red) two performing concepts for each category are highlighted. Only two of

the options were estimated to be profitable; the biochemical route to ethanol utilising concentrated HCl pretreatment and the thermochemical option of fast pyrolysis to bio-oil. The hybrid route generates the greatest loss (-€111M) due to the high costs to purchase and operate such a complex plant. The thermochemical route to hydrocarbon fuels performs badly in terms of TFCI, income and conversion efficiency, although these products would be the easiest to sell to the marketplace. In general it can be stated that the thermochemical options are more expensive in terms of TFCI, but have lower operational cost. This is because they do not use chemicals in pretreatment or expensive enzymes in the conversion process. The biochemical routes generally generate more income than the thermochemical routes.

Table 10.5 – Process model results, biochemical vs. thermochemical investigation based on 500 ktpa dry biomass input

	TFCI	Operational cost	Production cost	Product income	Profit/loss	Energy conversion efficiency	Ethanol produced
	€M	€M/annum	€M/annum	€M/annum	€M/annum	%	ktonnes/ annum
Biochemical -Steam explosion	397	118	191	120	-71	60%	115
Biochemical - AVIDEL	316	83	141	109	-32	52%	65
Biochemical - Organosolv	361	92	157	111	-46	40%	89
Biochemical – Mech alk	345	139	204	112	-92	49%	101
Biochemical - Conc. HCl	355	102	167	206	40	53%	126
ABNT base case	372	124	193	108	-85	75%	115
Thermochem - mixed alcohols	474	35	117	81	-36	37%	84
Thermochem - hydrocarbons	589	44	145	72	-73	28%	~
Thermochem - bio-oil	121	29	50	60	9	73%	~
Hybrid	494	118	208	118	-111	45%	~

The results of this investigation can be used to look at the best pretreatment method for producing ethanol. In terms of ethanol production the concentrated HCl pretreatment method produces the largest amount, followed by steam explosion, mechanical/alkaline pretreatment, Organosolv and AVIDEL. The concentrated HCl pretreatment generates the highest income because of the large amount of lignin produced.

10.2.3 PRODUCTS

Some further observations about the products are described in this section. Table 10.6 shows the total production for each of the 27 concepts. Looking at these results and the technologies included in the concepts some additional observations were made about the concepts.

Table 10.6 – Annual production, ktonnes/annum

Concept	Annual production, ktonnes/annum														
	Ethanol	Furfural	Phenolic fraction	ABE	Surfactants	Methanol	Butanol	Propanol	Bio-oil	Lignin	Xylonic acid	FDA	Gasoline	Diesel	Stillage for animal feed
0	90.0	12.0	3.6												
1	71.7	51.9	5.1												
2	80.4	49.7	7.5												
3	83.9					9.6	4.0	22.4							
4	46.7	20.2	6.4												
5	127.6					1.4	0.6	3.2							
6	46.7		6.4		64.2										
7	88.6		4.5												
8	52.4	18.1	9.4												
9	71.7	51.9							30.8						
10	71.7		5.1	39.6											
11	90.0			9.1						62.8					
12				97.3						62.8					
13	90.0	12.0								62.8					
14		57.7	11.2												
15									341.6						
16				86.9						86.4					
17	71.7									86.4	89				
18	70.9				49.5					83.9					
19					49.5					83.9		62.1			
20		20.2								128.1		45.6			
21															
22													24.8	36.2	
23	38.4					4.4	1.8	10.3							
24	101.0									62.8					
25	115.4														276.4
26	83.8	46.0								234.0					

- The highest ethanol yield was achieved by Concept 5. This makes sense as all streams are utilised for ethanol production following the steam explosion pretreatment
- The highest furfural yield is achieved by using the aquathermolysis pretreatment process in Concept 14. This concept also produces the highest yield of phenolic fraction.
- The best ABE yield is achieved in Concept 12, which utilises the mechanical/alkaline pretreatment process.

- The best surfactant yield is achieved in Concept 6 which uses the AVIDEL pretreatment process (there are no concepts with steam explosion, concentrated HCl or mechanical/alkaline pretreatment preceding surfactant production so it cannot be stated from these results which pretreatment gives the best yield. This may be interesting for further sensitivity analysis).
- Concept 3 gives a better yield of alcohols than if bio-oil is first produced and then gasified as is Concept 21. This option may be beneficial if used for decentralised fast pyrolysis plants with the bio-oil transported to centralised bio-oil processing plant.
- The best yield of dry lignin achieved in Concept 26 which uses the concentrated HCl pretreatment method.
- Xylonic acid is only produced in one concept (Concept 17); it is recommended that further investigations are carried out for xylonic acid production. Better yield may be achieved with alternative pretreatment methods for example.

10.2.4 ENVIRONMENTAL MODELLING RESULTS

The environmental model was created by JR and JRC (163, 164). The model was based on mass and energy balances from the 27 biorefinery concepts at a scale of 500,000tonnes dry biomass per annum. The environmental model was not integrated with the module and socio-economic models. From the material and energy flows the environmental performance was calculated. A selection of results is shown in Table 10.7. These are not the complete results but include the categories included in the biorefinery evaluation. For a short description of the categories see Section 5.7.

Looking purely at the environmental performance of each of the concepts Concept 15 appears to have the best performance, followed by Concept 3 and 21. Concept 15 has low emissions in nearly all of the categories included. The worst performing concepts from an environmental point of view were Concept 24 and 20. Concept 24 performs particularly badly in all of the categories, making it the worst performing concept in terms of environmental impact. This concept included mechanical/alkaline fractionation of wheat straw followed by the production of ethanol and a dry lignin product.

In the model created by JR further results are calculated and the results are compared to reference plants. This is typical of an LCA assessment with the biorefinery compared to a plant producing the same products using conventional methods. This allows the evaluation of the real environmental benefits of utilising biorefinery plants. All concepts were found to have lower CO_2 emissions than the corresponding reference case, with an average

reduction of 63% (163). On average a decrease of 32% in global warming potential was observed for nearly all concepts (163).

Table 10.7 – All concepts (Spain), environmental results

	Particles	Abiotic Depletion	Acidification Potential	Eutrophication Potential	Global Warming Potential	Ozone Layer Depletion Potential	Photochem. Ozone Creation Potential	Primary Energy Demand
	kg/t d.b.	kg/t d.b.	kg/t d.b.	kg/t d.b.	kg/t d.b.	mg/t d.b.	kg/t d.b.	GJ/ t d.b.
0	0.64	3.27	5.75	0.94	430.28	51.14	4.12	6.80
1	0.47	3.33	5.26	0.89	478.24	53.10	3.44	6.92
2	0.29	3.50	4.84	0.22	458.54	57.44	3.84	7.27
3	0.36	0.47	3.29	0.75	270.63	12.52	3.48	0.97
4	0.75	3.08	5.53	0.94	500.52	58.20	4.37	6.39
5	0.45	2.29	5.43	0.92	346.58	50.57	5.95	4.76
6	0.74	6.94	5.45	1.01	870.71	62.64	3.81	14.43
7	0.48	1.39	3.77	0.78	254.75	27.75	3.72	2.89
8	0.44	3.49	4.76	0.29	524.86	69.39	4.49	7.25
9	0.49	3.28	5.68	0.89	470.88	52.29	4.29	6.83
10	0.50	1.94	4.57	0.88	306.86	42.24	3.45	4.04
11	0.60	3.13	5.62	0.96	419.39	51.54	3.90	6.50
12	0.54	3.01	4.78	0.98	385.42	44.27	2.18	6.26
13	0.61	3.24	5.67	0.94	437.44	50.25	4.01	6.73
14	0.39	0.83	3.49	0.77	354.79	26.43	2.50	1.72
15	0.79	0.76	8.35	0.78	269.87	24.32	11.85	1.58
16	0.44	1.95	4.05	0.91	289.38	33.01	2.23	4.06
17	0.48	2.59	5.12	0.94	399.36	59.99	3.39	5.39
18	0.57	3.09	4.34	0.90	450.70	31.03	3.92	6.43
19	0.95	3.36	5.20	0.92	523.05	225.19	3.73	6.97
20	1.09	4.21	6.35	1.00	690.87	296.15	3.84	8.74
21	0.77	0.63	8.23	0.75	252.77	21.54	11.83	1.32
22	0.24	1.53	3.39	0.17	298.02	59.66	3.25	3.19
23	1.55	1.26	9.82	0.79	441.86	50.34	10.09	2.62
24	1.16	5.50	8.67	1.09	739.62	72.05	5.67	11.42
25	0.35	3.03	5.88	1.10	682.78	57.43	3.33	6.44
26	0.60	1.46	4.05	0.81	376.23	70.54	3.62	3.03

The environmental model results were further investigated by JR (163, 164), to evaluate which variables had the most influence on the environmental performance. These results are summarised in Table 10.8. It was found that the emissions from the auxiliary materials has a significant effect on the overall performance and that cultivation of the feedstock accounts for 32% of the total N_2O emissions (163). There is an increase in CO emissions for concepts using wood feedstocks, due to the heavier vehicles required (164).

Table 10.8 : Summary of dominating factors and concepts (164)

Indicator	Primary influence	Secondary influence	Best concepts	Worse concepts
CO_2	Biomass combustion	Auxiliary materials	3, 21	6, 20, 24
CH_4	Auxiliary materials		3, 14, 15, 21	6, 20, 24
N_2O	Cultivation	Biomass combustion	2, 8, 22	3, 14, 23
CO	Consumption of products		12, 15, 16 20, 21, 22	5, 24
SO_2	Auxiliary materials	Biomass combustion	3, 15, 16, 21, 22	23, 24
NO_x	Bio-oil use			15, 21, 23
NMVOC	Auxiliary materials	Biomass combustion	14, 15, 21	5, 6, 23, 24
PM10	Bio-oil use		2, 8, 22 (wood-based concepts)	15, 23 ,24
>PM10	Auxiliary materials		3, 14, 15, 21, 22, 23	6, 19, 20, 24
Abiotic depletion	Auxiliary materials		3, 14, 15, 21, 22, 23	6, 19, 20, 24
Acidification potential	Auxiliary materials	Biomass combustion	2, 3, 14, 22	15, 21, 23, 24
Eutrophication potential	Cultivation		2, 8, 22 (wood-based concepts)	24, 25
Freshwater Aquatic Ecotoxicity Potential	Auxiliary materials		3, 7, 14, 15, 21, 22, 23	17, 20, 24
Global Warming Potential	Biomass combustion	Auxiliary materials	22	6, 20, 24, 25
Human Toxicity Potential	Auxiliary materials		3, 14, 15, 21, 22, 23	6, 19, 20, 24
Marine Aquatic Ecotoxicity Potential	Auxiliary materials		3, 14, 15, 21, 22, 23	6, 19, 20, 24
Ozone Layer Depletion Potential	Auxiliary materials (specifically HCl)			19, 20
Photochemical Ozone Creation Potential	Bio-oil use			15, 21, 23
Terrestric Ecotoxicity Potential	Auxiliary materials		3, 14, 15, 21, 22, 23	17, 20, 24
Fossil energy use	Auxiliary materials		3, 14, 15, 21, 22, 23	6, 20, 24
Renewable energy use	Biomass combustion			14, 21, 23
Other energy use	Auxiliary materials	Biomass combustion	3, 14, 15, 21, 22, 23	20, 24
Total energy use	Biomass combustion	Auxiliary materials	15, 16, 22, 25, 26	4, 6, 23, 24

10.2.5 SOCIO-ECONOMIC MODELLING RESULTS

The socio-economic model was created by Aston (Patricia Thornley) to assess the socio-economic impact of the biorefinery concepts. The aim of the socio-economic model was to quantify socio-economic parameters for the different biorefinery concepts. The key focus of the model was employment and socio-economic interfaces to existing land-use patterns. The socio-economic results will not be discussed in detail in this thesis. The socio-economic model was integrated with the module models and process synthesis user interface to create a single system (see Appendix 5). It is possible using the model to investigate many more combinations for the five different countries; Netherlands, Spain, Germany, Poland and UK.

The results were generated based on a biorefinery located in Spain, shown in Table 10.9.

Table 10.9 – All concepts (Spain), socio-economic results

	Direct employment	Induced employment	Biomass consumption as % of national production	Land required for biomass supply	Land required for straw supply as % of regional agricultural land	Land required for straw supply as % of national agricultural land	Revenue from traded feedstock as % of agricultural GDP	Revenue from biorefinery products as % of national GDP (%)
	man years	man years	%	ha	%	%	%	%
0	14567	20240	10%	302973	5.84%	1.23%	0.071%	0.008%
1	19148	26837	10%	302973	5.84%	1.23%	0.071%	0.008%
2	44041	25698	4%	637750	~	~	0.005%	0.009%
3	20240	28288	12%	352803	6.81%	1.43%	0.083%	0.007%
4	16059	22388	10%	302973	5.84%	1.23%	0.071%	0.006%
5	20604	28918	10%	308937	5.96%	1.25%	0.073%	0.009%
6	14302	19858	10%	302973	5.84%	1.23%	0.071%	0.013%
7	17244	23962	12%	357614	6.90%	1.45%	0.084%	0.007%
8	39609	20156	3%	623631	~	~	0.005%	0.006%
9	18931	26524	10%	302973	5.84%	1.23%	0.071%	0.009%
10	20919	29220	13%	371489	7.17%	1.51%	0.087%	0.009%
11	13342	18476	10%	302973	5.84%	1.23%	0.071%	0.010%
12	16623	23201	10%	302973	5.84%	1.23%	0.071%	0.011%
13	13499	18702	10%	302973	5.84%	1.23%	0.071%	0.010%
14	13330	18430	11%	314832	6.07%	1.28%	0.074%	0.005%
15	7468	10018	10%	302973	5.84%	1.23%	0.071%	0.005%
16	24661	34775	10%	302973	5.84%	1.23%	0.071%	0.011%
17	19221	26942	10%	302973	5.84%	1.23%	0.071%	0.008%
18	16382	22661	13%	382411	7.38%	1.55%	0.090%	0.016%
19	26824	36905	24%	708242	13.66%	2.87%	0.167%	0.014%
20	19994	27751	14%	428071	8.26%	1.74%	0.101%	0.008%
21	13335	18466	10%	302973	5.84%	1.23%	0.071%	0.004%
22	47954	32174	3%	623631	~	~	0.005%	0.000%
23	27739	39207	10%	302973	5.84%	1.23%	0.071%	0.007%
24	15323	21329	10%	302973	5.84%	1.23%	0.071%	0.010%
25	16281	22708	10%	302973	5.84%	1.23%	0.071%	0.007%
26	18152	24678	20%	600900	11.59%	2.44%	0.141%	0.019%

Concept 23 and 16 are highlighted as having good socio-economic performance. They both have a high level of induced employment, bringing a large number of jobs to the region. The land required for supply of the straw feedstock is low. This is beneficial as it means that there should be adequate feedstock supply available. This is also indicated by the low % of land required as a proportion of agricultural land in Spain.

Concept 14 has the worst socio-economic performance as it brings the lowest level of direct and induced employment to the country. It also produces the lowest revenue from the biorefinery products as a % of national GDP.

For the MCDA not all of the socio-economic categories were included. This is to prevent double counting of the results leading to a skew in the final results. For more details on the chosen criteria see Section 9.3.1.

10.3 SENSITIVITY ANALYSIS

Using the model it is possible to carry out numerous different sensitivity analyses. The model is highly flexible so it is simple and quick to adjust a variable in order to assess the impact on overall performance. It is possible for the user to carry out their own sensitivity analysis using the model and methodology but it is not possible to include all permutations in this thesis. For this thesis only those described were carried out focussing on scale, feedstock price, TFCI, income, heat and power provision. The sensitivity results are displayed in charts with the slope of the line indicating which concepts are the most sensitive to the change made.

10.3.1 SCALE SENSITIVITY

To investigate the effect of scale on all concepts was not practical, so only those identified as most promising were investigated; Concepts 15, 17 and 26. The biorefineries were investigated for scales from 100,000 – 1,000,000 tonnes per annum of dry biomass, and the data was generated to view the impact on the profit/loss of the plant. It is possible for the user to carry out further scale investigations as the model is very flexible and customisable. The results of the impact of scale on the profit/loss are shown in Figure 10.7.

Concept 15 shows a typical scale relationship, with profit increasing with scale up to a certain point after which profit begins to decrease. This gives an indication that the cost estimations utilised are more realistic. The optimum scale for this plant appears to be 900,000tonnes biomass per year (dry basis).

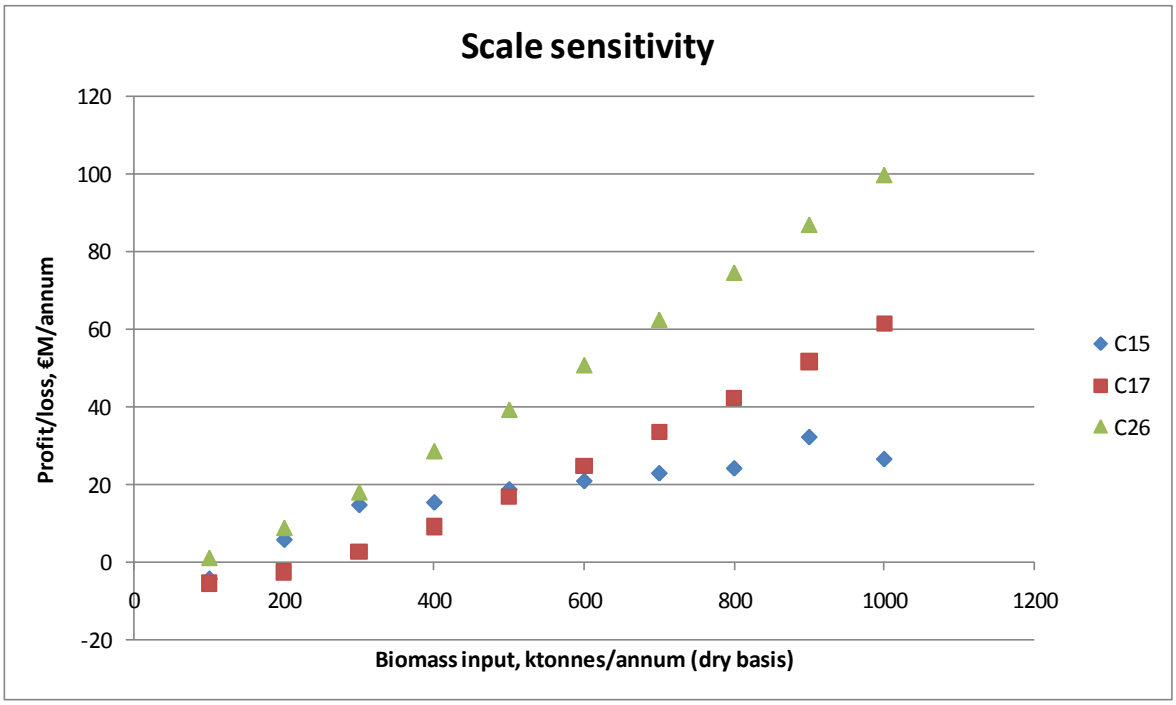

Figure 10.7 – Scale sensitivity, Concepts 15, 17 and 26

Concepts 26 and 17 have increasing profit for increasing biomass input and do not show a typical scale relationship. Profit continues to increase with increasing scale unlike the results for Concept 15. This may be due to the high level of uncertainty in the concentrated HCl pretreatment included in the concept. This is only at the lab stage and has not been successfully scaled up so the relationships derived do not appear to be the most accurate.

10.3.2 FEEDSTOCK PRICE

The feedstock price was varied by ±50% to investigate the impact on profit/loss. The resulting profit/loss for each concept is shown in Figure 10.8.

- Concept 26 remains profitable until feedstock price increases by 70%.
- Concept 17 remains profitable until feedstock price increases by 60%.
- Concept 19 - an increase in feedstock price of 10% makes this concept unprofitable. Decreasing the feedstock cost strongly affects the profit/loss of the concept because a large amount of additional biomass is required in order to provide heat and power.
- Concept 18 and Concept 20 become profitable if the feedstock price drops by 20%.

All other concepts remain unprofitable even when the feedstock costs are reduced by 50%. This indicates that substantial improvements are required to the overall performance of these concepts in order to create attractive biorefinery plants.

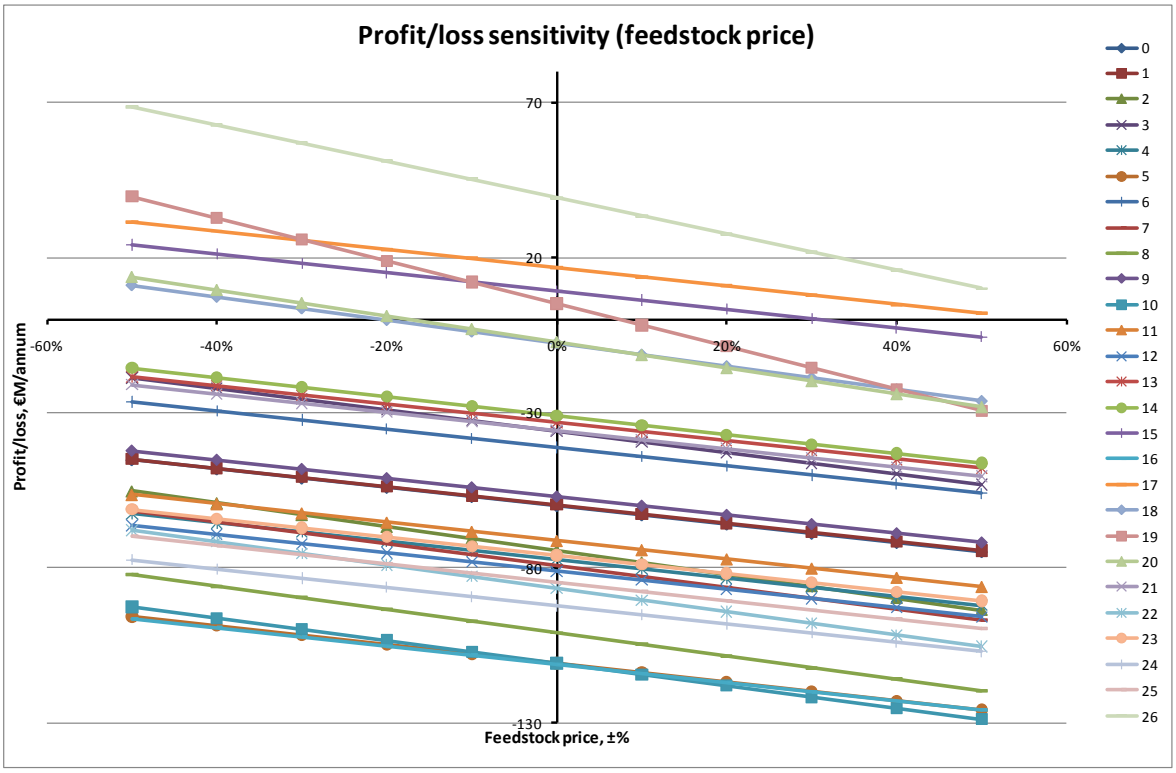

Figure 10.8 – Profit/loss sensitivity; feedstock price ±50%

Concept 19 is the most sensitive to feedstock price due to the additional of biomass required in order to provide the high demands for heat and power. The heat and power is not met by process residues so extra biomass has to be purchased in addition to the 500,000tonnes per annum (dry biomass). Concept 17 is the least sensitive to changes in feedstock price and all other concepts have a similar sensitivity.

10.3.3 TOTAL FIXED CAPITAL INVESTMENT

In this analysis the TFCI was increased and decreased by 50% to view the impact on the profit/loss of the biorefinery concepts. This is an interesting evaluation due to the estimated level of uncertainty in the cost estimates (see Section 10.1.1) and to view how changes to the TFCI affect the ranking of the biorefinery chains. From the process modelling results concepts 15 and 21 were identified as promising. The results of the TFCI sensitivity analysis are shown in Figure 10.9.

- Concept 26 remains profitable, even if there is an increase of 50% in the TFCI
- Concept 17 becomes unprofitable at an increase of 20% in the TFCI
- Concept 19 quickly becomes unprofitable at +5% but a drop in the TFCI has the largest impact on this concepts profit/loss. Concept 19 is the most sensitive to changes in TFCI and product price.
- Concept 15 remains marginally profitable until an increase in TFCI of 30%

The majority of the concepts remain unprofitable even at a decrease in TFCI of 50%.

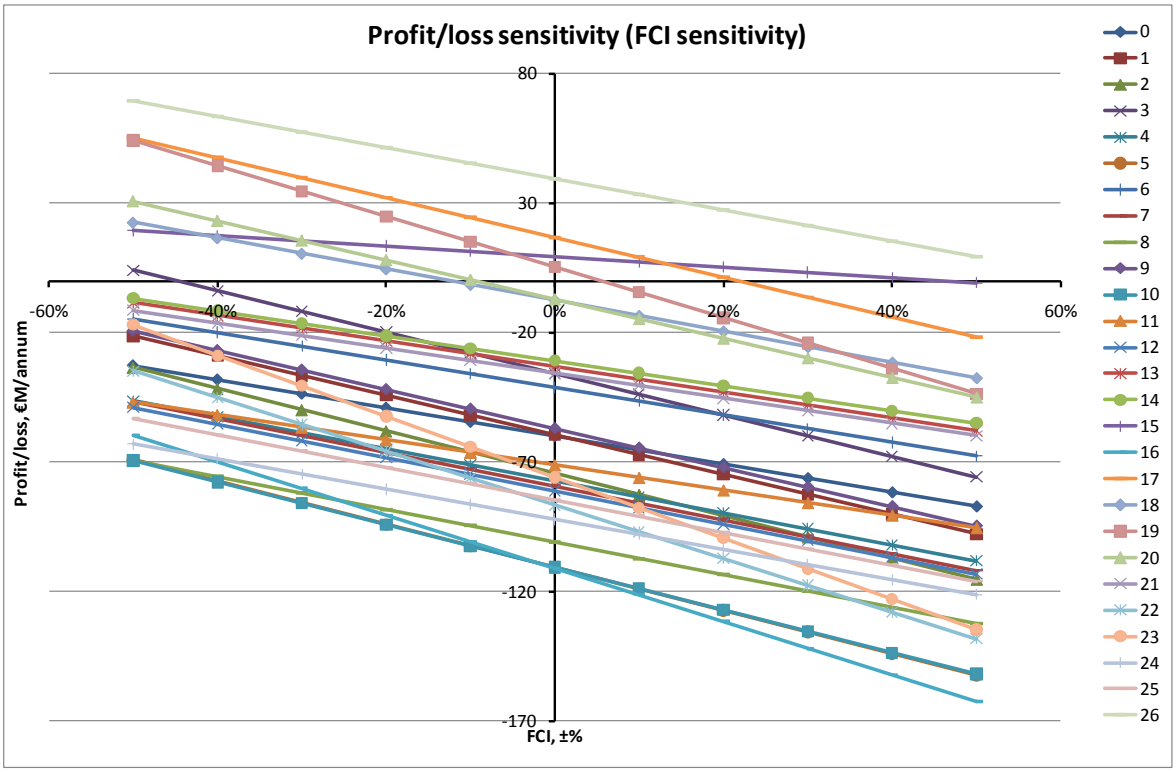

Figure 10.9 – Profit/loss sensitivity; TFCI ±50%

10.3.4 PRODUCT INCOME

In this investigation the product prices are increased and decreased by 50% and the impact on profit/loss calculated. The results are shown in Figure 10.10.

The products that have the highest value are the surfactants and FDCA (€1500/tonne) but it should be noted that these are speculative prices, as bio-based versions of these products are not yet on sale commercially. An estimate was made by the project partners on the likely product price for those products not commercially available or where prices were not freely available. The balance for product portfolios is between commodity products with large markets, but sold at a lower price and high value specialty products with smaller markets but higher selling price. The product income was increased and decreased by 50% in order to assess the impact on the concept profit/loss. Many of the biorefineries remained unprofitable irrespective of the increase in product income, and those that were marginally profitable soon become unprofitable as the product prices dropped. A drop in product price is likely as these plants come online, so the scenario of a decreased income is not unlikely. The commercial scale biorefinery plants should be able to cope with a level of fluctuation in the product prices. There is also some uncertainty in the prices assumed and this is represented in the chart.

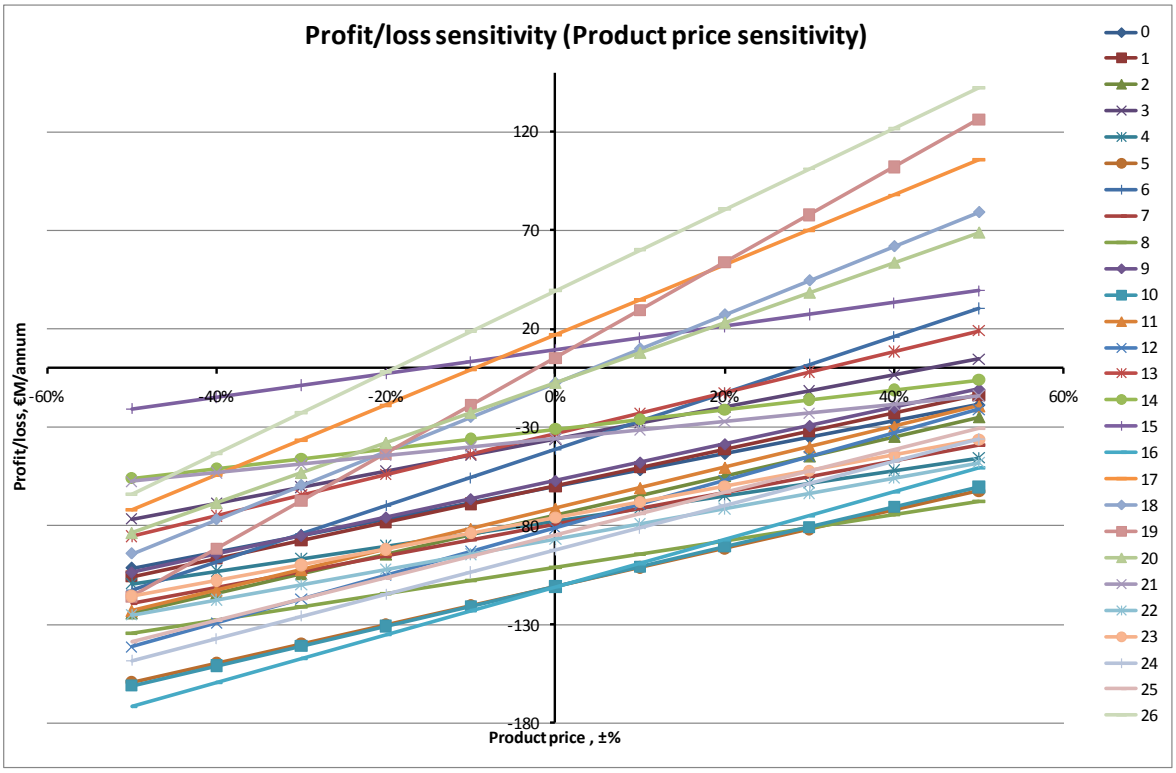

Figure 10.10 – Profit/loss sensitivity; product price ±50%

- If prices drop by 20% all concepts are found to be unprofitable. This is not an unlikely situation because of the uncertainty in the results
- The majority of concepts remain unprofitable, even with an increase in product prices of 50%
- Increasing product prices has the biggest impact on Concept 19

Figure 10.10 indicates how sensitive the profit/loss is to the product prices, with many of the profitable concepts becoming unprofitable even with a small drop in product prices. This indicates that much work needs to be continued on improving the biorefinery performance in terms of efficiency, operating and capital costs or that incentives need to be provided by governments to make these plants feasible.

Most concepts showed similar levels of sensitivity to changes in feedstock price, TFCI and product price. The sensitivity analysis showed that many of the concepts remained unprofitable no matter what changes were made to increase profit, such as a decrease in TFCI, increase in income or decrease in feedstock costs.

10.3.5 HEAT AND POWER SENSITIVITY

Module models were created to provide heat and power from biomass and/or process residues, to provide heat from biomass and/or residues with electricity purchased from the grid, or to provide all heat and power requirements from the combustion of natural gas and

electricity from the grid. In this section the results of an investigation into the impact of heat and power provision on the economics of the biorefinery concepts are described.

Concept 25 (ABNT base case) has been excluded from the heat and power sensitivity analysis. This concept has a defined heat and power arrangement with the lignin combusted to provide some process heat, any additional requirements provided by the combustion of natural gas.

The TFCI for each of the concepts is shown in Figure 10.11. The TFCI is displayed for each concept for the three different heat and power options. There is an overall reduction in TFCI if either heat and/or power are from non-renewable sources. Heat and power plants tend to be expensive whereas the conventional equivalents for connection to the electricity grid, or combustion of natural gas in a boiler are long established and hence available at a lower price. On average there is a reduction of 19% in the TFCI if heat is provided by biomass and electricity is purchased from the grid and a reduction of 44% in the TFCI if natural gas and electricity are purchased to provide the heat and power.

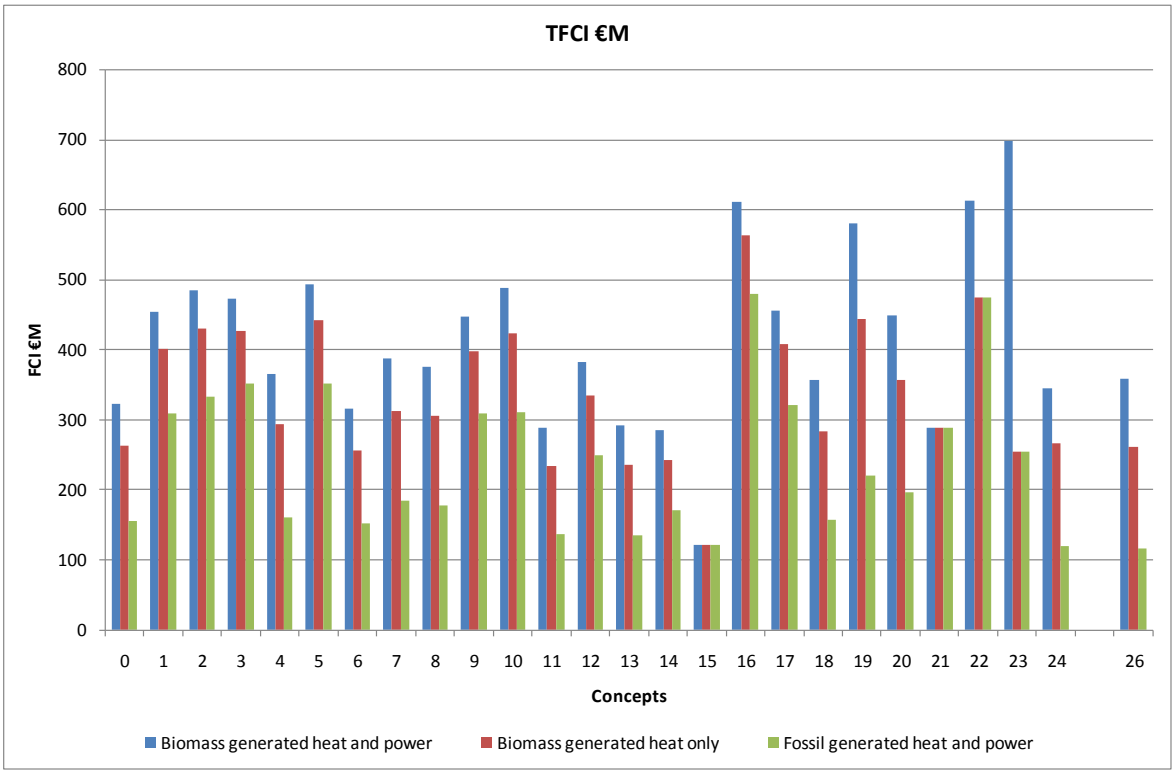

Figure 10.11 – Heat and power investigation TFCI

Biorefineries fuelled by biomass and residues any surplus electricity is sold to the grid to generate additional income for the plant. This does not occur if electricity is purchased from the grid and this leads to a drop in product income of 11% on average.

In Figure 10.12 the operational cost for each of the concepts is shown, for the three heat and power provision scenarios. As expected the operational cost increases if heat and/or power are purchased. If electricity is purchased with heat provided by biomass and residues this leads to an increase of 5% in the operational cost. If natural gas and electricity from the grid is utilised for heat and power this leads to an increase of 19% in the operational cost.

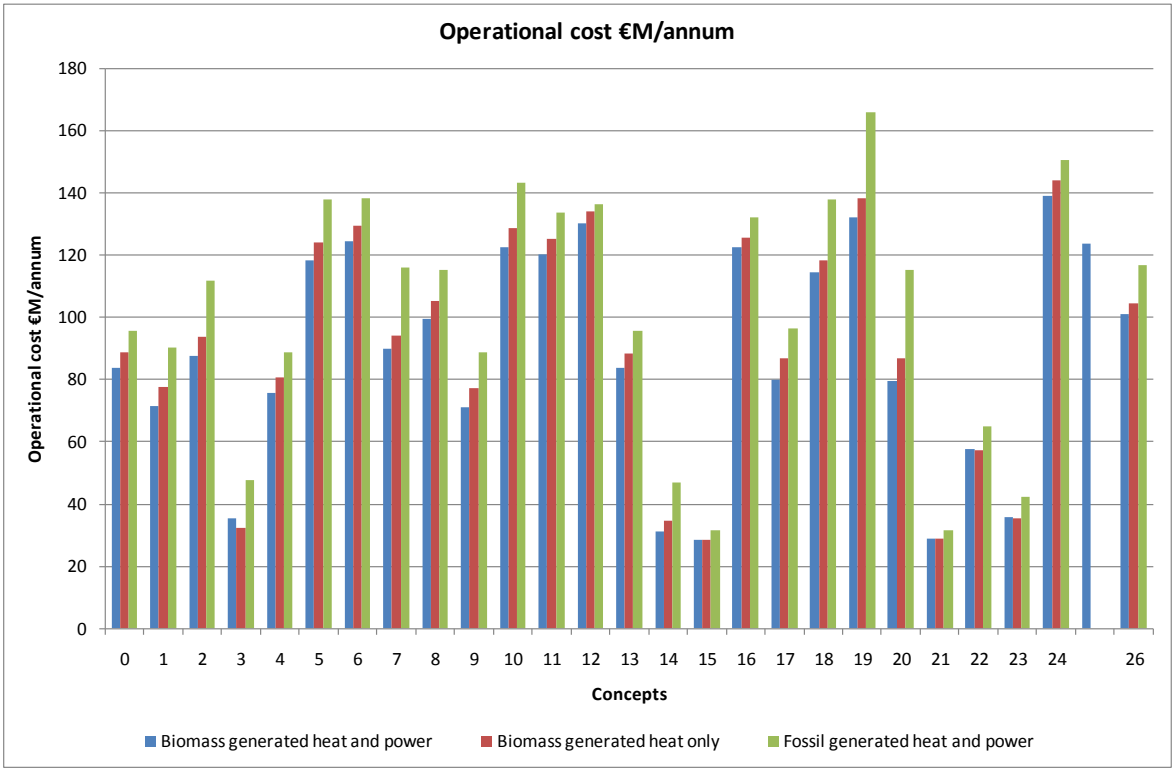

Figure 10.12 – Heat and power investigation operational cost, €M/annum

The production cost was calculated for the 27 concepts. The production cost takes into account the TFCI, capital expenses and operational cost. Overall there is a reduction in production cost as the increase in operational cost is outweighed by the reduction in TFCI. In comparison to biomass fuelled heat and power, the production cost decreases by 6% where only heat is provided by biomass and decreases by 8% for the case where electricity and natural gas are purchased.

The income and the production costs were used to make an estimate of the profit/loss achieved by the concepts (see Figure 10.13). In terms of profit/loss using heat from biomass and electricity from the grid decreases profits by on average 6% whereas purchasing electricity and gas to provide heat and power causes an increase in profits of 1% due to the reduced production cost.

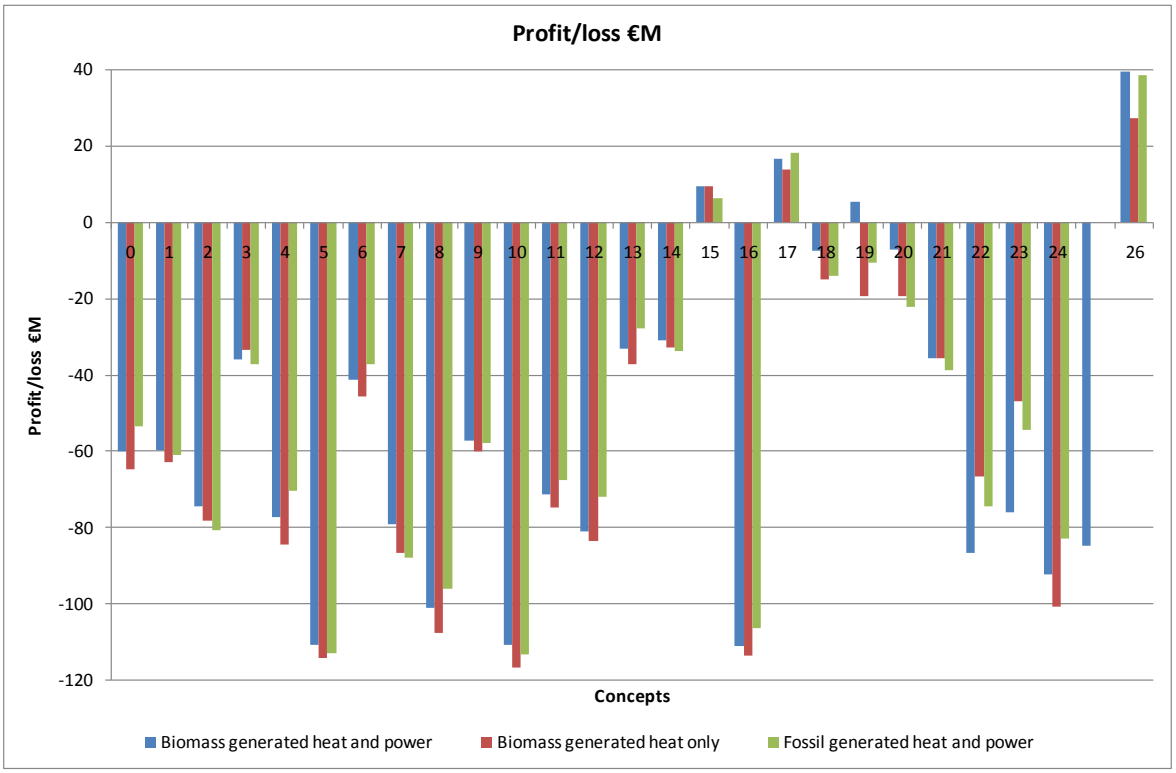

Figure 10.13 – Heat and power investigation profit/loss

This investigation looks at the options for heat and power purely on a financial basis, and does not take into account any other factors such as the environmental impact. It is anticipated that the environmental benefits of heat and power provision by biomass and residues would far outweigh any financial burden. It is recommenced that this exercise is repeated with the inclusion of environmental results. This would give an insight into whether the cost benefits in terms of TFCI of heat and power from non-renewable sources are outweighed by the reduced environmental performance.

10.4 MCDA RESULTS

The MCDA in Hiview uses the results from the modelling process and the weighting to give each of the 27 biorefinery concepts an overall score and identify the most promising. For more details on MCDA using Hiview see Section 9.3.2.The results were normalised to per tonne dry biomass input and the weightings applied as described in Section 9.3.3. The Hiview MCDA models for each of the five countries can be found in Appendices 6 to 10.

The criteria and sub-criteria chosen for the MCDA analysis were:

- Profit/loss
- Energy conversion efficiency
- Environmental
  - Particles
  - Abiotic depletion
  - Acidification potential
  - Eutrophication potential
  - Global warming potential
  - Ozone layer depletion potential
  - Photochemical ozone creation potential
  - Primary energy demand
- Socio-economic
  - Direct employment
  - Indirect employment
  - Biomass as a % national production
  - Feed revenue as % GDP
  - Product revenue as % GDP

Different weightings were applied in the MCDA analysis, as shown in Table 10.10. These weightings give a greater importance to the criteria with the higher weighting, and affect how the concepts are ranked.

Table 10.10 – Weightings applied in MCDA analysis

	Profit/loss	**Conversion efficiency**	**Socio-economic**	**Environment**
Equal	25%	25%	25%	25%
Techno-economic	50%	50%	~	~
Enviro-socio	~	~	50%	50%
Profit/loss bias	49%	17%	17%	17%
Efficiency bias	17%	49%	17%	17%
Socio-economic bias	17%	17%	49%	17%
Environment bias	17%	17%	17%	49%

10.4.1 EQUAL WEIGHTING, ALL COUNTRIES

In this analysis each of the four main criteria (profit/loss, energy conversion efficiency, environmental, socio-economic) were given an equal weighting of 25%. This was split equally between any sub-criteria. For example the overall socio-economic weighting is 25%; the individual socio-economic sub-criteria assigned 5% each. The MCDA results from the application of an equal weighing are shown in Table 10.11.

Table 10.11 – All concepts, all countries, equal weighting, overall MCDA score

Concept	MCDA overall score				
	Germany	Netherlands	Poland	Spain	UK
0	44	42	42	43	45
1	49	46	48	48	49
2	45	46	50	50	45
3	57	55	57	56	57
4	35	33	34	34	36
5	42	40	41	42	42
6	46	44	45	45	47
7	43	41	42	42	44
8	30	31	33	35	30
9	51	48	50	50	51
10	41	39	40	44	42
11	51	46	47	50	49
12	52	48	49	49	51
13	58	53	54	54	59
14	47	45	46	46	48
15	71	69	69	69	72
16	50	47	50	50	50
17	71	69	72	71	73
18	63	61	62	63	64
19	45	44	45	45	46
20	45	43	45	45	46
21	61	59	59	59	61
22	40	41	46	46	41
23	33	30	35	31	34
24	41	35	36	39	47
25	56	55	55	55	57
26	68	67	68	68	69

Table 10.12 - Most promising biorefineries: all countries, equal weighting

	Feed	Pretreatment	C5	C6	Lignin
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

This MCDA was carried out for all countries to assess whether the location has a big impact on the top and bottom 3 performing concepts. The modelling and MCDA methodology is internally consistent so the comparisons are valid.

The “best” biorefineries for each country were identified as Concepts 15, 17 and 26 shown in Table 10.12. The overall best biorefinery is Concept 17, located in the UK followed closely by Concept 17 located in Poland and Concept 15 located in the UK. Concepts 15, 17 and 26 perform consistently well, independent of the location of the plant.

The worst concepts are identified as Concepts 4, 8 and 23. The worst is Concept 8 located in either Germany or the UK, or Concept 23 located in the Netherlands. The overall results are only marginally different between countries, and they all agree as to the most and least promising concepts based on equal weighting.

The biorefineries that perform well when an equal weighting is applied could be judged to be the most promising from a balanced point of view, as the concept must obtain a good score for all criteria in order to achieve a higher ranking.

10.4.2 TECHNO-ECONOMIC WEIGHTING, SPAIN

In this analysis a techno-economic weighting was implemented. This is to assess the most promising biorefinery purely from a process efficiency and profit/loss basis. As noted in the literature (see Section 8.2) techno-economic evaluations are the most widely used form of biorefinery assessment. The profit/loss and the energy conversion efficiency criteria were each assigned a weighting of 50%, with the environmental and socio-economic criteria assigned a weighting of 0, eliminating them from the evaluation. The results of the MCDA analysis are shown in Figure 10.14.

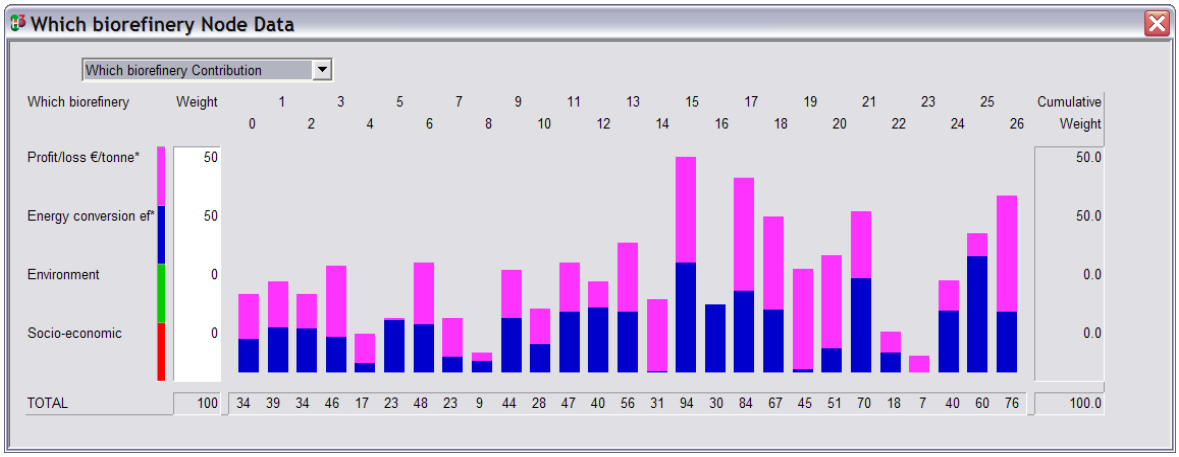

Figure 10.14 – All concepts (Spain), techno-economic weighting

Table 10.13 - Most promising biorefineries: techno-economic weighting

	Feed	Pretreatment	C5	C6	Lignin
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

The most promising biorefineries identified in this analysis are considered to be the best purely from a performance and cost point of view. This analysis completely disregards the environmental and socio-economic performance of the biorefinery concepts. From this techno-economic MCDA the most promising biorefinery is identified as Concept 15 and the worst performing was Concept 8. (See Table 10.13). Others with a high ranking were Concepts 17 and 26. It is interesting to note the variety of processing technologies in these concepts.

10.4.3 ENVIRONMENT-SOCIO WEIGHTING, SPAIN

This analysis focuses on the environmental and socio-economic performance of the biorefinery concepts. This type of analysis combining environmental and socio-economic performance was not found in the literature (see Section 8.2). In this analysis the environmental and socioeconomic criteria were each given a 50% weighting (split equally between sub-criteria); the profit/loss and energy conversion efficiency were weighted with 0. The MCDA results are shown in Figure 10.15.

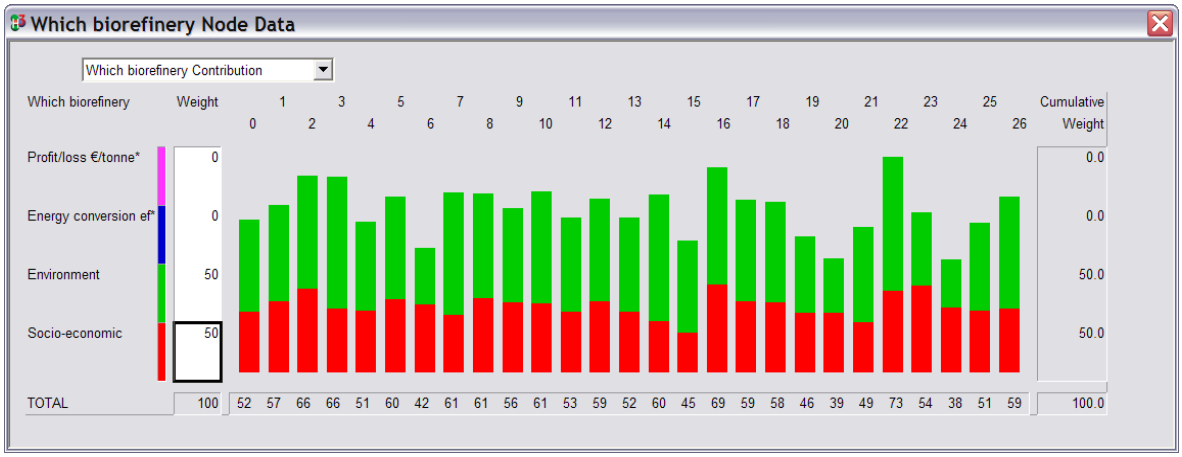

Figure 10.15 – All concepts (Spain), enviro-socio weighting

Table 10.14 - Most promising biorefineries: enviro-socio weighting

	Feed	Pretreatment	C5	C6	Lignin
22	Softwood	Gasification	Fischer-Tropsch synthesis to hydrocarbons		
16	Straw	Steam explosion	ABE fermentation		Dry lignin product
2	Softwood	Steam explosion	Furfural	Ethanol	Bio-oil phenolic fractionation

In this analysis the biorefinery is judged purely on its environmental and socio-economic performance, the efficiency and cost criteria are disregarded. From this enviro-socio MCDA analysis the most promising biorefinery is identified as Concept 22 (see Table 10.14) followed by Concepts 16 and 2. It is interesting to note that the concepts of interest from an enviro-socio aspect are very different to those in the previous techno-economic analysis. These concepts have the best performance purely from an environmental and socio-economic point of view. The worst performing biorefinery from this analysis was Concept 24. It performs particularly badly from an environmental point of view, as indicated in Figure 10.15 by the small size of the green bar in comparison to other concepts. It was found in the evaluation by Neil Bird et al. (163, 164) at JR that this was mainly due to the user of auxiliary materials. The auxiliary materials, especially acids and alkalis have a high environmental burden. It was not the biorefinery itself.

10.4.4 PROFIT/LOSS WEIGHTING BIAS, SPAIN

In this analysis the profit/loss criteria was given the highest weighting of 49%, the remaining criterion were given weighting of 17% each. This analysis gives the profit/loss criteria the largest impact on the final result but does not neglect the performance in other categories. The results are shown in Figure 10.16 with the best biorefineries listed in Table 10.15. This analysis would be useful for industrial stakeholders mainly interested in profit but with an understanding of the need for good performance in other areas.

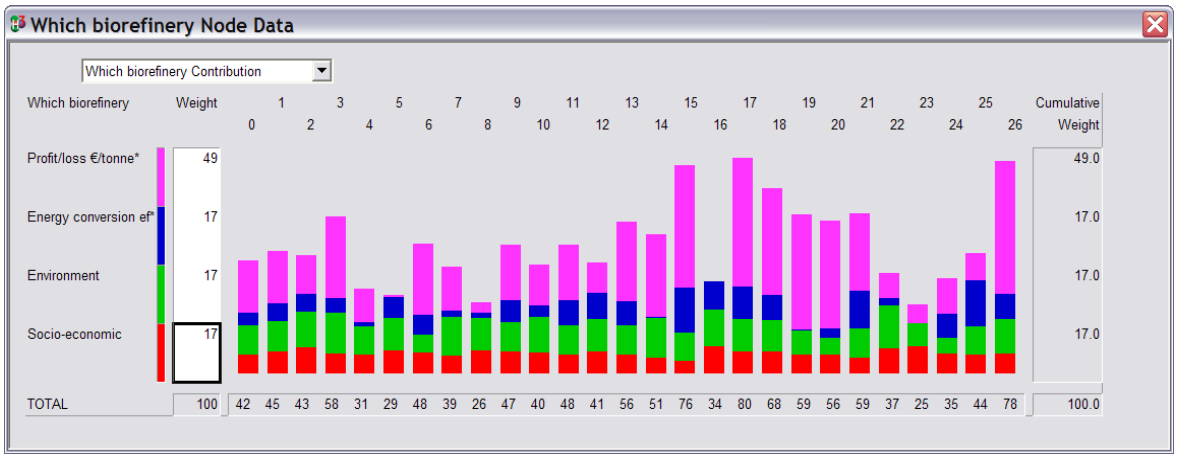

Figure 10.16 – All concepts (Spain), profit/loss bias

Table 10.15 - Most promising biorefineries: profit/loss bias

	Feed	Pretreatment	C5	C6	Lignin
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		

From this analysis the most promising biorefineries were identified as Concepts 17, 26 and 15. Concept 17 includes the steam explosion of wheat straw followed by xylonic acid and ethanol production from the C5 and C6 rich streams. The lignin stream is dried and sold. The worst performing biorefinery from this analysis was Concept 8. This concept includes the AVIDEL pretreatment of softwood, followed by the processing of the C5 and C6 streams to furfural and ethanol, and the fast pyrolysis of lignin and fractionation of the produced bio-oil to a phenolic fraction. These concepts were also identified as promising in the equal weighting and profit/loss biased MCDA analyses.

10.4.5 EFFICIENCY BIAS, SPAIN

In this particular analysis the focus is on the conversion efficiency of biomass to products (on a LHV basis). The efficiency criterion was given a weighting of 49% and all other criteria weighted equally at 17% (split equally between any sub-criteria). The best biorefinery identified by this analysis has the best conversion efficiency but must also

perform well in terms of cost, environment and socio-economics. The results are shown in Figure 10.17 with the contribution to the overall result indicated by the size of the coloured bar.

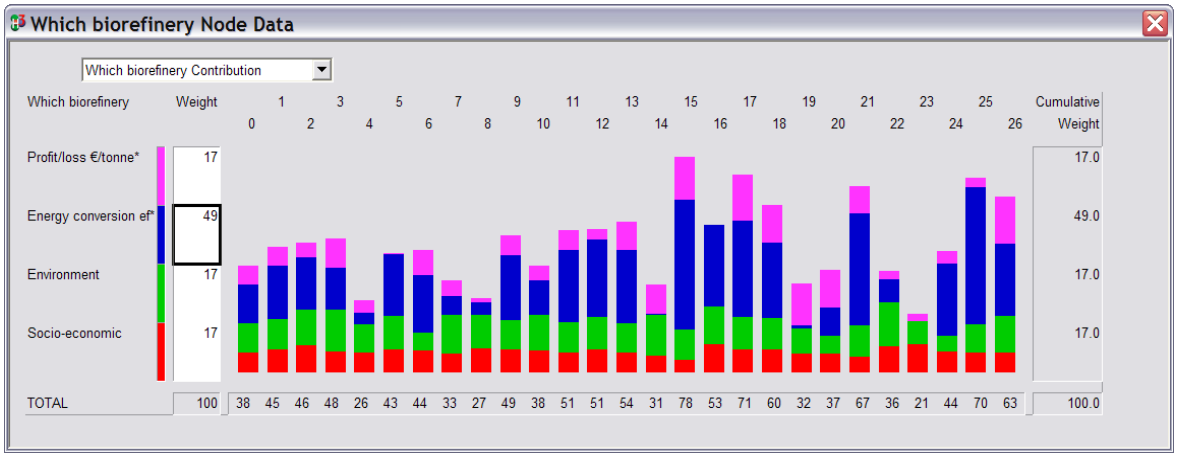

Figure 10.17 – All concepts (Spain), efficiency bias

Table 10.16 - Most promising biorefineries: efficiency bias

	Feed	Pretreatment	C5	C6	Lignin
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
25	Straw	Steam explosion	Ethanol, stillage to animal feed		Lignin combusted

The best biorefineries in this analysis with an efficiency bias are shown in Table 10.16. In this analysis Concept 15 performs the best. This concept involves the fast pyrolysis of wheat straw and then the gasification of the bio-oil followed by alcohol synthesis. The worst performing biorefinery was Concept 23. In terms of conversion efficiency this performs very badly as indicated by the size of the blue bar in Figure 10.17. Concepts 15 and 17 are repeatedly identified in the top 3 performing biorefineries.

10.4.6 ENVIRONMENT BIAS, SPAIN

The environmental criteria were given the highest weighting of 49% in this analysis, all other criteria were given a weighting of 17%. This analysis would be of interest to environmental stakeholders as it focuses on environmental performance, but still does not neglect all other criteria. The most promising biorefinery identified has a good environmental performance, but must also perform well in the other criteria.

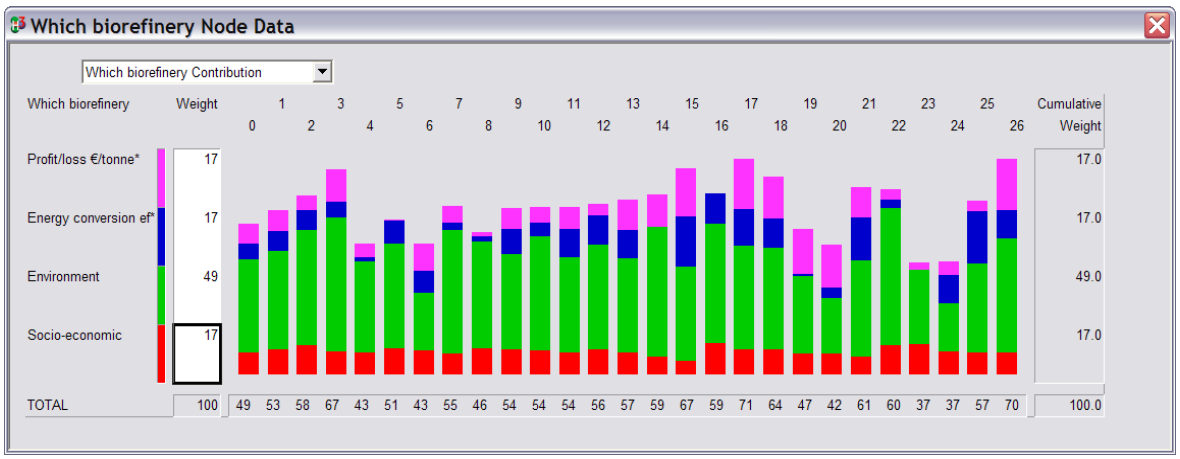

Figure 10.18 – All concepts (Spain), environmental bias

Table 10.17 - Most promising biorefineries: environmental bias

	Feed	Pretreatment	C5	C6	Lignin
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

In this analysis Concept 17 is identified as the most promising (see Table 10.17). The worst performing biorefinery was Concept 24 in which wheat straw undergoes mechanical/alkaline fractionation before being fermented ethanol, with the lignin dried and sold. Concept 24 was also identified as the worst concept in the enviro-socio analysis and by the environmental modelling results.

10.4.7 SOCIO-ECONOMIC BIAS, SPAIN

In this MCDA analysis the socio-economic criteria was given the highest weighting of 49% with all other criteria given 17%. The results are shown in Figure 10.19 with the most promising biorefineries listed in Table 10.18.

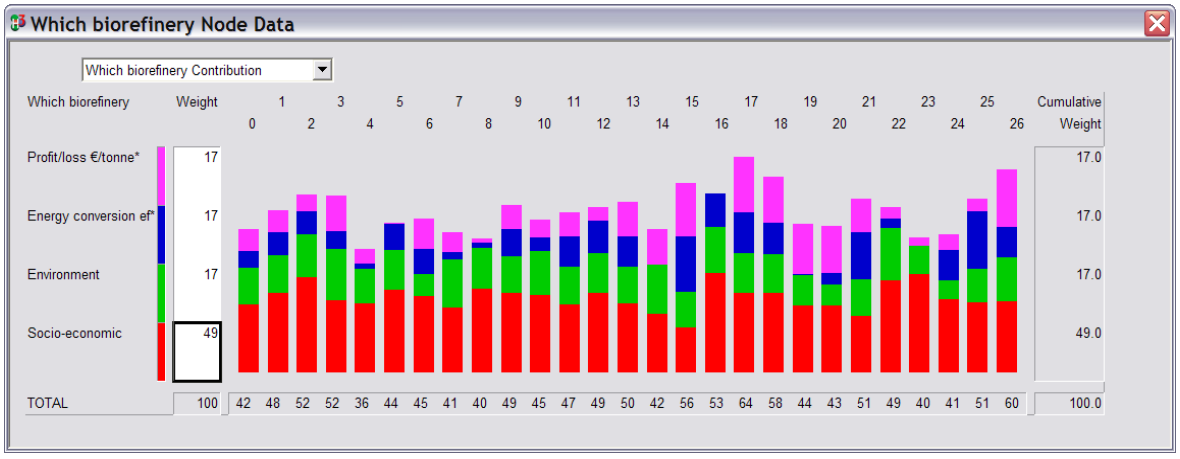

Figure 10.19 – All concepts (Spain), socio-economic bias

Table 10.18 - Most promising biorefineries: socio-economic bias

	Feed	Pretreatment	C5	C6	Lignin
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product
18	Straw	Organosolv	Surfactants	Ethanol	Dry lignin product

In this analysis the best biorefinery has a good socio-economic performance, but must also perform well for the other criteria. The best performing biorefinery in this analysis was Concept 17, followed by Concept 26 and 18. The worst performing was Concept 4 in which wheat straw undergoes AVIDEL pretreatment, the C5 stream is converted to furfural, the C6 to ethanol and the lignin to a phenolic fraction.

10.4.8 MCDA RESULTS SUMMARY

The results the different individual MCDA analyses are displayed in Table 10.19. Different weightings were applied in the evaluation (see Table 9.5) to adjust the objectives of the analysis. In Table 10.19 the top (green) and bottom (red) 3 biorefinery concepts are highlighted for each of the analysis. This allows a quick overview of all of the results.

Table 10.19 – Summary of MCDA results

	Equal weighting	Techno-economic	Enviro-socio	Profit/loss bias	Efficiency bias	Environment bias	Socio-economic bias
0	43	34	52	42	38	49	42
1	48	39	57	45	45	53	48
2	50	34	66	43	46	58	52
3	56	46	66	58	48	67	52
4	34	17	51	31	26	43	36
5	42	23	60	29	43	51	44
6	45	48	42	48	44	43	45
7	42	23	61	39	33	55	41
8	35	9	61	26	27	46	40
9	50	44	56	47	49	54	49
10	44	20	61	40	38	54	43
11	50	47	53	48	51	54	47
12	49	40	59	41	51	56	49
13	54	56	52	56	54	57	50
14	46	31	60	51	31	59	42
15	69	94	45	76	78	67	56
16	50	30	69	34	53	59	53
17	71	84	59	80	71	71	64
18	63	67	58	68	60	64	58
19	45	45	46	59	32	47	44
20	45	51	39	56	37	42	43
21	59	70	49	59	67	61	51
22	46	18	73	37	36	60	49
23	31	13	54	25	21	37	42
24	39	40	38	35	44	37	41
25	55	60	51	44	70	57	51
26	68	76	59	78	63	70	60

It appears from the MCDA results that some concepts perform consistently well, or consistently badly independent of the weighting applied. The only real difference in results is viewed when considering only environmental and socioeconomic criteria. Concepts 15, 17 and 26 perform well in all of the analyses, apart from the enviro-socio assessment.

From a purely environmental and socio-economic viewpoint different concepts are identified as most promising. These are Concepts 2, 3, 16 and 22. It is interesting to note this difference as it indicates what may be most promising from a techno-economic point of view (techno-economic bias results) is not necessarily the most promising from an environmental or socio-economic viewpoint. It indicates the lesser environmental and socio-economic performance of concepts 15, 17 and 26 is outweighed by the profit/loss and efficiency of these concepts. These concepts have good techno-economic performance, but below average enviro-socio performance.

Although MCDA was used to generate the overall results, a judgement can be made using tables similar to those shown in Section 10.2 , highlighting good and bad performance. From early analysis of the results (Section 10.2) concepts 17, 15 and 26 had already been identified as having good performance from a cost, efficiency, environmental and socio-economic point of view. It may be possible for the user to make judgements without the MCDA step, and without having to purchase the Hiview software, as long as they are aware of all results. The advantage of using the MCDA software is that it allows the use of weightings and gives further analysis tools not described in this thesis for gaining a deep insight into the biorefinery rankings.

Overall the most promising biorefineries were identified as Concepts 15, 17 and 26 at the scale of 500,000tpa, located in Spain.

10.5 LIMITATIONS OF METHODOLOGY AND RESULTS

Although the objectives of the project have been achieved there are a number of limitations to the methodology and results. It was hoped at the beginning of the project that the process, environmental and socio-economic models would be integrated to give one system. Unfortunately this was not achieved. The process and socio-economic models were integrated successfully, offering complete flexibility with process and socio-economic results generated for whatever modules were chosen by the user. Due to time restraints and the differing levels of flexibility between models it was not possible to integrate the environmental model. The environmental model created by JR did not offer the same level of flexibility as the other models. Environmental results could only be

generated for the 27 concepts chosen by the partners. These results were used in the MCDA evaluation, but were not fully integrated into the process and socio-economic models.

Another limitation of the methodology and results is that no market data was included. It was originally part of the Biosynergy WP6 work plan to include market information into the system. This task was assigned to JRC but unfortunately the results produced were not suitable for integration in the model. As identified by the IAB (see Section 9.3.1) the market situation for the products is an important criterion in biorefinery assessment. The market situation of the chosen products is crucial, because if the products cannot be sold then the biorefinery will fail.

The focus for the module models and the results described in this chapter were the 27 concepts chosen for detailed analysis. Although it is possible to evaluate other routes using the methodology, the assumptions have not been optimised for different combinations, so the results may not be as accurate. One example is the gasification followed by Fischer-Tropsch synthesis modules. This was created based on assumptions used for Concept 22 using softwood as a feedstock. It is possible using the model to evaluate the gasification of wheat straw and obtain results, but as the model was based on the gasification of softwood, the assumptions and resulting data may not be as accurate.

The level of uncertainty is another limitation of the results. The uncertainty varies between modules but this has no impact on the final results. This should be taken into account in any further studies.

A possible limitation of the results was the use of energy conversion efficiency as a measure of the performance of the biorefinery concepts. The lower heating value was used to calculate the energy content of the products and compared to the energy content of the biomass input to give a measure of the biomass conversion efficiency. This may not be the most accurate measure, as a number of the products cannot be classed as “energy based” products; products such as furfural or surfactants. It may also be argued that the efficiency of the plant is inherent in the results of the models and so is represented by the cost, environmental and socio-economic results, as these are all based on the mass and energy balances. For this reason the efficiency criteria used in the MCDA may actually be double counting of the results and may be having an unwanted effect on the final results. It is recommended that this criteria is removed from any future developments of the finished system.

It may have been interesting to include a case study based on the interests of a particular user of the system, not focussing on the 27 Biosynergy concepts. Taking it from the very start in the generation of the process chains through to the evaluation of the results and the weighting used in the MCDA. This may have illustrated more clearly how the methodology may be used in the future.

11 CONCLUSIONS

The outcomes from this project are twofold. The first outcome is the creation of the flexible methodology for the generation, analysis and evaluation of biorefinery process chains. The second outcome is the use of this methodology for the identification of the most promising biorefineries from those studied in the Biosynergy project.

A robust, flexible and reproducible methodology for the generation and evaluation of biorefinery process chains has been created and developed with a user friendly interface. The methodology brings a new and unique contribution to the field of biorefinery evaluation and comparison, whilst the results give detailed insight into promising biorefinery configurations.

11.1 BIOREFINERY GENERATION, EVALUATION AND COMPARISON METHODOLOGY

- A simple three step methodology was created in order to achieve the objective of the Biosynergy project; to identify the most promising biorefineries. The model is available for users to quickly generate, evaluate and compare biorefinery process chains (See attached model on CD – Appendix 5). The methodology consists:
    - Process chain generation (process synthesis) – The user can generate biorefinery process chains using the user interface in order to choose scale, location, feedstock and processing routes. The user makes choices from drop down menus, with subsequent decisions displayed, based on inbuilt logic and relationships
    - Modelling – Once the user has chosen the process chain the modelling results are generated. A modular structure was chosen to allow greater flexibility with inbuilt logic rules to govern the connection of modules. Each module represents a distinct process step. Results are generated to describe the processes in terms of mass and energy, cost, profitability and socio-economics. If the biorefinery chain specified is one of the 27 defined Biosynergy concepts, environmental results are also available.
    - Evaluation – The results from the modelling are used as the input for MCDA which is used in order to assess different biorefinery process chains. The biorefineries are evaluated in terms of performance, costs including profit/loss, efficiency, environment and socio-economic performance with the objective of the evaluation set by the weighting of these criteria. Environmental assessment

is only available for the 27 concepts studied in the project. Those criteria considered to be of more importance can be assigned a higher weighting. The result of the MCDA is ranking of the biorefineries according to the objectives set by the weighting.

- The methodology was used to evaluate the 27 concepts chosen by Biosynergy partners (see Table 10.1) for the five countries chosen (Netherlands, UK, Germany, Poland and Spain) but it has the potential to evaluate many more configurations, at any scale, in any of the five countries included, as defined by the user. Due to the modular structure it would be easy to add further technologies and feedstocks which make this a valuable tool for the evaluation of biorefineries.
- The methodology created for this project offers a new approach for the generation, evaluation and comparison of biorefineries. The ability to consistently generate and evaluate biorefinery plants was identified from the literature as a gap in the research. It has been widely acknowledged in the literature that the main problem with biorefineries is identifying the optimum configuration in order to gain the most value from the biomass. The methodology created is user friendly, highly flexible and transferable. It can be used not just for the processes included in this project but may be extended to include more processes or applied to a different problem.
- The methodology created provides an important tool to help direct future research and development, and is capable of taking into account the viewpoints of different users through the weighting of criteria in the MCDA analysis.
- The advantages of this methodology are consistency and repeatability. The user can be confident in comparing results generated using the methodology because it is internally consistent although there are concerns over the extent and degree of uncertainty in different modules. Another advantage is the speed at which results can be generated. Conventional techno-economic evaluations are time consuming and limit the number of biorefineries that can be included in the evaluation.
- The optimum configuration is available for analysis, because all possible configurations of the technologies included are available within the system. This is a huge advantage as in many of the conventional evaluations it cannot be assured that the optimum route has been included, as the choice of biorefineries to be evaluated is made by the researchers and is fixed.
- The methodology provides a long lasting tool which documents the Biosynergy project. The tool is not static and the models can be updated as new breakthroughs are made to follow the progress of the research. The tool allows virtual experiments of numerous

scenarios and because all options are included, this guarantees that the optimum has also been included within the system.

- Microsoft Excel was chosen with the advantages of flexibility, transferability and familiarity. Excel was also used to create the socio-economic and environmental models. The socio-economic model was integrated with the process module models to automatically generate socio-economic data for the processes included. Unfortunately time and resources did not allow the integration of the environmental model.
- The ranking of the biorefineries was carried out using MCDA according to objectives set by the weighting. This has been used extensively in renewable energy planning and for aiding decision makers in UK government. This project was the first time MCDA has been applied to biorefineries, in order to rank them according to objectives set by the weighting. These methods were successfully applied to this project with the identification of the most promising biorefinery chains.

11.1.1 IDENTIFICATION OF MOST PROMISING BIOREFINERIES

The second result of the project was the use of the methodology for the identification of the most promising biorefineries. An extensive evaluation of the modelling results took place in order to identify the most promising biorefineries, from the 27 studied within the Biosynergy project. The raw results from the modelling process were evaluated and these results were used in an MCDA analysis in order to rank the concepts according to objectives set by the weighting.

The results of the MCDA for the weightings applied are summarised in Table 10.19. This was based on plants processing 500,000 tonnes biomass per annum (dry basis) with the plant located in Spain. Heat and power was provided by biomass and residues. Due to the level of uncertainty in the results (estimated ± 40%, see Section 10.1.1) it would not be appropriate to definitively state the best and worst biorefinery. For this reason the top 3 concepts for each category are highlighted in green and the worst 3 highlighted in red. This allows overall performance to be viewed at a glance to identify the strongest and weakest biorefineries and act as guidance for decision makers.

Using this methodology and analysing the 27 concepts it appears that the best option is for biomass to undergo fast pyrolysis to generate bio-oil (see Table 11.1). Although this was the overall result it does not include any kind of market analysis and in reality this may not be as attractive due to the question of the availability of a market for the bio-oil. Other promising biorefineries generate high value specialty chemicals such as surfactants or

furfural in addition to ethanol. The lignin is not used to generate heat and power but is dried and sold as a product. Again there is the issue of the market for these products, but this indicates the impact that the high value speciality chemicals have on a biorefinery processing scheme. These results indicate that the production of high value added specialty materials/products has a positive impact on the overall performance of a biorefinery, in terms of economics and efficiencies. It has illustrated the requirement for the inclusion of a market assessment. These results are particularly interesting because literature evaluations have not been found of such an extensive product portfolio as those contained in the 27 concepts.

Table 11.1 - Most promising biorefineries: overall result

	Feed	Pretreatment	C5	C6	Lignin
17	Straw	Steam explosion	Xylonic acid	Ethanol	Dry lignin product
15	Straw	Fluidised bed fast pyrolysis	Bio-oil		
26	Straw	Conc. HCl pretreatment	Furfural	Ethanol	Dry lignin product

As well as the most promising biorefineries, the least promising were also identified (See Table 11.2). Two of least promising included the AVIDEL pretreatment method which indicates that this particular pretreatment method requires further research before it will become attractive. The other concept with poor performance was the fast pyrolysis of wheat straw, followed by gasification of the bio-oil and mixed alcohol synthesis. The complexity and uncertainty of this configurations results in poor performance.

Table 11.2 - Least promising biorefineries: overall result

	Feed	Pretreatment	C5	C6	Lignin
4	Straw	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
8	Softwood	AVIDEL	Furfural	Ethanol	Bio-oil phenolic fractionation
23	Straw	Fast pyrolysis	Bio-oil gasification → alcohol synthesis		

Out of the 27 concepts only 4 were estimated to generate a profit. This indicates that there is the requirement for incentives or significant performance improvements (in terms of efficiency, cost, environmental and socio-economic) in order to make biorefineries more attractive. Even when a sensitivity analysis was carried out to estimate the impact on profit/loss of variations to the feedstock price, product prices, TFCI and scale the vast majority of the concepts remained unprofitable (see Section 10.3). The results illustrate that a number of concepts are not attractive even if feedstock costs are dramatically reduced or if the product income is increased. This helps direct future research in that the researchers can target areas that need to be improved for those biorefineries that do not perform so well, or these concepts can be eliminated from further evaluations. The breakdown of the data makes it possible for the user to investigate which particular area is

having the biggest negative impact on the biorefinery. The results will help direct future research on these technologies and prevent researchers following “dead ends”.

The results from the analysis of the 27 concepts give further insights into the feasibility of biorefinery plants. Most studies in the literature focussed on ethanol based plants, but the results of this study indicate fast pyrolysis as a promising route. In addition, the production of high value co-products such as xylonic acid or surfactants was also indentified as promising. These results indicated that there should be further development and research into the co-products in order to make the biorefineries more attractive from an economic, efficiency, environmental and socio-economic point of view and that ethanol production may not be the optimum use for biomass.

The results can be used to support further research. For example, in terms of pretreatment methods, the most promising for the production of ethanol was identified as concentrated HCl. This is a relatively new concept developed by the Biosynergy partner Bioref. The other concept (Concept 26) containing this pretreatment method was also identified as one of the most promising from the 27 studied. This strongly supports further research on this pretreatment method.

The results provide additional information about more unusual co-products such as xylonic acid, surfactants and phenolic fraction by bio-oil. These products have not been included in previous biorefinery evaluations in the literature and help highlight the potential benefits of coproducing such products with ethanol. None of the evaluations in the literature were found to evaluate so many options or include so many different technologies.

A major benefit of the methodology created is that it is internally consistent. The same models and procedures are followed each time with a consistent set of data and assumptions. The use of a defined methodology removes the possibility of bias in the evaluation by the project partners. Project partners have a particular interest in processes that they have studied so the methodology takes away the possibility of adjustment of the evaluation results as all partners have to use the same methodology.

The results of the project have successfully utilised elements of process synthesis, process modelling and evaluation techniques to create a highly valuable methodology that will aid biorefinery research. The application of the methodology had clearly identified areas of interest for researchers, industry and policymakers, as well as identifying areas requiring further development.

12 RECOMMENDATIONS

Based on the results and conclusions of the thesis some further recommendations for future research are given in this chapter. With the implementation of each of these recommendations over time the system will evolve into a more robust and comprehensive system.

- It is recommended that a more detailed investigation is carried out into utilisation of lignin. The investigation carried out for this thesis was carried out at a relatively early stage in the modelling process, using only basic information and without properly considering the most recent developments (see Section 5.4.1). It would be interesting to repeat the analyses using more models with greater detail and including potential market information for derived products to identify the most promising processing route for lignin.
- Improve integration of the modules in terms of mass and energy balances, to improve efficiency and to more accurately represent a complete integrated biorefinery plant. One possible way to achieve this is to create steam headers at different temperatures and pressure levels, which feed into and out of the modules with the same concept for chemicals, water and other auxiliary materials. This will increase the level of integration and optimisation over the entire biorefinery concept and improve processing efficiency. The integration of the cost factors should also be considered, as those used in this initial model are likely to overestimate the likely labour, instrumentation and control costs for example.
- Include a market analysis for all of the products as this will potentially affect the overall results and their impact. The potential and existing market situation should be assessed in detail in terms of market size, impact on price and the willingness of consumers to accept the products. It is predicted that the bio-oil options would drop down the ranking substantially if the market failed to develop as predicted. The ability to sell the products produced by the biorefinery is crucial. An assessment is needed of how the quantities produced impact on the market situation for each of the products. For example, it is pointless to produce high volumes of a high value specialty if the market is only small. It has been stated that there are few organic chemicals or polymers with markets large enough to serve as primary products for a full sized biorefinery (4) especially as no one plant can expect to hold the full market share.
- Independent external validation of the module models. The modules were validated by partners involved in the project and by comparing results with those found in the

literature. To ensure the real accuracy and robustness of the models the assumptions and results should be validated by experts independent to the project.

- Improved heat and power provision investigation. An economic analysis was carried out for different heat and power scenarios (see Section 10.3.5), but no environmental or socio-economic evaluation. It is predicted that the environmental benefits of heat and power from biomass would outweigh the economic burden (Section 10.3.5).
- Allow further splitting of pretreated biomass streams - for example, making more than one product from the C6 stream, or using a portion of the lignin for heat and power and a portion for other products (this was shown to be beneficial in the work by Black and Veatch (25)).
- Carry out a more thorough sensitivity analysis to identify the variables that have the most impact on performance. For example, using tornado diagrams or spider plots.
- Integration of the environmental model. The environmental model was not integrated with the module and socio-economic models and exists as a standalone model, providing result only for the 27 concepts. It does not offer the same level of flexibility as the other models. It would be valuable and beneficial to integrate the environmental model so that the results are generated automatically depending on the modules included, as for the module and socio-economic models. This would mean that by using one system process, socio-economic and environmental results could be generated.
- Automatic linking of the process model to the MCDA to generate final results. It would be valuable to create a single integrated model capable of carrying out all functions
- Consider the biomass supply chain by being more specific about plant location. It would be particularly useful if the exact location of the plant is known with the biomass availability in that particular region. If feedstock cannot be obtained cost effectively for plants above a certain size this should also be taken into account. The size of the plants should be considered more carefully based on specific locations. For this thesis the socio-economic model focussed on the country as a whole rather than a specific region. It would be interesting to consider the flexibility of feedstock, to overcome the stumbling block of seasonality and feedstock availability.
- Identify data with the highest uncertainty and take steps to reduce it. It is recommended that a more accurate calculation of the uncertainty be included, as certain modules contain a greater level of uncertainty than others. It is recommended that the uncertainty for each of the modules is calculated, and then combined to give an overall

estimated uncertainty level for the biorefinery configuration under investigation. This should then be included as a criterion in any subsequent evaluations.

Further biorefinery configurations that should be considered are:

- Xylonic acid production with different pretreatment methods, coupled with different products from the C6 stream.
- Concentrated HCl pretreatment coupled with different products (xylonic acid should definitely be included as one of the combinations tested).
- Aquathermolysis with the solid residue used for heat and power provision, or processed as a C6 stream.
- Surfactant production following all pretreatment methods.
- Xylonic acid production following all pretreatment methods.
- Identification of the best pre-treatment method for ethanol production.

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APPENDIX 1 – LIGNIN ANALYSIS RESULTS

For the second batch of concepts chosen (concepts 11-26), the decision about processing of the lignin component was not made immediately. It was important to choose the optimum processing route for lignin, as it has a large impact on the overall efficiency of the plant, but due to the time pressures only processing options from within the Biosynergy project could be considered. Using the lignin purely for heat and power may not give the optimum benefits, but one of the problems with lignin processing is the variability depending on the biomass source and the processes used to recover it ([1]).

Additional analysis was carried out to assess the best option for the lignin stream. There were a number of questions that needed to be answered:

- Should lignin fractionation be included in the pretreatment step? Most pre-treatment processes offer the option of fractionating the biomass into two streams; a solid cellulose/lignin stream and a liquid C5 rich stream or into three separate fractionated streams; cellulose, lignin and C5. Including the lignin fractionation step is expensive in terms of operating costs and fixed capital investment. Is the increased capital and operating costs outweighed by the benefit of the income from the purer lignin stream?

- How should the lignin be used?

There were four options investigated for the processing of lignin. The processing options were based on the technologies included within the Biosynergy project.

- Fractionation followed by fast pyrolysis of the lignin stream. The bio-oil then processed to obtain a phenolic fraction that may be substituted for phenols in phenol-formaldehyde resins.
- Fractionation followed by combustion of the lignin stream for heat and power purposes.
- Fractionation followed by drying of the lignin stream. The pure dry lignin then sold as a finished product.
- Without fractionation, lignin rich stillage from the fermentation of cellulose and lignin used for heat and power generation.

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[1] Holladay, J.E., Bozell, J.J., White, J.F., Johnson, D., *Top Value-Added Chemicals from Biomass - Volume II—Results of Screening for Potential Candidates from Biorefinery Lignin*. 2007, PNNL.

To identify the optimum route for the lignin two analyses were carried out to assess these options. The processes were modelled using information available at the time and the results then compared to identify the optimum using the MCDA software Hiview.

The first analysis was based around Concept 1, shown in Table 1 with lignin processed in the four routes described.

Table 1 – Lignin options based around Concept 1

	Feedstock	Pre-treatment	Lignin fractionation included?	C6	C5	Lignin
1a	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin fast pyrolysis followed by bio-oil fractionation
1b	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin combustion for heat and power
1c	Wheat straw	Steam explosion	Fractionation	Ethanol	Furfural	Lignin dried and sold
1d	Wheat straw	Steam explosion	No fractionation	Ethanol	Furfural	Lignin rich stillage for heat and power

The second analysis was based around Concept 11. The four options are shown in Table 2.

Table 2 – Lignin options based around Concept 11

	Feedstock	Pre-treatment	Fractionation included?	C6	C5	Lignin
11a	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin combustion for heat and power
11b	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin fast pyrolysis followed by bio-oil fractionation
11c	Wheat straw	Mechanical/ alkaline fractionation	Fractionation	ABE	Ethanol	Lignin dried and sold
11d	Wheat straw	Mechanical/ alkaline fractionation	No fractionation	ABE	Ethanol	Lignin rich stillage for heat and power

Data was generated for these options using the process modules. This data was then used as the input for the Hiview to carry out a simple MCDA comparison. This was carried out at a relatively early stage in the modelling before the models had been completed and validated.

Results

The overall MCDA results for the Concept 1 and Concept 11 lignin variations are shown in Figure 1and Figure 2. The results indicated that the most promising route for lignin

processing from the four options was to include fractionation in the pre-treatment step, dry the lignin and then sell it as a dry lignin product. Therefore for all concepts between 11 and 26 generating a lignin stream, this is dried and sold.

For future work it is recommended that a more thorough analysis be carried out. The analysis for this project was carried out at a relatively early stage, when the models were not finalised. The analyses did not take into account environmental, socio-economic impacts or the markets associated with the finished products. These extra criteria should be included in a more detailed study. In addition, only four options for processing lignin were considered when there are many other available. The study should be expanded to include the further options for processing lignin.

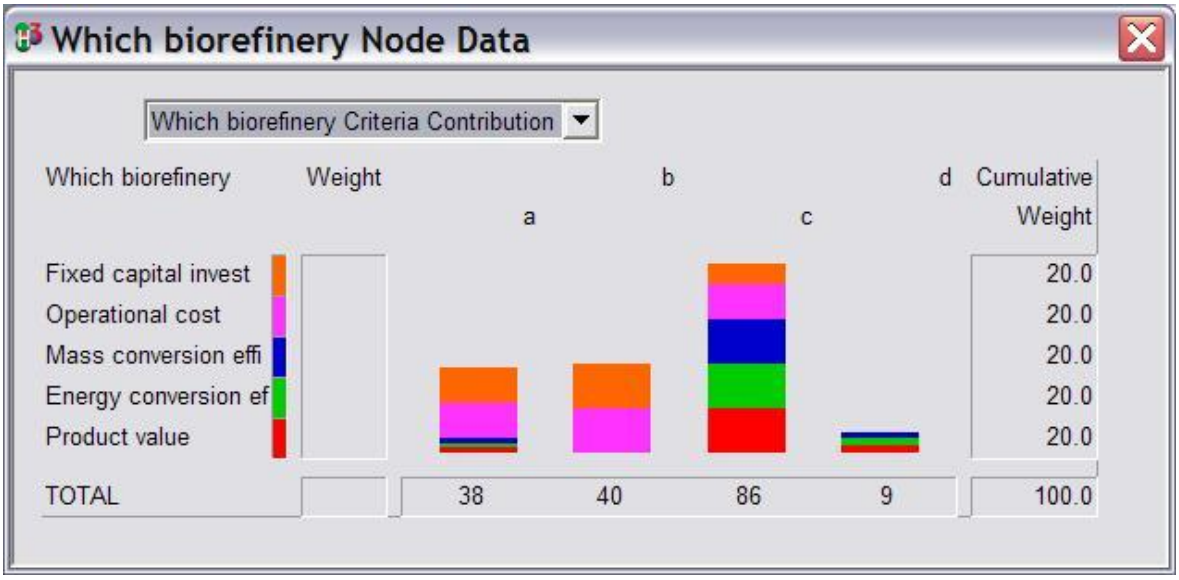


Figure 1 – MCDA results, Concept 1 variations

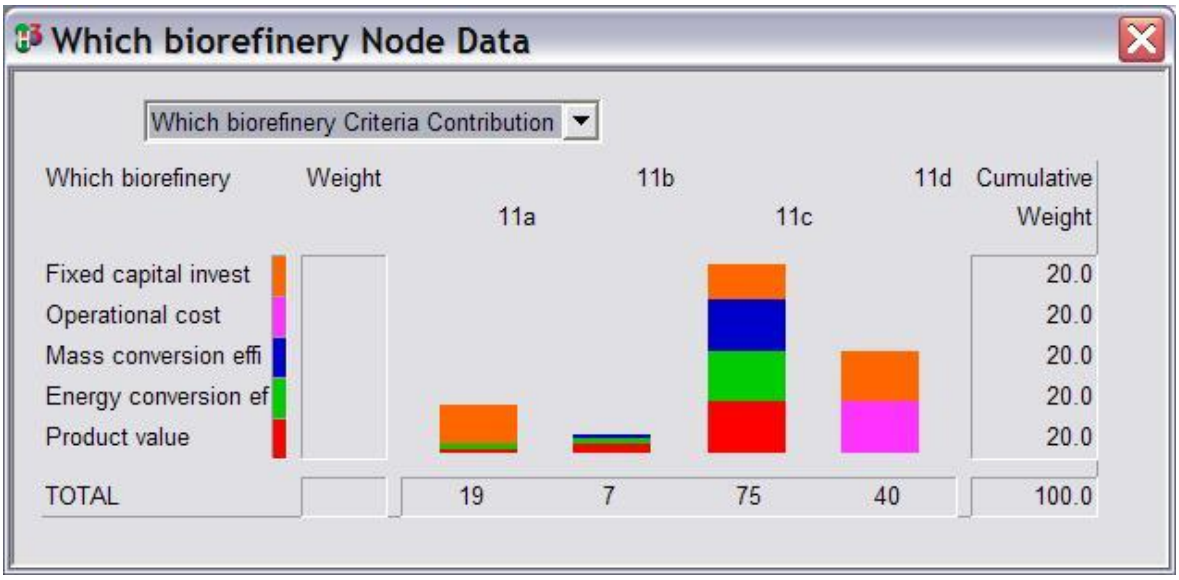


Figure 2 – MCDA results, Concept 11 variations

APPENDIX 2 – DATASHEET

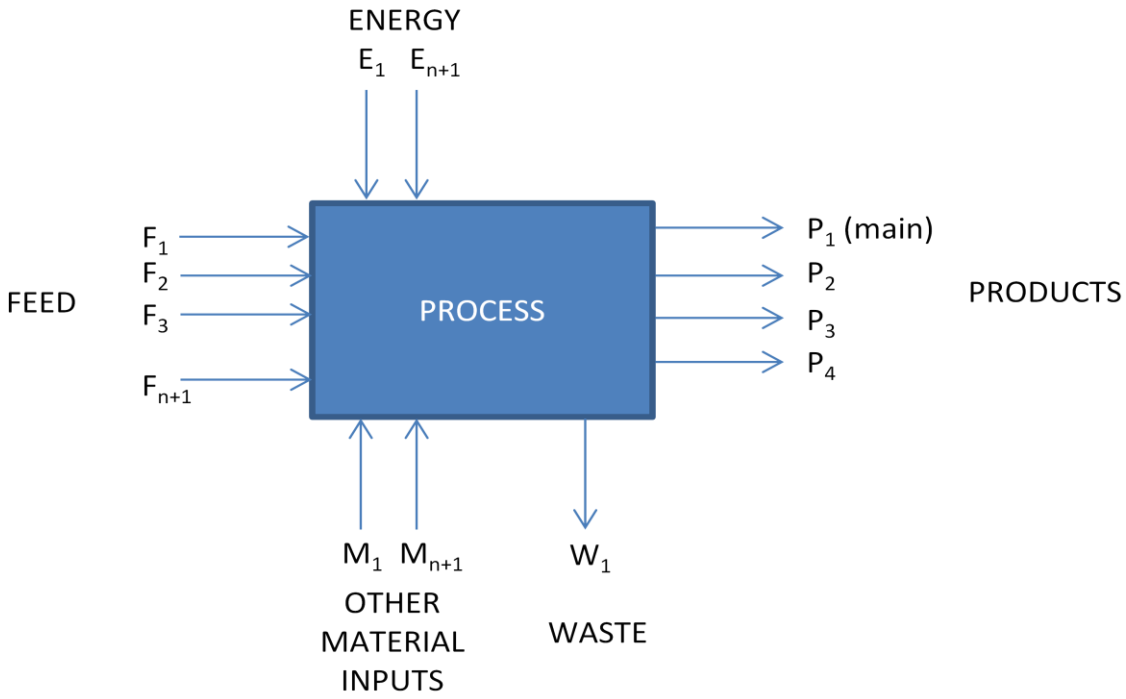
Data Collection

Date modified:

WP

Process unit

Please add as much information as possible to enable accurate modelling. Add extra rows and columns if needed.



Please state design basis, choose from the dropdown list or state:

Basis

PROCESS Short process description	**[Units]**				**Data Source:** where does the data come from
Mass conversion efficiency	%		to primary product		
Energy efficiency	%				
Full-load operational hours	[h/a]				
economic data (if available)	€ per tonne feed	capital		(from preceding unit)	
	€ per tonne feed	operating		(from preceding unit)	
feed rate basis			e.g. per kg dry biomass, per kg dry lignin		
state of technology			i.e. lab scale, pilot scale, commercial		
operating temperature	°C				
operating pressure	bar				

further information			e.g. reaction mechanisms	
Scale				
operating capacity	t/h		basis of this data	
minimum capacity	t/h			
maximum capacity	t/h			
Reaction mechanisms				

FEED

		F_1	F_2	F_3		
description						
mass flow	t/h					
from which preceding unit:						
water content	%					
composition	eg, C, H, O, N				(depending on the process, please input as much detail as possible)	
condition					eg. chipped biomass, slurry etc	
further information						
temperature	°C					
pressure	bar					
lower heating value	MJ/kg					

ENERGY

electrical, steam

		E_1	E_2	E_3	
description					
electrical energy supplied	kWh/h				
steam supplied	t/h				
steam pressure	bar				
steam temperature	°C				
further information					

OTHER MATERIAL INPUTS

for example, chemicals, water

		M_1	M_2	M_3		
description						
mass flow	t/h					
composition	eg. C, H, O, ash				dependent on material	
temperature	°C					
pressure						
moisture	%					
lower heating value	MJ/kg					
further information						

PRODUCTS

		P_1 (main product)	P_2 by-product	P_3 (by-product	
description					
mass flow	t/h				
composition	eg. C, H,				

	O, ash					
market value	€ per tonne					
condition					eg. bio-oil, electrical energy,	
temperature						
moisture	%					
lower heating value	MJ/tonne					
further information						
to which process/consumer						

WASTE

WS (solid waste)

description				
mass flow	t/h			
moisture	%			
quality				
condition			eg. metals, stones, DDGS	
composition	eg. C, H, O, ash			
further information				

WL (liquid waste)

description				
mass flow	t/h			
quality			e.g. COD, BOD	
composition	eg. C, H, O, ash			
further information				

WV (air emissions)

description				
mass flow	t/h			
pressure	bar			
temperature	^{o}C			
quality				
composition	eg. CO2, CH4			
further information				

APPENDIX 3 – USER MANUAL

BIOSYNERGY PROCESS SYNTHESIS MODEL – USER MANUAL

The Biosynergy Process Model allows the user to generate biorefinery chains beginning at the scale of operation and feedstock, through to the final products. Once a complete biorefinery chain has been defined by the user receives an output file containing performance, cost, efficiency and socio-economic data.

The model was created in Excel and is controlled by the "USER INTERFACE" page. The model contains a large number of processing options in the form of modules, in addition to a fully integrated socio-economic model. Each process module is contained within a separate worksheet within the model. The full list of worksheets contained within the model is shown in Table 3 with the colour coding of the tab and a short description of each worksheet.

The tabs/worksheets in **dark green** contain the socio-economic model, created by Patricia Thornley. Each sheet contains the calculations for a different element of the socio-economic model with the overall results displayed in the "SoEc Results" sheet. These are also integrated in the "RESULTS SUMMARY" sheet.

A general user will only need to use the "USER INTERFACE" (see Figure 3 and Figure 4) in order to generate biorefinery concepts and a results summary. The contents of the results summary are shown in Table 4.

Table 3 – Process synthesis model worksheets

		Worksheet	Description
Socio-economic model		Comments	
		Direct facility development	
		Direct facility construction	
		Direct facility operation	
		Direct agricultural	
		Direct transport logistics	
		Techno-economic data	
		Economic labour indices	
		SoEc Results	Displays a summary of the socio-economic results
User interface		USER INTERFACE	
Integrated results		RESULTS SUMMARY	Summary of all results for the chosen biorefinery configuration
Process module models		A1 RSH	Feedstock reception, storage and handling. This module included in all biorefinery configurations.
		B1 Steam explosion	Steam explosion pre-treatment
		B2 AVIDEL	AVIDEL pre-treatment
		B3 Organosolv	Organosolv pre-treatment
		B4 Mech alk (2)	Mechanical/alkaline pretreatment
		B5 Conc HCl	Concentrated HCl pre-treatment
		B6 Aquathermolysis	Aquathermolysis pre-treatment
		F1 Fractionation	Fractionation of steam exploded biomass to either a cellulose/lignin and a C5 stream or separate cellulose, lignin and C5 streams
		T1 gasification CFB	Gasification in a circulating fluidised bed
		T2 gasification BtL	
		T3 Bio-oil heat and power	
		T4 Bio-oil gasification	
		P1 C5 ethanol	Fermentation of C5 stream to ethanol
		P2 C5 ABE	Fermentation of C5 stream to ABE
		P3 C5 to furfural	Processing of C5 stream to furfural
		P4 C5 surfactants	Processing of C5 stream into surfactants
		P5 C5 xylonic acid	Processing of C5 stream to xylonic acid
		H1 C6 ethanol	Fermentation of C6 stream to ethanol
		H2 C5 C6 ABE	Fermentation of C6 or C5 and C6 stream to ABE
		H3 C6 FDCA	Processing of C6 to FDCA
		L1 pyrolysis	Fast pyrolysis
		L2 lignin drying	Lignin drying
		S1 Alcohol synthesis	Mixed alcohol synthesis of syn-gas following gasification
		S4 phenolics	Fractionation of bio-oil from fast pyrolysis to produce phenolic fraction
		R1 Ethanol dist.	Distillation of beer stream from ethanol fermentation
		R2 Mix alc. Dist.	Distillation of mixed alcohols from mixed alcohol synthesis
		Stillage drying	Drying of lignin rich stillage from fermentation, in the ABNT base case only
		Water & Residues	Calculation module
		Water treatment	Processing and treatment of wastewater streams
		Heat & Power	Heat and power provision from biomass and process residues
		Heat only	Heat from biomass and residues, electricity from grid
		NO heat & power	Heat from combustion of natural gas, electricity from grid

Table 4 – Contents of results summary

Concept summary			
Biomass requirement	kg/h, a.r.		
	kg/h, dry		
	tpa, dry		
Electrical power requirement	MW		
Fixed capital investment	€M		
Product summary	kg/h		
	tonnes/annum		
	Price, €/t		
	€/h		
	€/annum		
	Energy in products (LHV basis), MJ/h		
Surplus electricity sold to grid	kWh		
	MW/annum		
	€/kWh		
	€/h		
	€/annum		
Energy in feedstock	MJ/h		
Mass conversion efficiency (dry basis)	%		
Energy conversion efficiency (dry basis including electricity)	%		
Energy conversion efficiency (dry basis excluding electricity)	%		
Operational cost	€/h		
	€/annum		
Production cost	M€/annum		
Steam requirements	kg/h		
	MW		
Steam generated by heat recovery	kg/h		
	MW		
	^{o}C		
Socio-economic results			
Employment			
Direct employment	facility	*development*	man years
		construction	
		operation	
	agricultural	*operational*	
	supply & logistics	*operational*	
Induced employment	regional/national	*development*	
		construction	
		operation	
Agricultural and land assessment for biorefinery plant			
Wheat straw consumption as % of regional production			
Wheat straw consumption as % of national production			
Land required for straw supply (ha)			
Land required for straw supply as % of regional agricultural land			
Land required for straw supply as % of national agricultural land			
Trade assessment for biorefinery plant			
Revenue from traded feedstock (euro pa)			
Revenue from traded feedstock as % of agricultural GDP			
Revenue from biorefinery products (euro pa)			
Revenue from biorefinery products as % of national GDP (%)			
Overall mass balance, kg/h	all inputs and outputs summarised, kg/h		

1.1 USING THE SYSTEM

When opening the model, please enable macros.

Beginning on the "USER INTERFACE" worksheet. Make sure previous choices have been cleared by clicking on the "RESET ALL OPTIONS" button.

1. Begin by entering dry biomass input (kg/h) into cell B18
2. Choose country from drop down menu in cell B19. There are five choices; Germany, Spain, UK, Netherlands, Poland
3. Choose feedstock from dropdown menu in cell A41. There are two choices; wheat straw and softwood
4. Choose from the dropdown menus as highlighted for pretreatment and subsequent processes. Depending on the pre-treatment method chosen, different dropdown menus will be displayed (see Figure 3).
5. Once all of the processing steps have been chosen choose from the drop down menu in cell A58 the heat and power provision. There are three choices; heat and power from biomass, heat only from biomass, heat and power not from biomass. See Figure 4.
6. Finally click on "CREATE SUMMARY" to receive results summary for chosen biorefinery.
7. To clear choices and begin again click on "RESET ALL OPTIONS"

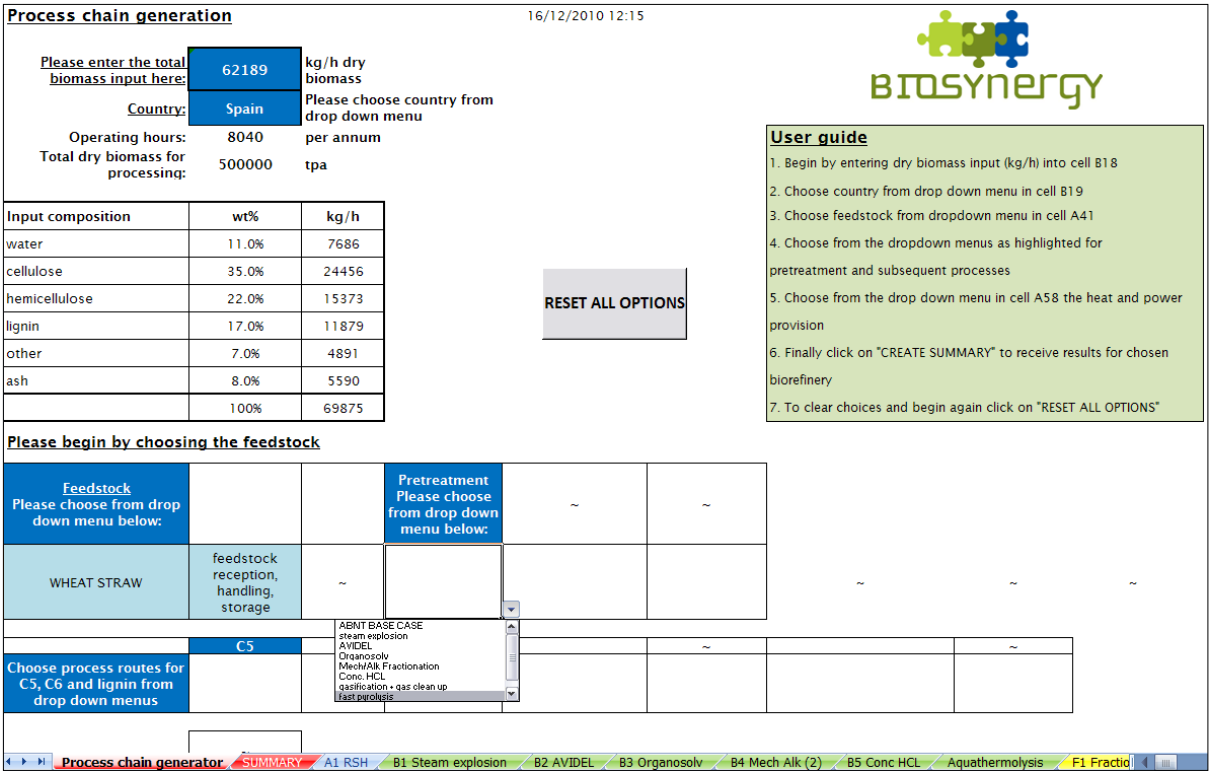


Figure 3 - User interface screen grab 1

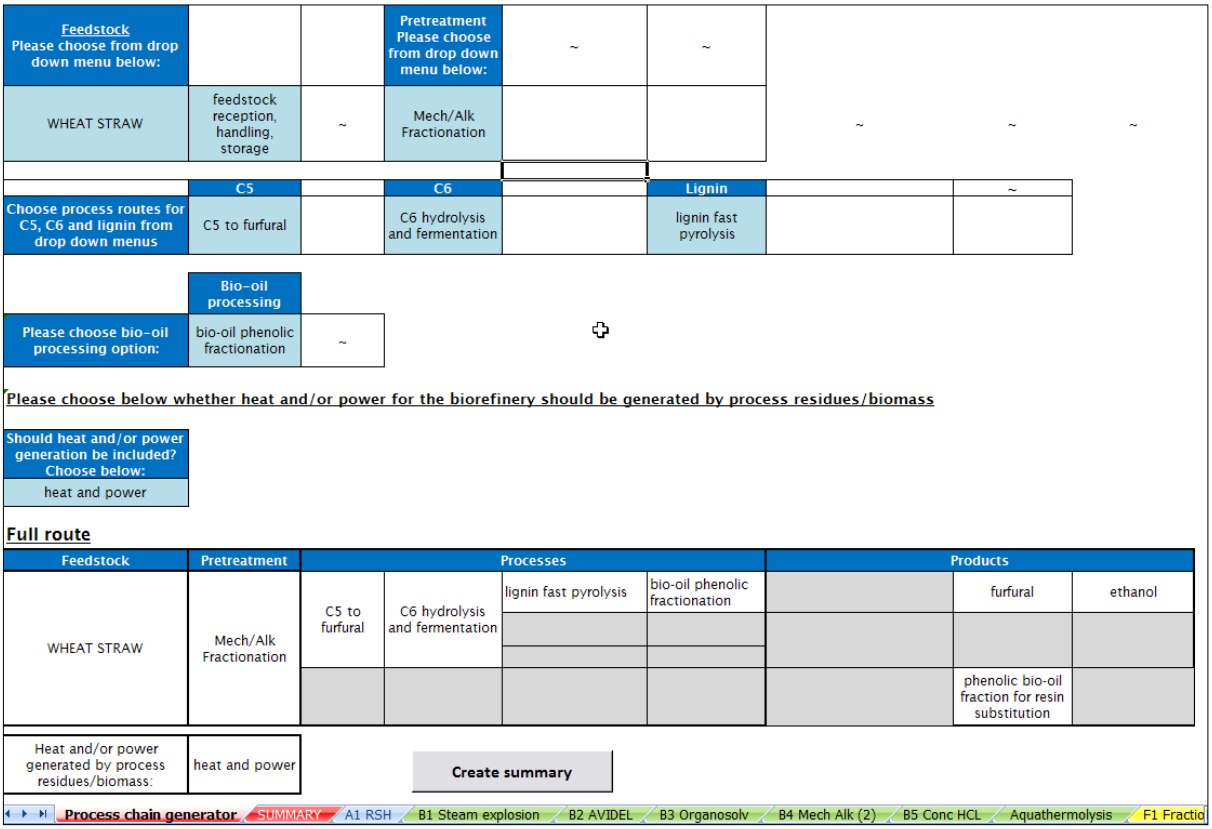


Figure 4 - User interface screen grab 2

SENSITIVITY ANALYSES

It is possible carry out further analyses using the process model by adjusting the assumptions on which the module models are based. Within each process module the user definable elements are highlighted in **bold blue** font. These can be adjusted to view the impact on the overall performance of the biorefinery. Please note that great care should be taken by the user if these assumptions are changed.

APPENDIX 4 – SUMMARY SHEET FROM MODEL

Summary	Country:	Spain	Operating hours	8040	per annum	28/10/2010 10:06

Feedstock	Pretreatment	Processes	Products
WHEAT STRAW	ABNT BASE CASE		ethanol stillage for animal feed

Heat and/or power generated by process residues/biomass:	Heat and power from fossil sources

	kg/h, a.r.	kg/h, dry	tpa, dry
Biomass input	69875	62189	500000

Electrical power requirement summary

	MW
RSH	**0.5**
steam explosion	**1.7**
AVIDEL	0.0
Organosolv	0.0
Mech/alk pretreatment	0.0
Conc. HCl	0.0
aquathermolysis	0.0
fractionation	**3.6**
C5 to ethanol	**2.8**
C5 to ABE	0.0
C5 to furfural	0.0
C5 to surfactants	0.0
C5 to xylonic acid	0.0
C6 to ethanol	**5.9**
C6 (&C5) to ABE	0.0
C6 to FDA	0.0
gasification (alc. synthesis)	0.0
gasification (BtL)	0.0
pyrolysis	0.0
drying	**0.9**
bio-oil gasification (entrained flow)	0.0
mixed alcohol synthesis	0.0
bio-oil to phenolics	0.0
ethanol distillation	**1.3**
mixed alcohol distillation	0.0
wastewater plant	**2.0**
Total electrical power requirement	**18.6**

Fixed capital investment

Fixed capital investment summary	€M (2009)
RSH	**19.3**
steam explosion	**87.3**
AVIDEL	0.0
Organosolv	0.0
mech/alk pretreatment	0.0
Conc. HCl	0.0
aquathermolysis	0.0
fractionation	**76.2**
C5 to ethanol	**9.8**
C5 to ABE	0.0
C5 to furfural	0.0
C5 to surfactants	0.0
C5 to xylonic acid	0.0
C6 to ethanol	**29.6**
C6 (&C5) to ABE	0.0
C6 to FDA	0.0
gasification (alc. synthesis)	0.0
gasification (BtL)	0.0
pyrolysis	0.0

drying	**40.1**	
bio-oil gasification (entrained flow)	0.0	
mixed alcohol synthesis	0.0	
bio-oil to phenolics	0.0	
ethanol distillation	**9.9**	
mixed alcohol distillation	0.0	
Bio-oil heat and power plant	0.0	
wastewater plant	**32.8**	
heat and power plant	0.0	
heat plant	**66.9**	
gas boiler	**0.3**	
Total fixed capital investment	**€ 372**	**M**

Products

Products	**kg/h**	**tonnes/annum**	**Price, €/t**	**€/h**	**€/annum**	**Energy in products MJ/h**
ethanol	**14356**	115422	700	10,049	80,795,700	414387
furfural	0	0	625			0
phenolic fraction	0	0	750			0
ABE	0	0	910			0
surfactants	0	0	1500			0
methanol	0	0	300			0
butanol	0	0	1000			0
propanol	0	0	300			0
bio-oil	0	0	175			0
lignin	0	0	400			0
xylonic acid	0	0	1000			0
FDA	0	0	1500			0
gasoline	0	0	1337			0
diesel	0	0	1117			0
Stillage for animal feed	**34374**	276370	100	3,437	27,637,037	378119
	kWh	**MW/annum**	**€/kWh**	**€/h**	**€/annum**	
Surplus electricity sold to grid	0	0	0.04	0	0	0
Heat	0	0	0.024	0	0	(based on cost of producing an equal amount of heat from natural gas) 0
				Totals:	80,795,700	792505

Energy in feedstock	1052903	MJ/h

Mass conversion efficiency (dry basis)	78%		
Energy conversion efficiency (dry basis, including electricity)	75%	Energy conversion efficiency (dry basis, excluding electricity)	75%

Operational cost

Operational cost (feedstock,chemicals, additives etc)	**€/h**	**€/annum**
RSH	**3519**	€ 28,293,713
steam explosion	**39**	€ 312,294
AVIDEL	0	€ -
Organosolv	0	€ -
mech/alk pretreatment	0	€ -
Conc. HCl	0	€ -
aquathermolysis	0	€ -
fractionation	**699**	€ 5,616,718
C5 to ethanol	**6634**	€ 53,333,964
C5 to ABE	0	€ -
C5 to furfural	0	€ -
C5 to surfactants	0	€ -
C5 to xylonic acid	0	€ -
C6 to ethanol	**3089**	€ 24,831,581
C6 (&C5) to ABE	0	€ -
C6 to FDA	0	€ -
gasification (alc. Synthesis)	0	€ -
gasification (BtL)	0	€ -
pyrolysis	0	€ -

bio-oil gasification (entrained flow)	0	€	-
mixed alcohol synthesis	0	€	-
bio-oil to phenolics	0	€	-
ethanol distillation	0	€	-
mixed alcohol distillation	0	€	-
Bio-oil heat and power plant	0	€	-
wastewater plant	**123**	€	988,385
heat and power plant	0	€	-
heat plant	**90**	€	720,391
gas boiler	**2**	€	12,406
fresh water	**5**	€	36,368
fresh boiler make-up	0	€	-
natural gas	**466**	€	3,746,844
electricity	**743**	€	5,971,526
TOTAL	€ 15,406	€	123,864,191

Production cost = ((OpEx + 0.16FCI)/0.95) =	193.1	M€/annum

Steam requirement

Steam requirements	**kg/h**	**MW**
steam explosion HP	**47999**	**37**
steam explosion LP	**4995**	**4**
AVIDEL	0	0
Organosolv (reactor heating)	0	0
Organosolv (ethanol flash)	0	0
Organosolv (cellulose flash)	0	0
Mech/alk	0	0
Conc. HCl	0	0
Aquathermolysis (heating)	0	0
Aquathermolysis (stripper)	0	0
T1 gasification (fluidising)	0	0
T1 gasification HP (SMR)	0	0
T1 gasification (acid gas removal)	0	0
T2 gasification and FT (BTL)	0	0
T4 bio-oil gasification	0	0
C5 furfural HP	0	0
C5 furfural LP	0	0
C5 ABE distillation	0	0
surfactants	0	0
C6 to FDA	0	0
phenolics	0	0
ethanol distillation	**31552**	**24**
mixed alc. Distillation	0	0
drying	**11980**	**9**
TOTAL	**96526**	**74**

Steam generated	**kg/h**	**MW**	**°C**
T2 gasification (BtL)	**0.0**	**0.0**	
From cooler	0.0	0.0	0.0
From FT reactor	0.0	0.0	0.0
From HC recovery	0.0	0.0	0.0
From HC recovery	0.0	0.0	0.0
Bio-oil gasification	**0.0**	**0.0**	**0.0**

Socio-economics

Employment assessment for biorefinery plant

			Total employment (man years) Straw	Forestry
Direct employment	**facility**	***development***	7,235	
		construction	5,817	
		operation	825	
	agricultural	***operational***	1,893	0
	supply & logistics	***operational***	511	0
Induced employment	**regional/national**	***development***	10,418	0
		construction	8,376	0
		operation	3,914	0
		Total	38,989	0

Agricultural and land assessment for biorefinery plant

Wheat straw consumption as % of regional production	36.99%		
Wheat straw consumption as % of national production	10.26%	***Wood consumption as % of national production***	**0.00%**
Land required for straw supply (ha)	302,973	***Forested area required to supply wood (ha)***	0
Land required for straw supply as	5.84%		

% of regional agricultural land			
Land required for straw supply as % of national agricultural land	1.23%		

Trade assessment for biorefinery plant

Revenue from traded feedstock (euro pa)	**28,089,888**	*Revenue from traded feedstock (euro pa)*	**0**
Revnue from traded feedstock as % of agricultural GDP	**0.07%**	*Revnue from traded feedstock as % of agricultural GDP*	**0.00%**
Revenue from biorefinery products (euro pa)	80,795,700		
Revenue from biorefinery products as % of national GDP (%)	0.007%		

Overall Mass Balance, kg/h

Includes all processing plant, except heat and power, wastewater treatment. These considered separately

	Input, kg/h	Output, kg/h	
biomass	**69875**		
biomass to heat and power generation		0	sent to generate heat and power for plant
H_2SO_4 (98%)	**7385**	0	
steam explosion	**270**		
Mech/alk	0		
fractionation	**7115**		
C5 to ethanol neutralisation	0		
C5 to ABE neutralisation	0		
furfural production	0		
C5 surfactant	0		
C6 ethanol neutralisation	0		
C6 C5 ABE	0		
C6 FDA (neutralisation)	0		
NaOH (50%)	**1686**		
Mech/alk	0		
fractionation	**1259**		
C5 to ethanol neutralisation	**427**		
C5 to ABE neutralisation	0		
C5 surfactant	0		
C6 ethanol neutralisation	**0**		
bio-oil fractionation	0		
C6 C5 ABE	0		
C6 FDA (neutralisation)	0		
C6 FDA (reactor)	0		
Xylonic acid	0		
Xylonic acid inoculum prodn	0		
HCl	0		
Conc HCl pretreatment	0		
C6 FDA	0		
Toluene	0		
Yeast	**1258**		
Enzymes	**917**		
C6 ethanol enzymes	**917**		
C6 (&C5) ABE enzymes	0		
C6 FDA enzyme	0		
Fermentation gases	0	**13726**	
CO2		**13605**	sent to atmosphere
O2		**121**	sent to atmosphere
H2		0	sent to atmosphere
Medium (inolulum production)	0		
Organic acid (acetic and formic mixture)	0		
ethanol	**0**		
Organosolv	0		
butanol	**0.00**		
C5 surfactants	0		

air	**603843**	**603843**	sent to atmosphere
steam explosion	**603843**	**603843**	
gasification char combustor (T1)	0		
gasification (T1 - OLGA)	0	0	
xylonic acid	0	0	
xylonic acid (inoculum prodn)	0	0	
gasification (T2)	0	0	
gasification (T4)	0	0	
FDCA production	0	0	
char to char combustor (T1 gasification)		0	
CO2 (acid gas removal)		0	sent to atmosphere
T1 gasification		0	
T2 gasification BtL		0	
T4 bio-oil gasification		0	
Flue gas (char combustor)		0	sent to atmosphere
Sand	0		For T1, T2 bed material, T4 flux agent)
T1 gasification	0		
T2 gasification BtL	0		
T4 bio-oil gasification	0		
Boiler feedwater chemicals (T3 Bio-oil heat and power)	0		
Solid waste (stones, etc)		**311**	sent to landfill
Ash and unburnt solids		0	sent to landfill
T1 gasification		0	
T2 gasification BtL		0	
T4 bio-oil gasification		0	
L1 pyrolysis		0	
Elemental sulphur (acid gas removal)		0	sent to landfill
T1 gasification		0	
T2 gasification BtL		0	
T4 bio-oil gasification		0	

Not included in overall input/output of plant as made up of recycled process water from wastewater treatment, with a small amount of make-up if required.

Process water	**Input**	**Return**
steam explosion	**26165**	
AVIDEL	0	
Organosolv	0	0
Mech/alk (with alkaline to reactor)	0	
Mech/alk (washing)	0	
Strong HCl	0	0
Fractionation (solid/liq sep)	**436898**	
fractionation (NaOH dilution)	**11329**	
fractionation (H2SO4 dilution)	**809**	
Aquathermolysis	0	0
T1 gasification	0	0
T2 gasification and FT	0	0
T4 bio-oil gasification	0	
C6 cooling	0	0
C6 SSF (dilution)	**118669**	
C6 (and C5) ABE dilution	0	
C6 (and C5) ABE cooling	0	0
C6 FDA cooling water	0	0
C6 FDA dilution water	0	
C6 FDA reactor	0	
C6 FDA washing water	0	
C6 FDA water	0	
C5 fermentation	0	
C5 furfural	0	
surfactants	0	0
mixed alcohol synthesis	0	0
Bio-oil fractionation	0	
Bio-oil fractionation (NaOH dilution)	0	
lignin pyrolysis (quench)	0	0
TOTAL	**593869**	0

Not included in overall input/output of the plant

as made up of recycled condensate and a small amount of make-up if required

Steam requirements	Input	Condensate return
steam explosion HP	**47999**	
steam explosion LP	**4995**	**43395**
AVIDEL	0	0
Organosolv (reactor heating)	0	0
Organosolv (ethanol flash)	0	
Organosolv (cellulose flash)	0	
Mech/alk	0	0
Conc. HCl	0	0
Aquathermolysis (heating)	0	0
Aquathermolysis (stripper)	0	
T1 gasification (fluidising)	0	
T1 gasification HP (SMR)	0	0
T1 gasification (acid gas removal)	0	
T2 gasification and FT (BTL)	0	0
T4 bio-oil gasification	0	0
C5 furfural HP	0	0
C5 furfural LP	0	
C5 ABE distillation	0	0
surfactants	0	0
C6 to FDA	0	0
phenolics	0	0
ethanol distillation	**31552**	**52727**
mixed alc. Distillation	0	0
drying	**11980**	**11980**
TOTAL	**96526**	**108102**

Water vapour	0	**5668**	sent to atmosphere
RSH		0	
lignin drying		**5668**	
pyrolysis prep		0	
C6 FDA		0	

Products		**48730**
furfural		0
surfactant		0
xylonate		0
bio-oil		0
lignin		0
phenolic fraction		0
ethanol		**14356**
MeOH		0
PropOH		0
ButOH		0
ABE		0
FDA		0
gasoline		0
diesel		0
Stillage for animal feed		**34374**

steam generated (T2 & T4))		0	
Waste pyrolysis gases		0	sent to CHP to generate heat and power
Char combusted		0	combusted to provide heat for pyrolysis
Unconverted syn-gas		0	sent to CHP to generate heat and power

Total liquid waste stream to dewatering (prior to wastewater treatment)	0	**594979**
Fractionation		**37789**
C5 ABE neutralisation losses		0
C5 ABE wastewater		0
C5 ABE pervaporation waste		0
furfural		0
surfactants		0
phenolic fractionation waste water		0
aqueous soluble fraction		0
alkaline insoluble fraction		0
ethanol distillation stillage		0

mixed alcohol waste		0
T1 gasification		0
T2 gasfication BtL		0
T4 gasification of bio-oil		0
C6 ABE solids		0
C6 ABE neutralisation losses		0
C6 ABE wastewater		0
C6 FDA waste 1		0
C6 FDA waste 2		0
C6 FDA waste 3		0
C6 FDA waste 4		0
lignin		**10750**
Xylonic acid production liquid waste		0
Xylonic acid production waste 2		0
Xylonic acid production waste 3		0
Aquathermolysis waste 1		0
Aquathermolysis waste 2		0
Aquathermolysis waste 3		0
stillage drying		**546440**
TOTAL	**1375359**	**1375359**

Freshwater	**56542**	0	
Fresh process make-up	**56542**		The rest of the water requirement is made up of recycled water from the wastewater treatment plant
boiler make-up	0		The rest of the boiler feedwater requirement is made up of recycled condensate
Wastewater output		0	Wastewater emitted by biorefinery

Wastewater treatment

Liquid input	**539179**	
Nutrients	**328**	
air	**218867**	
vapours		**222593**
sludge to heat and power		**817**
biogas to heat and power		**3807**
cleaned process water		**531157**
TOTALS	**758374**	**758374**

Heat and power

Pyrolysis waste gas	0	
Unconverted syn-gas	0	
Residues	**55801**	
Wastewater sludge	**817**	
Bio-gas wastewater treatment	**3807**	
Bio-oil	0	
TOTAL	**60425**	
biomass	0	

Air input	**193359**		
Flue gas output		**252703**	sent to atmosphere
Solid residues (ash & unburnt feed)		**1080**	sent to landfill
TOTAL	**253783**	**253783**	

Information about heat and power plant

Heat Production η	70%	
Electrical Power Generation η	30%	
LHV of biomass (incl. moisture/water)	15.07	MJ/kg
Biorefinery requirements:		
Steam Requirement	74	MW
Electricity requirement	19	MW
Steam + electrical requirement	92	MW

Boiler feed water chemicals	1	kg/h							
Total residues:	60425	kg/h							
Provided by residues	89	MW	90%	combustion efficiency					
From residues:									
heat	56.19	MW	Heat required by biorefinery			0	MW		
electricity	0.00	MW	Surplus heat used to generate electricity			0	MW		
Total	0.00	MW							
From biomass needed:									
heat	0.00	MW	90%	combustion efficiency					
energy in straw	0.00	MW							
biomass required	0.00	kg/h							
heat produced	0.00	MW							
electricity produced	0.00	MW							
Total	0.00	MW							
Total electricity sold to grid	0.00	MW		Natural gas purchased	1835	kg/h	466	€/h	
Heat to be sold	0.00	MW		Electricity from grid purchased	18.57	MW	743	€/h	

APPENDIX 5 – (ON CD) BIOSYNERGY PROCESS SYNTHESIS MODEL

APPENDIX 6 – (ON CD) HIVIEW MCDA MODEL, GERMANY

APPENDIX 7 – (ON CD) HIVIEW MCDA MODEL, NETHERLANDS

APPENDIX 8 – (ON CD) HIVIEW MCDA MODEL, POLAND

APPENDIX 9 – (ON CD) HIVIEW MCDA MODEL, SPAIN

APPENDIX 10 – (ON CD) HIVIEW MCDA MODEL, UK