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Executive Summary

The ButaNexT project has focused on the production of ligno-cellulosic biobutanol, developing an integrated process at pilot scale, and investigating its use as a blend component in vehicle fuel. The value proposition of biobutanol within the transport sector rests on its ability to reduce GHG emissions compared to conventional fossil fuels. Therefore this study aims to provide a GHG assessment of biobutanol produced both in the integrated pilot plant which has been constructed during the ButaNexT project, and in a conceptual commercial-scale plant, calculated according to RED methodology.

The mass and energy balance for the pilot plant is based on actual data from the operating plant. The mass and energy balance for the conceptual commercial-scale plant was put together in collaboration with the members of the ButaNexT consortium, and models the biobutanol production process at a commercial scale of 450 ktonnes/annum of straw input (moisture content 12%). This produces 39 ktonnes/year of butanol based on yields achieved to-date in the pilot plant, and 67 ktonnes/year of biobutanol based on yields considered achievable at commercial scale by the project consortium (high conversion efficiency scenario).

In the pilot plant, all heat and steam demands are provided by electrically heated boilers, therefore all of the energy required by the process is provided by electricity. The total electricity demand is 1,100 MJ/kg butanol.

In the conceptual commercial-scale plant, the overall power demand of the process is 22MJ/kg butanol produced, and the overall heat demand is 43MJ/kg butanol produced. The majority of the heat demand comes from separation and purification of the biobutanol, whilst the power demand is roughly 2/3 attributable to enzymatic hydrolysis and 1/3 attributable to fermentation, separation and purification.

Based on the commercial plant mass and energy balance and using the RED GHG calculation methodology, an assessment of the greenhouse gas emissions of the biobutanol was carried out. Comparison of the GHG emissions across a number of heat and power provision scenarios was carried out, considering on-site combustion of by-product biomass (scenario A), gas boiler with CHP (scenario B), gas boiler with electricity from the grid (scenario C), and gas turbine CHP (scenario D). Across these scenarios, the lowest GHG emissions can be achieved when the by-product biomass is combusted on-site to provide heat and power to the process. In addition, a number of scenarios for improved plant performance were also investigated: lower heat and power demand and high conversion efficiency of the process. When both low heat and power demand and high conversion efficiency occur together, and heat and power is provided by on-site biomass combustion (heat and power scenario A), biobutanol has a GHG emissions intensity of 38 gCO₂eq./MJ (Figure 1). This is equivalent to a GHG saving of 55% compared to the RED fossil fuel comparator, approaching the 60% GHG saving threshold that is required for biofuels produced in new plants under the RED.
Figure 1  GHG emissions of butanol, under plant performance scenario 4: Low heat and power demand and high conversion efficiency. Dashed line refers to fossil fuel comparator (Ref. European Commission, 2009)

Without CO₂ capture, ligno-cellulosic biobutanol can make moderate GHG savings, comparable to current corn ethanol plants, but higher than those of ligno-cellulosic bioethanol (Figure 2). This is largely due to the low yield of biobutanol compared to bioethanol, and the high heat and power demand of the production process. As the biobutanol process is developed and scaled up, key actions to further reduce GHG emissions are: improving overall conversion efficiency of feedstock to product, reducing heat and power demand of the biobutanol production process, for example through process integration, and exploring increased use of by-products such as hydrogen for on-site energy provision.

Figure 2  GHG emissions of biobutanol compared to crop-based and LC ethanol, across a number of different plant performance scenarios. Dashed line refers to RED fossil fuel comparator, and data labels show % GHG saving compared to this.
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<th>Full Form</th>
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<tr>
<td>Capex</td>
<td>Capital expenditure</td>
</tr>
<tr>
<td>CENER</td>
<td>National Renewable Energy Centre of Spain</td>
</tr>
<tr>
<td>GBL</td>
<td>Green Biologics</td>
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<tr>
<td>GHG</td>
<td>Greenhouse Gas</td>
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<tr>
<td>LC</td>
<td>Ligno-cellulosic</td>
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<td>LCA</td>
<td>Life cycle assessment</td>
</tr>
<tr>
<td>LCI</td>
<td>Life cycle inventory</td>
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<tr>
<td>LHV</td>
<td>Lower Heating Value</td>
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<tr>
<td>Opex</td>
<td>Operational expenditure</td>
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<td>RED</td>
<td>Renewable Energy Directive</td>
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<tr>
<td>TR</td>
<td>Tecnicas Reunidas</td>
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<td>TYIR</td>
<td>Nutrient mixture used in butanol production</td>
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<td>VITO</td>
<td>Flemish Institute for Technological Research</td>
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1 Introduction and aims of the study

1.1 The ButaNexT project

The ButaNexT project, funded through the Horizon 2020 programme, aims to develop new and improved processes and techniques for the cost-effective production of biobutanol. Whilst butanol has a wide range of uses in the chemicals sector and can be used as a transport fuel, the focus of the ButaNexT project is on butanol used within the transport sector.

Lignocellulosic biofuels (2nd generation biofuels) are produced from feedstocks which are not food or feed crops. When derived from agricultural/forestry waste or residues, they present a reduced risk of land-use-change impacts compared to conventional biofuels. In addition, it is anticipated that waste/residue-based lignocellulosic biofuel routes will have significant greenhouse gas reductions compared to fossil fuels and conventional biofuels. Whilst ligno-cellulosic ethanol production is currently being produced at commercial-scale by several companies in Europe and the USA, to-date there has been limited research or deployment of ligno-cellulosic biobutanol production.

The ButaNexT project brings together partners with expertise in each step of the biobutanol production process (Figure 3). Over the course of the project they have optimised each step of this process, and have brought all the elements of the process together in an integrated pilot plant operating at scale of around 100L fermentation tank.

1.2 The technology and partners

Each stage of the biobutanol production process is being developed either individually or by a combination of two of the ButaNexT consortium partners (Figure 4). Ligno-cellulosic biomass (Miscanthus and cereal straw) undergoes mechanical pre-treatment (milling) and thermochemical pre-treatment in order to break apart the cellulose, hemicellulose and lignin in the biomass. Enzymatic hydrolysis is used to break polymeric sugars contained in cellulose down into monomeric sugars that can be more easily digested by the fermentation organisms. Vacuum filtration is then required to remove the recalcitrant biomass stream, which is largely lignin and undigested sugars. Finally, fermentation produces acetone, butanol and ethanol (ABE), and in-situ pervaporation is used to recover these ABE solvents.

Over the course of the ButaNexT project, several technologies used throughout the production process have been scaled up from lab scale (TRL 4) to pilot scale (TRL 5/6). These novel elements of the process (milling, enzymatic hydrolysis, fermentation and pervaporation) which were the focus of the ButaNexT
project, have been combined with other more established processes (soaking and pre-treatment, and vacuum filtration) in an integrated pilot plant.

1.3 Aims of this study
This study aims to refine and revise the preliminary energy balance and greenhouse gas (GHG) assessment carried out in deliverable D6.2, based on the final feedstock selection in work package 2 and the actual data which is now available from the integrated pilot plant.

At this stage in the project, operational data are now available from the integrated pilot plant, which is operated by CENER. Therefore a GHG calculation of the products produced in the pilot plant, based on data obtained from the pilot plant, was carried out. Due to its small scale and limited optimization of the integrated process, the GHG intensity of biobutanol produced in the pilot plant is unlikely to accurately reflect the potential GHG intensity of a commercial biobutanol production process. Therefore a theoretical mass and energy balance of a commercial-scale biobutanol plant has been extrapolated on the basis of expected yields and large-scale processes, in order to assess the likely GHG impact of butanol in commercial production.

Whilst butanol can be used as a fuel or a chemical feedstock, the focus of the ButaNexT project has been on the use of butanol as a liquid transport fuel. Therefore the GHG assessment will be carried out in line with the Renewable Energy Directive (RED) (European Commission, 2009) GHG assessment methodology, which is used to assess the GHG emissions of transport fuels within the EU, in order to assess each Member State’s progress towards renewable energy targets. The GHG emissions of Biobutanol production via the ButaNexT process will be compared with the GHG emissions of first generation and cellulosic ethanol production, and conventional gasoline and diesel.

1.4 Structure of this report
Having defined the goal of the study in this introduction, chapter 2 addresses the scope of the study. Chapter 2 is split into two sections, first addressing scope of the GHG assessment of the operating pilot plant, and then addressing the scope of the GHG assessment of the conceptual commercial-scale biobutanol production plant, stating for each the product function and functional unit, the functional flow and the system boundary. Chapter 3 describes the method that was followed for this study, discussing the overall method principles that were followed, and then specifically how allocation was dealt with, data requirements for the study, and the emission factors used. The mass and energy balance of the pilot plant is provided in chapter 4. The mass and energy balance of the commercial-scale plant is provided, along with a discussion of underlying assumptions, and explanation of the scenarios that were analysed, in chapter 5. Chapter 6 contains the results of the study for the pilot plant (6.1) and the conceptual commercial plant (6.2), and finally a comparison with other fuels (6.3). Finally in chapter 7 the results are summarized and key conclusions and areas for future work are identified.
2 Scope of the study

In this study, an energy balance and GHG assessment is carried out on biobutanol produced in the pilot plant, as established at CENER premises by the ButaNexT consortium, and on butanol produced in a conceptual commercial-scale plant. The scope of the energy and GHG assessments are slightly different for the pilot and commercial plants. The scope of the pilot-scale study is addressed in section 2.1, followed by the scope of the commercial-scale study (section 2.2).

2.1 GHG assessment of pilot-scale biobutanol production

2.1.1 Product function and functional unit

At the pilot plant, the processes only goes as far as mixed acetone, butanol and ethanol (ABE) production, so in order to accurately reflect the experimental set-up of this plant, the functional unit for the pilot-scale assessment is 1MJ of ABE produced in the pilot plant. This is calculated as an average of the LHV of acetone, butanol and ethanol according to the composition of the ABE stream. In a commercial plant, ABE would be further processed to separate the butanol from acetone and ethanol (see section 2.2) but this does not happen within the pilot plant.

2.1.2 Functional flow

The functional flow of the pilot-scale GHG assessment is the well-to-gate lifecycle of ABE produced in the pilot plant, including the production of feedstock, pre-treatment, and fermentation-pervaporation. Separation out of the individual biobutanol stream is not included within the functional flow. It should be noted that this does not cover the full well-to-tank process, which is required under the Renewable Energy Directive, because isolation and purification of butanol was not carried out in the pilot plant.

It should be noted that whilst the flows are given in per MJ of ABE, the mixed ABE permeate stream produced in the pilot plant contains around 79% water and 21% ABE solvents, meaning it has a lower heating value of 0 MJ/kg. Therefore in order to provide a meaningful result to illustrate the principle GHG burdens of butanol production in the pilot plant, the GHG emissions are expressed per MJ pure ABE solvents, as though this water had been removed.

2.1.3 System boundary

The system boundary of the pilot-scale GHG assessment is illustrated in Figure 5, showing those production steps in blue which are implemented at the pilot plant.

2.2 GHG assessment of commercial-scale biobutanol production

2.2.1 Product function and functional unit

For the commercial-scale assessment, the functional unit is 1MJ of biobutanol used as a fuel in a vehicle.
2.2.2 Functional flow
For the commercial-scale GHG assessment, the functional flow is the well-to-tank lifecycle of biobutanol produced through the ButaNexT process, comprising all stages of production, including the production of the feedstock (or feedstock collection only if it is a waste / residue), and storage and transport of the final product to petrol pumps for vehicle re-fuelling.

2.2.3 System boundary
The system boundary of the commercial-scale GHG assessment is illustrated in Figure 6. Production steps implemented at the plant are coloured blue, and those that are not are orange. This system boundary is in line with that required for RED-compliant GHG calculations. In line with the EU RED, the GHG intensity for feedstock production and processing of agricultural/forestry waste and residue is zero. Furthermore, the system boundary includes a generic transportation step to filling station step. The emissions from the fuel in use are taken to be zero for biofuels.

![Figure 6 System boundary of commercial-scale GHG assessment (orange modules are outside the physical boundary of the plant, blue modules are within the plant)](image)

The study will not consider the manufacture of machinery and chemical plant infrastructure as this is not included in the calculation of default values in the RED or in calculation of fossil fuel comparator values (European Commission, 2009).
3 Method

3.1 Overview
The focus of the ButaNexT project is on biobutanol produced as a next-generation transport fuel. Therefore the methodology used for the GHG calculation will be that defined in Annex V of the Renewable Energy Directive (RED), which is used across Europe for assessing the GHG emissions of biofuels used in transport and bioliquids. The process steps laid out in ISO 14044 for LCA studies have been broadly followed, although this study is not a full LCA and is not fully compliant with ISO 14044, which would also require a peer review of the work. If there is any conflict between ISO 14044 and RED methodologies then RED has been followed. This approach ensures results are compliant with EU regulation, and are easily comparable with the GHG emissions of other fuels and biofuels which have been calculated using the same method. The RED method takes into account CO$_2$, CH$_4$, and N$_2$O when calculating GHG emissions, with CO$_2$ equivalents of:

- CO$_2$ : 1 kgCO$_2$eq/kgCO$_2$
- CH$_4$ : 23 kgCO$_2$eq/kgCH$_4$
- N$_2$O : 296 kgCO$_2$eq/kgN$_2$O

3.2 Allocation
When a production process produces multiple products (i.e. co-products), GHG emissions from that process must be allocated between the different co-products. Several possible different methods of allocation can be used. In consequential LCA an ‘avoided emissions’ approach would be taken, which assigns each co-product a ´credit´ equal to the avoided environmental impact of producing that product by an alternative process.

In an attributional LCA, emissions must be allocated between products and co-products on the basis of either their masses, energy contents, or economic value. Under the RED GHG methodology, emissions must be allocated on the basis of the lower heating value (LHV) energy content of co-products. Given that RED methodology is used in this study, co-product allocation has been carried out based on the respective LHV of the different co-products. In the case of wet or aqueous co-products, the LHV used is the LHV of the wet product.

When excess electricity is exported to the grid from a co-generation plant (except when the fuel used for the cogeneration is a co-product other than an agricultural crop residue) a credit is given for the excess electricity that is equal to the amount of greenhouse gas that would be emitted when an equal amount of electricity was generated in a power plant using the same fuel as the cogeneration unit (European Commission, 2009). In this study, the only case where excess electricity is exported to the grid is when it is generated in a gas CHP on-site. Therefore in this case a credit is given to this electricity equal to the GHG intensity of electricity generated in a CCGT natural gas plant.

3.3 Data requirements
For the purposes of carrying out a GHG assessment of the butanol produced in the ButaNexT process, the key data requirements are: full mass and energy balance detailing all inputs and outputs required for the production of a unit of product, and GHG emissions factors for all inputs and outputs of the process.

The mass and energy balance for the pilot plant was provided by CENER, based on data recorded in the pilot plant (see section 4 for more information). The mass and energy balance for the theoretical commercial-scale plant was put together based on process modelling of the ButaNexT process at a larger scale, consultation with equipment providers, and literature values, as detailed in section 5.

GHG emissions factors used in the GHG assessment are detailed in section 3.4.
It is common practice in LCA studies, and allowed under ISO 14044, to use lower quality data or proxies for less relevant processes if data is not available. In this study a cut-off value of 0.1% of the overall GHG impact is used, so that data gathering efforts can be focussed on those processes which contribute the most significant portion of the overall burden.

3.4  GHG emission factors

3.4.1  Approach
GHG emission factors quantify the GHG intensity (in gCO$_2$eq.) of each input/output in the production process. The emissions factor of each input to the plant includes the emissions required to produce and transport that input to the butanol facility. The emissions factor of each output from the plant includes the emissions required to dispose of those outputs. Emissions from the manufacture of machinery and equipment were not taken into account, in line with the requirements of the RED methodology. Emission factors used in this study were obtained from the consortium partners or from literature sources.

Each GHG assessment, and therefore each emissions factor, is specific to given geographic area, a specific time-period, technology type etc. Emission factors used in this study were chosen to be as specific as possible to the technology used in biobutanol production. For the pilot plant, emission factors specific to Spain were chosen where possible, and if these were not available those specific to Europe were used. For the study on the commercial biobutanol plant, the location within Europe is not fixed so emission factors applicable to Europe were used. This has a particularly big impact in the case of electricity emissions factors, and is discussed in more detail in section 3.4.2.

For the purposes of this GHG assessment, which is carried out in line with the RED methodology, emission factors from the RED-compliant Biograce database (Biograce, 2015) were used where available, and where this was not possible other reputable scientific sources were used, including those contained in the Ecoinvent database. Where data from the Ecoinvent database were used, the global warming potential was calculated using the method: ReCiPe 2016 Midpoint (H) V1.00. Whilst the methodology for calculating global warming potential in ReCiPe 2016 is not exactly in line with that stipulated by the RED, for example a wider range of chemical emissions contribute to the global warming potential under the ReCiPe method, it is generally acceptable to use these emissions factors in RED-compliant GHG calculations where emissions factors calculated exactly using the RED-compliant method are not available. In the following sections 3.4.2 and 3.4.3 the source and justification of the emission factor used for each input and output is given.

3.4.2 Emission factors for process inputs

_Emission factors for Miscanthus_

In the literature, GHG emissions associated with Miscanthus vary between 0.5 gCO$_2$eq./MJ (Giuntoli et al., 2014) and 11.61 gCO$_2$eq./MJ (McCalmont et al., 2017). The emissions can even be negative in some cases if the Miscanthus sequesters soil organic carbon.

This range in reported GHG emissions is partially due to variations in cultivation method: because Miscanthus cultivation and harvesting is still a developing technology, there are a range of techniques that may be used, for example in terms of the amount of fertilizer used and type of equipment. Assumptions around soil organic carbon also contribute to the range of emission factor values for Miscanthus. Whether Miscanthus growth sequesters organic carbon in the soil depends on a number of factors, including the type of soil. For example, Miscanthus grown on carbon-depleted soils such as actively farmed cropland is more likely to sequester additional carbon in the soil. However, this sequestration would only occur for a 20 – 50 year period until the soil reaches sink capacity (Scown et al., 2012).

In order to account for the diversity of emissions factors for cultivation, 'low’ ‘middle and ‘high’ Miscanthus emission factors were used, as defined in Table 1. These are based on the range of values reported in
the literature. We did not include any scenario with negative GHG emissions for Miscanthus due to the large uncertainty and very site-specific nature of modelling soil carbon fluxes. These emission values include 100km of transport by truck, which would be the average collection distance if the feedstock was uniformly distributed in a 150km radius around the plant.

<table>
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<th>Scenario name</th>
<th>GHG emissions incl. transport (gCO₂eq./kg)</th>
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<tr>
<td>Miscanthus (Low)</td>
<td>16</td>
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<tr>
<td>Miscanthus (Med)</td>
<td>97</td>
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<tr>
<td>Miscanthus (High)</td>
<td>178</td>
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Table 1 Different Miscanthus emission factors used in the GHG calculation

Growing Miscanthus on arable land could cause that food production to be shifted to other currently-unused land. The GHG emissions associated with this ‘indirect land use change’ (ILUC) can be substantial. Deliverable D1 reviewed only Miscanthus grown on land that is currently un-utilised or marginal for butanol production, suggesting that there could be sufficient land of this type in Europe to supply a biobutanol plant. Therefore, in this study no ILUC emissions from Miscanthus cultivation are included. Moreover, inclusion of iLUC factors is not compulsory under the RED calculation methodology.

**Emission factors for straw**

Under the RED, zero emissions are assigned to agricultural residues such as straw, up to the first point of collection, since all GHG emissions from cultivation are attributed to the crop.

However, cereal residues can provide a valuable environmental service when left on the land, in terms of erosion control, nutrient recycling, maintaining soil structure and regulating water retention (Whittaker et al. 2014), and their removal can in some cases lead to adverse environmental impacts, including GHG impacts.

There are a number of ways in which straw removal from the land can contribute to GHG emissions:

- Additional GHG emissions due to additional nutrients required to replace the nutrients removed with the cereal residues, in order to avoid losses in grain yields.
- Avoided emissions if straw is removed from the land, because it does not break down and release N₂O into the atmosphere.
- Removing agricultural residues from the field can lead to lower levels of Soil Organic Carbon (SOC), which may lower the overall carbon sequestered in soil.

Whittaker et al (2014) assessed the GHG emissions of straw removal. The direct GHG emissions, which are composed predominantly of soil organic carbon losses and N₂O emissions, are 22.8 gCO₂eq./MJ. Compared to a ‘reference system’ where straw is chopped and left on the field, the authors conclude that the average GHG impact of straw removal is 27.8 gCO₂eq./MJ straw. However there is a large uncertainty in this data, particularly concerning the GHG impacts of the soil organic carbon change, which constitutes the majority of these emissions.

Generally other reviews of this subject, for example that carried out by Searle and Bitnere (2017) for the International Council on Clean Transportation point to the uncertainty in the net effect of residue removal on soil health and carbon storage in any one particular farm. What does seem certain is that to ensure the environmental benefits of cereal residues are maintained, some residue should be left on the field. Monforti et al. (2015) nevertheless assert that sustainable straw collection can be practiced in order to preserve soil organic carbon levels.

Therefore in this study, a straw base-case will be applied, assuming the straw has zero emissions at the point of collection, and adding emissions from baling (46.1 gCO₂eq./kg as given in the UK Solid and Gaseous Biomass Carbon Calculator) and 100 km transport by truck to give a GHG emissions factor of
straw as delivered to the biobutanol plant of 54.3 gCO₂eq./kg straw, 12% moisture. In a worst-case scenario, the GHG figure reported by Whittaker et al. (2014) will be used, combined with 100km of truck transport, to give a worst-case GHG emissions factor of 404 gCO₂eq./kg.

The ButaNexT partners have now decided to focus solely on straw as the most promising feedstock for biobutanol production (see Deliverable 4.2 for more discussion on this), therefore the RED-compliant straw GHG emissions of 54.3 gCO₂eq./kg will be used in the commercial-scale GHG assessment. Sensitivity on feedstock emissions will be applied only to the pilot-scale assessment.

**Emission factor for electricity**

The ButaNexT pilot plant is situated in Spain, therefore the emissions factor for Spain’s grid electricity was used in the GHG assessment of the pilot plant (352 gCO₂eq./kWh). This emissions factor was taken from Ecoinvent (2017).

In the GHG assessment of the theoretical commercial plant, the average GHG emission factor for Europe from Ecoinvent (2017) was used (447 gCO₂eq./kWh). In order to account for the variability of the electricity mix across different European countries, a range of electricity emissions factors was used in the sensitivity analysis to reflect the different impacts that might be incurred if the plant was located in different European countries (see section 5.3.3 for more information).

Actual GHG emissions from grid electricity change with policy decisions such as the phase-out of nuclear power and support for increased renewable generation capacity, which are observed in many European countries. Because the process to collect and process nationwide data on electricity emissions factors can be slow, the data available in LCA databases is often several years old. Ecoinvent currently offers the most up to date set of data covering all EU countries, based on IEA data from the year 2014. Whilst more up-to-date data is available for some particular countries, this harmonised data set across all countries was used here in order to ensure comparability between countries.

**Emission factors for nutrients**

In the pilot plant, a nutrient mixture called ¼ TYIR has been used, comprising yeast extract (2.5 g/L), tryptone (2.5 g/L), iron sulphate (0.025 g/L) and ammonium sulphate (0.5 g/L). The emission factor for ¼ TYIR is 4.4gCO₂eq./kg; it was calculated as the weighted average of the emission factors of yeast extract, iron sulphate, ammonium sulphate and process water from the Ecoinvent database. There was no emissions factor available for tryptone nor was a suitable proxy available, so this component was not included in the overall emissions factor for the pilot plant nutrients. The impact of this is anticipated to be significantly less than 0.1% of the overall emissions, based on the size of the change if the emissions factor for yeast extract were used instead, so well below the cut-off criteria.

In the theoretical commercial-scale plant, the nutrients would likely be a cheaper option than ¼ TYIR, for example corn steep liquor. Therefore for the nutrients used in the commercial-scale plant, a GHG emission factor for corn steep liquor obtained from the US Life Cycle Inventory (US LCI) database, and accessed via SimaPro is used: 9.09 gCO₂eq./kg.

**Emission factors for microorganisms**

Fermentation microorganisms for biobutanol production are inputs to the pilot plant. They are produced in Oxford by Green Biologics. Fermentation microorganisms are also required in the commercial plant, but in this case they would be produced on-site in seed fermenters. Therefore in the commercial plant a separate emission factor is not applied to the microorganisms – instead the emissions from the inputs required for their production (heat, power and nutrients) are accounted for separately.
Literature data on the GHG emissions associated with the production of microorganisms is sparse, as the production process tends to be proprietary, and is usually included on-site within a process. The microorganisms used in the pilot plant are grown on-site from lyophilised bacteria, which are produced by Green Biologics and sent to CENER by courier. Therefore, to estimate the emissions associated with the nutrients which enter the pilot plant, the emissions associated with transportation of lyophilised bacteria from Oxford-based Green Biologics (around 1% of the mass of nutrients that enters the pilot plant) are included. This is 1600km by air, equivalent to London to Madrid, and 470km by road, equivalent to Oxford to London and Madrid to Pamplona. This gives an emission factor of 18.4 gCO₂eq./kg microorganisms. A small amount of nutrients and energy for heating and stirring would be required when the microorganisms are produced. Given the small volume of microorganisms required as input to the pilot plant, and the fact that even when transport emissions are included microorganisms only constitute 0.07% of the overall GHG intensity, heating and stirring required for their production was not further investigated.

**Emission factors for enzymes**

A recent GHG assessment of similar enzymes to those used in the pilot plant (Pursula et al., 2016), which was carried out specifically on MetGen enzymes, calculates a cradle to gate lifecycle of the enzyme of 1.87 kg CO₂eq./kg enzyme. This value refers to the pure enzyme that comprises about 5% of the enzyme formulate which is used in the process. The enzyme formulate also contains 20% by weight of glycerol (also known as glycerine) and the rest is assumed to be water. This is a close approximation, validated by MetGen, because in reality the enzyme formulate would be different for every application. Emission factors from Ecoinvent are used for glycerine and water, so that a weighted average emissions factor of the enzyme formulate is calculated to be 782 gCO₂eq./kg enzyme formulate.

<table>
<thead>
<tr>
<th>Component</th>
<th>% composition by mass of enzyme formulate</th>
<th>Global warming potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enzymes</td>
<td>5%</td>
<td>1870 g CO₂eq./kg enzyme</td>
</tr>
<tr>
<td>Glycerine</td>
<td>20%</td>
<td>3442 g CO₂eq./kg glycerine</td>
</tr>
<tr>
<td>Water</td>
<td>75%</td>
<td>0.03 gCO₂eq./kg water</td>
</tr>
<tr>
<td>Weighted average total</td>
<td>782 gCO₂eq./kg enzyme formulate</td>
<td></td>
</tr>
</tbody>
</table>

Transport must be added on to this emissions factor to reflect the burden of transporting the enzyme from the factory to the butanol plant. For the pilot plant, the enzyme formulate is transported by air from Helsinki to Madrid, and by road from MetGen’s site to Helsinki and then from Madrid to Pamplona. Because of this substantial transportation burden, this brings the overall emission factor of the enzymes to 3,167 gCO₂eq./kg.

For the commercial plant, transport distance would depend on plant location. In order to minimise costs, the transport distance of the enzymes should not be too great in the commercial plant, and with increasing deployment of advanced fermentation technologies throughout Europe, it may be possible to source enzymes from a nearby location. Therefore in this study truck transport of 400km is modelled, which brings the overall GHG intensity of the enzymes to 815 gCO₂eq./kg.

**Emission factors for other inputs**

<table>
<thead>
<tr>
<th>Input</th>
<th>Emission Factor</th>
<th>Unit</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂SO₄</td>
<td>207.7</td>
<td>gCO₂eq./kg</td>
<td>Biograce v4d</td>
</tr>
<tr>
<td>NaOH</td>
<td>469.3</td>
<td>gCO₂eq./kg</td>
<td>Biograce v4d</td>
</tr>
</tbody>
</table>
### Emission factors for process outputs

#### Emission factor for biomass sludge

Biomass sludge is an output of the waste water treatment plant, and has been dewatered to 20% insoluble solids content (Steinwinder, 2011). It could be used as fertiliser, or dried further and used as a source of fuel in a biomass boiler. In some plants, sludge from AD can be dried using only waste heat from the process, and research is also ongoing to improve the efficiency of this process (Makela et al., 2017). Experiments suggest that biomass sludge from the pulp and paper industry can be dried using secondary heat (70°C) to between 19 and 68% solids content. Whether this could be achieved in the ButaNexT process depends on the heat integration around the plant. Therefore in the absence of concrete information on the feasibility of further drying and use of biomass sludge within the plant, it is assumed here that the sludge is not combusted on-site, and instead leaves the plant as a co-product. Therefore emissions are allocated to it on the basis of its energy content, as for all other co-products (section 3.2). Due to the low mass of this stream, and high moisture content, allocation of emissions results in a reduction in overall GHG emissions of butanol of roughly 3%.

Biomass sludge is only an output of the commercial-scale plant as there is no on-site waste water treatment in the pilot plant.

#### Emission factor for material waste, stones and dust

The emission factor for the disposal of inert material waste such as stones and dust is taken from Ecoinvent (1 kg Inert waste, for final disposal {CH} | market for inert waste, for final disposal | Alloc Def, S (of project Ecoinvent 3 - allocation, default - system) which results in an emissions factor of 7.84 gCO₂eq/kg waste material. A generic ‘EU-wide’ figure was not available, but this process is not anticipated to differ substantially between Switzerland and the rest of the EU. Even if the emissions factor in other regions was five times greater or smaller than Switzerland, the overall impact would be below the cut-off percentage.

This emission factor is applied to the material waste from both the pilot and commercial-scale plant.

#### Emission factor for brine

Brine is produced as a waste from waste-water treatment. It is composed primarily of water, with some dissolved salts and other impurities. The emission factor associated with its disposal is based on a generic waste-water treatment process available in Ecoinvent (Wastewater, average {CH} | treatment of, capacity 1.1E10l/year | Alloc Def, S) giving an emissions factor of 0.35 gCO₂eq/kg of processed brine. As for the emissions factor for waste, stones and dust, variation in the emissions factor between Switzerland and other European countries is anticipated to be small, and the overall impact on the result is small.

Brine is only an output of the commercial-scale plant as there is no on-site waste water treatment in the pilot plant. Nevertheless condensates are produced in the pre-treatment stage in the pilot plant. The emission factor for disposal of brine is used as a proxy for the GHG emissions associated with disposal of ‘condensates’ which is also a largely aqueous waste water stream.

#### Emission factor for ash

Ash is produced when the recalcitrant biomass is burned on-site (heat and power scenario A). The emission factor for treatment of this waste is obtained from the Ecoinvent database, for disposal of ash in landfill. Value: 19.95 gCO₂eq/kg (database entry: Wood ash mixture, pure {Europe without Switzerland} | treatment of wood ash mixture, pure, sanitary landfill | Alloc Def, S).
Ash is only an output of the commercial-scale plant as there is no on-site biomass combustion in the pilot plant.

**Emission factor for fermentation off-gas stream**

Off-gases from ABE fermentation consist of 3.95 mol CO₂ / mol butanol and 2.41 mol H₂ / mol butanol in a mixed gas stream (Jones and Woods, 1989). This stream is assumed to be a waste, as the gases are at low concentration and mixed with impurities. However no GHG emissions are allocated to this stream because the CO₂ is biogenic, therefore does not constitute a net GHG emission. Whilst hydrogen may have indirect GHG impacts in the upper atmosphere (Derwent et al. 2006), these are not currently modelled under the RED methodology. This approach is adopted for both the pilot-scale and commercial-scale GHG assessment, although a scenario around CO₂ capture is also investigated (section 5.3.4).

**Emission factors for other outputs**

The other outputs from the process are acetone, ethanol and recalcitrant biomass. These are all classed as co-products from the process, therefore emissions are allocated to them on a LHV basis, as outlined in section 3.2.

### 3.5 Plant mass and energy balances

In an LCA study, a life cycle inventory (LCI) of all of the process inputs and outputs is required. In the life cycle inventory all material and energy inputs and outputs to the process are expressed in terms of the functional unit. The greenhouse gas impact of each of these inputs and outputs are then assessed per functional unit, summing together to give the overall GHG impact per functional unit. The life cycle inventory is derived from the plant mass and energy balance, which describes the overall material and energy inputs and outputs of the process.

In section 4 the mass and energy balance of the pilot plant is described, which was used to derive the life cycle inventory of the pilot plant.

In section 5 the mass and energy balance of the conceptual commercial-scale plant is described, which was used to derive the life cycle inventory of the commercial-scale plant.
4 Mass and energy balance of pilot plant

The mass and energy balance for the pilot plant was put together based on information obtained from CENER pertaining to the integrated pilot plant constructed during the ButaNexT project. The product of the pilot plant is a mixture of aqueous ABE products – the different solvents are not separated from this mixed stream. Whilst it is possible to estimate the yield of butanol as a proportion of the total ABE yield (roughly 60% by mass of the aqueous ABE stream), the separation itself can be an energy-intensive process. Therefore, the mass and energy balance (and consequently the greenhouse gas assessment) is carried out on the basis of per kg of ABE products, to reflect only those processes that actually operate in the pilot plant.

In the pilot plant, all heat and steam demands are provided by electrically heated boilers, therefore all of the energy required by the process is provided by electricity. The electricity consumption per 100kg slurry, as provided by CENER, and the electricity consumption per kg ABE products, as used in the GHG assessment, is given in Table 4. The total electricity demand is 214 kWh/kg ABE products (Table 4). This is equivalent to 771 MJ/kg ABE products, or 1,100MJ/kg butanol based on the theoretical butanol yield.

Table 4 Energy balance in pilot plant.

<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-process</th>
<th>Electricity consumption (kWh/100 kg slurry)</th>
<th>Electricity consumption (kWh/kg ABE products)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chopper</td>
<td></td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td>Micronizing prototype</td>
<td></td>
<td>55</td>
<td>22</td>
</tr>
<tr>
<td>Soaking &amp; mixing</td>
<td></td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>Pretreatment</td>
<td>Boiler</td>
<td>176</td>
<td>71</td>
</tr>
<tr>
<td></td>
<td>Reactor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Enzymatic hydrolysis</td>
<td>Stirrer</td>
<td>141</td>
<td>57</td>
</tr>
<tr>
<td></td>
<td>Heating</td>
<td>80</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Boiler</td>
<td>166</td>
<td></td>
</tr>
<tr>
<td>Filter</td>
<td>Centrifugue pump</td>
<td>28</td>
<td>11</td>
</tr>
<tr>
<td>Fermentation</td>
<td>Decalcified water</td>
<td>not representative</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Compressed air</td>
<td>not representative</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Stirrer**</td>
<td>88</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Boiler</td>
<td>117</td>
<td>47</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>214</td>
<td></td>
</tr>
</tbody>
</table>

The mass balance from the pilot plant was obtained from deliverable D4.1 and updated by operational pilot plant data from CENER (Table 5). Rows in grey indicate theoretical yields that can be obtained from the fermentation broth (34kg ABE solvents / 330 kg LC biomass) and the pervaporation permeate (20kg ABE solvents / 330 kg LC biomass). Theoretical yields are used, because in the pilot plant complete purification and isolation of the product is never carried out. The yield of ABE solvents from LC biomass after pervaporation (0.06kg ABE solvents / kg LC biomass) was used as the theoretical ABE yield from which to calculate all GHG emissions.
<table>
<thead>
<tr>
<th>Process</th>
<th>Material</th>
<th>Input (kg)</th>
<th>Output (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mechanical pre-treatment</td>
<td>LC biomass</td>
<td>330.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Material losses</td>
<td>1.64</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(pre-treatment)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Soaking</td>
<td>Water (soaking)</td>
<td>262.68</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Acid catalyst</td>
<td>5.91</td>
<td></td>
</tr>
<tr>
<td>Thermochemical pretreatment</td>
<td>Steam</td>
<td>488.32</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Condensates</td>
<td>264.39</td>
<td></td>
</tr>
<tr>
<td>Enzymatic hydrolysis</td>
<td>Water (hydrolysis)</td>
<td>615.66</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Enzymes</td>
<td>28.73</td>
<td></td>
</tr>
<tr>
<td>Filtration</td>
<td>Material losses</td>
<td>71.83</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(filtration)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Solid cake</td>
<td>366.32</td>
<td></td>
</tr>
<tr>
<td>Fermentation</td>
<td>Nutrients</td>
<td>9.55</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Microorganisms</td>
<td>102.71</td>
<td></td>
</tr>
<tr>
<td></td>
<td>ABE products</td>
<td>33.83</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(theoretical)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Media</td>
<td>1044.30</td>
<td></td>
</tr>
<tr>
<td>Pervaporation</td>
<td>Permeate</td>
<td>95.08</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Butanol (theoretical)</td>
<td>14.22</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Acetone (theoretical)</td>
<td>5.33</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ethanol (theoretical)</td>
<td>0.83</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water (theoretical)</td>
<td>74.71</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>1843.56</td>
<td>1843.56</td>
</tr>
</tbody>
</table>

Table 5  Mass balance in pilot plant
5 Mass and energy balance of theoretical commercial-scale plant

This section outlines first the key methodological principles which have been followed in putting together the mass and energy balance for a conceptual commercial-scale plant. Then a summary of the mass and energy balance is provided, followed by detail on the key data sources and assumptions for each sub-process. Finally, a number of different scenarios are described, which are used to explore the range of results that could be obtained, given the uncertainty in modelling a substantially scaled-up plant based on technology which only operates at pilot-scale.

5.1 Key principles

5.1.1 Technology selection

The technology of the commercial—scale plant is assumed to be the same as in the ButaNexT pilot plant configuration, in order to provide a result that is most appropriate to the consortium and can be reasonably compared with the pilot plant. Nevertheless, the upscaling from pilot to commercial plant would modify some processes due to the requirements of operating at larger scale. Therefore each step in the conceptual commercial-scale process will reflect as closely as possible the ButaNexT process, to the extent that this is realistic at commercial-scale. The one exception to this, is in the inclusion of pervaporation as a separation technique after fermentation. The pervaporation process used in the pilot plant was developed specifically for the ButaNexT project and therefore does not yet operate at a larger scale. Nevertheless, given that it is a key innovation of the ButaNexT project, it has been included here. No distinction has been made between the equipment or process flows for Miscanthus compared to wheat straw, as data at this level of detail was not available.

5.1.2 Data gathering

The data for the mass and energy balance was gathered from a number of sources, in the following order of priority. It is indicated in brackets which subsections of the process were modelled using this type of data:

1. Process modelling of the technology used in the ButaNexT pilot plant, scaled up to commercial scale (fermentation, pervaporation, purification)
2. Information from equipment providers of commercial-scale equipment which is the equivalent to that used at pilot scale in the ButaNexT plant (milling, filtration)
3. Literature data or engineering studies (Feedstock handling and storage, pre-treatment, hydrolysis, waste-water treatment)

It should be emphasized that the aim of this data gathering exercise was not process optimization, but simply to provide a credible theoretical mass and energy balance for a commercial-scale butanol plant. In some cases, there were clearly trade-offs between, for example different choices of equipment or different processing conditions. In these situations we tried to reflect the most likely or most probable set-up, and highlight in sections 5.2.1 to 5.2.12 the key trade-offs that are made between the different options. Future engineering studies would likely focus on process optimization to achieve the best outcome, where such trade-offs exist.

5.1.3 Plant size

In earlier deliverables a commercial plant size of 50 ktonnes / annum of butanol was considered. However, given the current conversion efficiency of feedstock to butanol obtained in the pilot plant (7 kg butanol/kg wet feedstock), approximately 750,000 tonnes/annum of feedstock would be required to produce this amount. 750,000 tonnes/annum of feedstock is roughly double that processed by the largest existing ligno-cellulosic ethanol facilities; DuPont’s ligno-cellulosic ethanol plant (USA), for example, has capacity...
of roughly 400,000 tonnes wet/annum of corn stover (DuPont, 2015). Given the challenge of handling large volumes of feedstock, and the fact that substantial feedstock requirements can lead to long transport distances, which can adversely affect both plant economics and GHGs, it was decided to downsize the commercial plant to 450,000 tonnes/annum of feedstock input. This is a similar feedstock capacity to the largest ligno-cellulosic ethanol plants operating today.

5.2 Commercial-scale mass and energy balance

5.2.1 Mass and energy balance summary
The mass balance for the butanol process is summarized in Table 6, both in per unit biomass input and per unit butanol output.

<table>
<thead>
<tr>
<th>Mass Inputs</th>
<th>Mass flow (kg wet/tonne wet biomass input)</th>
<th>Unit mass flow (kg/kg butanol output)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ligno-cellulosic biomass</td>
<td>1,000.00</td>
<td>11.62</td>
</tr>
<tr>
<td>H2SO4</td>
<td>34.80</td>
<td>0.40</td>
</tr>
<tr>
<td>NaOH</td>
<td>30.45</td>
<td>0.35</td>
</tr>
<tr>
<td>Enzyme formulate</td>
<td>60.90</td>
<td>0.71</td>
</tr>
<tr>
<td>Nutrients</td>
<td>26.16</td>
<td>0.30</td>
</tr>
<tr>
<td>NaOH (WWT)</td>
<td>19.80</td>
<td>0.23</td>
</tr>
<tr>
<td>Water</td>
<td>54.27</td>
<td>0.63</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mass outputs</th>
<th>Mass flow (kg wet/tonne wet biomass input)</th>
<th>Unit mass flow (kg/kg butanol output)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stones and dust</td>
<td>4.98</td>
<td>0.06</td>
</tr>
<tr>
<td>Solid cake (recalcitrant bior</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Butanol</td>
<td>86.10</td>
<td>1.00</td>
</tr>
<tr>
<td>Acetone</td>
<td>33.21</td>
<td>0.39</td>
</tr>
<tr>
<td>Ethanol</td>
<td>3.69</td>
<td>0.04</td>
</tr>
<tr>
<td>Waste brine</td>
<td>54.27</td>
<td>0.63</td>
</tr>
<tr>
<td>Biomass sludge</td>
<td>36.18</td>
<td>0.42</td>
</tr>
<tr>
<td>Biogas</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Ash</td>
<td>15.04</td>
<td>0.17</td>
</tr>
<tr>
<td>Off-gas</td>
<td>207.63</td>
<td>2.41</td>
</tr>
</tbody>
</table>

The overall power demand of the process is 22MJ/kg butanol produced, and the overall heat demand is 43MJ/kg butanol produced. For comparison, the overall energy demand of the pilot plant, in terms of electricity required for both heat and power, is 1,100 MJ/kg butanol.

In the following sections the data sources and assumptions that lie behind this mass and energy balance are described in more detail, taking each key element of the plant in turn, as shown in Figure 7.
5.2.2 Feedstock handling
Feedstock handling is required to get the feedstock from delivery trucks into the plant. The modelled commercial plant will require an input of around 57 tonnes/hour of biomass, based on the plant size (section 5.1.3). Therefore unlike at the pilot plant, a system of feedstock storage, conveyors and feeders will be required to process such large volumes of feedstock. Across this process, material losses of 0.5% (by mass) are assumed, based on the work carried out by TR. The power requirement for the equipment is taken from a similar system reported in the literature, 8.26 kWh/tonne wet biomass (Humbird, 2011). No material inputs apart from the biomass itself are required for feedstock handling.

5.2.3 Feedstock drying
Experiments in the pilot plant were carried out on feedstock with moisture content of 10%, but discussions with suppliers of lignocellulosic-biomass indicated that they usually supply biomass at around 15% moisture content. Whilst developing the milling equipment for the ButaNexT project, Technicas Reunidas (TR) considered biomass with a maximum moisture content of 12%. Therefore 12% was chosen as the average moisture content of the biomass modelled for this study.

A feedstock drying step is not included within the plant mass and energy balance. Miscanthus moisture content at harvest depends on a wide range of factors, but in-field drying can reduce the moisture content to at least 15%, and likely to 12%. Similarly, the moisture content of straw at collection may be high or low depending for example on weather conditions, but natural drying of straw in the field can generally reduce this to ~10% (Zhang et al., 2012). Drying prior to pre-treatment is also not assumed necessary in other published LCAs, such as Wang et al (2013), and JEC (2014).

5.2.4 Mechanical pre-treatment
Mechanical pre-treatment reduces the size of the biomass particles to enable more effective downstream processing. It is assumed that biomass is delivered to the plant with a length of 50mm (i.e. some chopping has been carried out at the point of collection of the feedstock). Under this assumption, a single-stage of milling is required to reduce the size to 0.5mm, using technology based on that developed by Tecnicas Reunidas for the ButaNexT project.
Based on information provided by TR on their milling equipment, material losses of 0.5% (wt.) and power use of 40 kWh/tonne of wet biomass processed, are used in this assessment.

5.2.5 Thermochemical pre-treatment

Thermochemical pre-treatment breaks down the biomass to release sugars for fermentation. Existing commercial pre-treatment processes tend to be unique to the companies who have developed them and highly confidential. There are also a wide range of pre-treatment techniques which can potentially be used, including acid, hot water, alkali, and steam explosion (or combinations of these) (Kumar and Murthy, 2011). In the ButaNexT pilot plant, a process of soaking, followed by acid and stream treatment at high pressure is used, although development and optimisation of this process has not been a focus of the ButaNexT project. Therefore, for the purpose of modelling thermochemical pre-treatment for commercial butanol production, a process similar to that used currently in the pilot plant is assumed, requiring sulphuric acid, steam and pressure.

Mass and energy requirements for thermochemical pre-treatment were estimated by CENER based on experience operating the pilot plant. Water is added to the milled biomass to bring it to 50% moisture content. H2SO4 at 2wt.% concentration is required, in a ratio of 0.02kg acid/kg wet biomass (at 50% moisture content). It was estimated by CENER that the electrical energy required for the screw-feeder would be 675kW, and the electrical energy required for each of the three reactor vessels would be 45kW. Whilst only one screw-feeder is required, three reaction vessels with a residence time of around 3 minutes in each would be required. Heat energy required to heat the reaction to 175°C is 9.2MW (162 kWh/tonne wet biomass). This is supplied in the form of steam.

The heat demand in pre-treatment is substantial, but is also a significant source of uncertainty in the data, given the limited published literature. Humbird (2011) models a comparable dilute-acid pre-treatment process for the production of ligno-cellulosic ethanol, and estimate that roughly 33kWh heat/tonne wet biomass is required. This is 79% lower than the value estimated by the ButaNexT partners. Given the large variation in process configurations that can be used for pre-treatment, moisture content, and the fact that no heat integration or optimization studies have been carried out on the commercial ButaNexT process, this large difference does not seem unrealistic. Nevertheless, whilst figures provided by the ButaNexT consortium were used in the ‘baseline’ assessment, sensitivities are explored around reducing both heat and power demand of the process (see section 5.3.2).

5.2.6 Enzymatic hydrolysis

Enzymatic hydrolysis further breaks down polymeric sugars to provide monomeric sugars for fermentation. In the ButaNexT pilot plant, hydrolysis is followed by filtration to remove the insoluble solids, and by fermentation with in-situ pervaporation. Filtration is required, because it is likely that the presence of insoluble solids in the fermentation broth would reduce the efficiency of the pervaporation, and could damage the membranes. Given that the use of in-situ pervaporation is a key aspect of the commercial-scale butanol process modelled here, filtration must also be included at commercial scale, between the hydrolysis and fermentation steps.

It should be noted that in some commercial ligno-cellulosic fermentation processes, hydrolysis and fermentation happen simultaneously, which can allow for lower investment costs as fewer separate vessels are required, and can increase hydrolysis yields by the continual removal of sugars (Paulova et al., 2015). There can also be drawbacks to this approach, for example due to the presence of solids in the fermentation broth. This simultaneous hydrolysis and fermentation setup could be investigated further in future work, but has not been considered here, so a filtering step was also included in the commercial plant (See section 5.2.8). The fermentation step is further detailed in section 5.2.9.

Hydrolysis is a challenging stage in the lignocellulosic-butanol production process. The initial slurry is extremely viscous, which makes it difficult to mix in order to obtain the required conditions for enzymatic activity, such as oxygen transfer into the bulk mixture. Adding additional water to reduce solids content
can mitigate this problem, but creates a higher-volume of hydrolysate with a lower concentration of sugars and therefore a higher demand for distillation capacity downstream. There is therefore a trade-off (both in terms of cost and energy use) between adding water to facilitate the hydrolysis process, and increasing the volume of the reactant.

The time over which the hydrolysis reaction takes place is also a trade-off, as longer reaction times generally give a higher yield of sugars, but require a larger number of hydrolysis vessels and more power for stirring.

It is clear therefore that the equipment and process design of the hydrolysis process is crucial in maximising the efficiency and minimising overall costs. However, the scope of this report is not to conduct such optimisation. Therefore for the purposes of this study an indicative process has been assumed which broadly represents a commercial hydrolysis process.

For the purposes of this study, a hydrolysis process lasting 72 hours is modelled, with a slurry at initial solids loading of 20% (by mass), which corresponds to a very high viscosity. As the hydrolysis process progresses the viscosity decreases and it becomes easier to mix. A two-stage process is adopted, whereby for the first 24 hours the mixture is split across a large number of smaller vessels, with a high power demand for stirring (2 kW/m$^3$). For the remaining 48 hours the mixture is transferred into larger vessels with a lower power demand for stirring (1kW/m$^3$). Power requirements for stirring were estimated from standard engineering estimates (Dalian University, 2010).

There is ongoing work on the design of the hydrolysis reactor in order to improve the efficiency of the process and reduce the power required for mixing, as this can be substantial with such a viscous reaction mixture. For example, in Humbird (2011), a design is given for a continuous high-solids reactor which is an empty tower with the slurry entering at the top and flowing down with gravity, with minimal power requirement for mixing. The residence time in this first stage is 24 hours, and then the slurry is batched to one of a number of smaller reactors where hydrolysis continues for another 60 hours, with much lower power requirements for stirring.

Therefore it is possible that improvements in equipment and process design could further reduce the power required for stirring during hydrolysis, and this is addressed in section 5.3.2.

It is assumed that the sugars concentration in the hydrolysate after hydrolysis is 150 g/L, which is judged to be a realistic and achievable yield to attain, if the process conditions and equipment are optimised at commercial scale. For comparison, in the pilot plant a yield of 110 g/L has been achieved with a solids content of 20% during hydrolysis.

5.2.7 Production of hydrolysis enzymes

Hydrolysis enzymes can either be produced on-site at a ligno-cellulosic biofuels plant, or brought in from a specialist supplier. Both of these options have been implemented in existing commercial ligno-cellulosic ethanol plants to-date. On-site enzyme production is likely to require higher-capital expenditures (capex) and lower operational expenditures (opex) compared to buying enzymes from an external supplier. The most optimal is likely to be specific to the particular plant and process. Given that raising financing for capex can be challenging for first-of-a-kind plants this assessment assumes that hydrolysis enzymes are brought in from an off-site supplier.

On-site production could offer some advantages, but has not been further investigated in this study. For example, Clariant’s sunliquid process, which is currently the subject of an FP7 grant for construction of an industrial-scale demonstration plant, proposes on-site enzyme production. This allows lower overall production costs and insulation from supply shortages and price volatility (Sunliquid, 2017). DSM state that on-site enzyme production enables use of carbon sources that are already available on-site and
remove several steps such as formulation and packaging of the enzymes, hence results in lower costs (Pel, 2015). Construction of an on-site enzyme manufacturing process for the POET-DSM project Liberty plant in Iowa was announced in February 2017 and is currently underway.

5.2.8 Filtration
In the pilot plant a filter press is used to filter the hydrolysate prior to fermentation, in order to separate out the liquid hydrolysate from the solid recalcitrant biomass. The recalcitrant biomass is composed largely of lignin and un-hydrolysed sugars, with more detail available in Deliverable D2.6. At commercial scale there are several options for the exact filtration equipment that should be used, including filter press, vacuum belt filter and centrifuge. After filtration some hydrolysate, containing dissolved sugars, remains in the solid fraction. This can be removed by washing this solid fraction with water, but a trade-off exists because washing also dilutes the sugars, lowering the fermentation yield and increasing the energy required to evaporate off the water in distillation.

Sievers et al., 2014 evaluated technical and economic trade-offs in choosing different lignin separation technologies, investigating the use of pressure filtration, vacuum filtration and basket centrifugation to separate insoluble solids from a dilute-acid pre-treated corn stover slurry. They exclude the centrifuge from their economic analysis as its capital cost per unit area was an order of magnitude higher than the pressure and vacuum filtration techniques. They conclude that the vacuum belt filter is lower cost than the pressure filter, and that a wash ratio of 2 is the lowest cost option across a whole biorefinery. There are some differences in the process modelled in this paper compared to the ButaNexT process, for example simultaneous hydrolysis and fermentation is assumed in Sievers et al., so the conclusions should be treated with some caution.

Figure 8 illustrates how increasing washing reduces the amount of solute remaining in the solid fraction, where the wash ratio W is defined as:

\[
\frac{\text{volume of wash water used (L)}}{\text{cake liquid volume (L)}}
\]

![Fraction of solute remaining in filter cake as a function of wash water use for a range of different filtration techniques (Sievers, 2014).](image)

Filtration technology providers contacted for this assessment recommended use of a filter press, and provided data on power use of such equipment. They claimed to be able to reduce the moisture content of the insoluble solids fraction to 39%, but literature sources tended to estimate a higher possible moisture content.
content of around 60% to 70%. Therefore for this modelling exercise an average value of 50% moisture content is assumed. A wash ratio of 2.5 is used, which results in a high recovery rate of sugars.

Further studies would be required to optimise the choice of filter technique and the amount of water added in the washing stage. Some academic work has been carried out on this already, for example by Sievers et al. (2015).

5.2.9 Fermentation
In the commercial-scale plant, it is assumed that fermentation takes place in four fermenters operating in parallel on a staggered 100-hour cycle. This is based on the fermentation set-up currently operated in commercial ethanol plants, the corn butanol plant run by Green Biologics, and the expertise of Green Biologics fermentation engineers.

As an alternative configuration, a two-stage fermentation, with two fermentation tanks in series, was discussed with the ButaNexT partners. The second fermenter could be used to fully consume the xylose (a five-carbon sugar), and would in addition increase the concentration of solvents in the fermentation broth, therefore reducing the demands on downstream processing and purification. However this was not tested in the pilot plant, and is not examined further in this study.

The theoretical yield of the fermentation process is roughly 0.4kg of ABE solvents / kg of sugars. Based on the yields achieved in the pilot plant, the consortium agreed that a yield of 0.3kg\text{ABE/kg sugars} represented a realistic and achievable yield for the commercial-scale plant. Therefore in the theoretical commercial-scale butanol plant modelled in this study, a yield of 0.3kg/kg has been modelled, with the ratio of butanol:acetone:ethanol at 70:27:3.

A ‘high-yield’ scenario has been investigated (see section 5.3.2), incorporating an overall yield of 0.35kg ABE solvents / kg sugars and a B:A:E ratio of 78:20:2. This is considered optimistic but achievable with further technology development.

As well as the ABE solvents, CO$_2$ and hydrogen are also produced during fermentation, in a ratio of 3.95 mol CO$_2$/mol butanol and 2.41 mol CO$_2$/mol butanol respectively (Jones and Woods, 1986). Capture of these off-gases has not been practiced in the pilot plant, so in the base-case for the commercial-scale plant no capture is assumed. A scenario is investigated where CO$_2$ capture is implemented (section 5.3.4). The hydrogen is at low concentrations, so hydrogen capture and use is not investigated in this study, but it could be a useful extension of this work.

In a commercial fermentation plant, the microorganisms that carry out the fermentation must be grown in a series of smaller vessels known as seed trains. Generally they are grown in the same fermentation media that is used to produce the alcohol. Given the fermentation setup outlined in section 5.2.9, it is estimated that 2 seed trains would be required, with each seed train having 5 vessels: two at lab scale, one at 1000L, one at 10,000L and one at 100,000L. Nutrients required by the seed trains are assumed to be corn-steep-liquor. Electricity requirements for stirring is estimated to be 1kW/m$^3$ for the three largest vessels. Any additional low-temperature heating that might be required by the seed train vessels is assumed to be provided by waste heat from elsewhere in the plant.

5.2.10 Pervaporation
The in-situ pervaporation technology used in the commercial-scale plant is used to separate out the ABE solvents (along with some water) from the fermentation vessel. This separated stream is known as permeate. The pervaporation technology assumed in the commercial-scale plant is based on that developed for the pilot plant over the course of the ButaNexT project, using a poly(octyl methyl siloxane) (POMS) membrane. There are some technical challenges in scaling up the pervaporation membranes to the required scale. In particular, Integration of the required pervaporation surfaces with the fermenters is
still challenging as temperature and concentration gradients along the length of the module will lead to decreased solvent fluxes. These challenges have been discussed and addressed by project partners VITO in other deliverables.

The mass and energy flows through the fermentation-pervaporation process were based on process modelling carried out by VITO (van Hecke, 2015; van Hecke, 2018). Electricity is required for operating the vacuum pump for the pervaporation unit (2MJ electricity / kg butanol), and for chilling water for the condensers (5.07MJ/kg butanol).

5.2.11 Separation and purification

Purification is required to remove water from the ABE solvent stream, and to separate out the individual solvents. In the pilot plant, purification was not carried out, therefore in the GHG assessment for a theoretical commercial plant, the technology used for purification is based on that modelled by VITO for a commercial-scale butanol plant (van Hecke, 2015). Under this set-up, the permeate from the pervaporation units is sent to a series of distillation towers to separate out the acetone, butanol and ethanol. The effluent from the fermenters is treated in a beer stripper, with remaining solvents sent back into the distillation towers, and the solvent-depleted bottom stream sent to a multiple-effect evaporator. Under this setup, the steam use for fermentation, pervaporation and butanol purification is 36.6MJ/kg butanol.

5.2.12 Waste water treatment

First generation biobutanol production facilities using conventional sugars as feedstocks tend to be reuse most water within the plant, with very little waste. Purification of the water can be done by reverse osmosis (RO) or by filtration, as the waste water is generally not too contaminated. The solid waste stream from waste water treatment, containing dead organisms and spent fermentation media (undigested sugars and minerals) can be sold as fertilizer.

However, literature sources suggest that the waste-water streams from lignocellulosic ethanol plants are likely to be substantially more challenging to treat, due to the high level of inorganics such as fertilizers that are typically found on the non-food portion of a crop, and the chemicals that are added in pre-treatment to overcome biomass recalcitrance (Humbird, 2011). Indeed Luiz et al. (2014) suggest that in cellulosic ethanol production wastewater treatment can account for 20 – 33% of the total process cost.

Therefore for the purposes of this study, waste water treatment is modelled on that outlined in Steinwinder et al., (2011) which was developed specifically for a techno-economic study on a cellulosic ethanol plant. It requires anaerobic treatment to remove the organic material (represented by a reduction in COD), aerobic treatment to further remove organic material and remove some inorganics, reverse osmosis for salt removal, and sludge dewatering. Two streams undergo waste water treatment: the waste stream from thermochemical pretreatment, and the wet fermentation broth solids (FBS) from biobutanol purification. It is known that operating cellulosic ethanol plants, such as that operated by Poet-DSM, also use anaerobic digestion for water purification at their plant (Dishman, 2017).

For the biobutanol production process modelled here, it was estimated that the wet FBS stream, after multiple-effect-evaporation of fermenter effluent, has a COD of roughly 130,000ppm. When diluted by the other input stream to the wastewater treatment plant, from pre-processing, the total COD of treated water is estimated to be 41,000ppm. Electricity and chemical requirements, and outputs of biogas are calculated from Humbird (2011) by scaling from the waste-water treatment plant modelled in that study for processing an input stream of 64,000ppm COD. It is assumed that of the water treated in the waste water plant, 90% is recovered as water for reuse within the plant, 5% by mass as sludge (79% moisture content) and 5% by mass as purge water. The purge water must be disposed of, and the sludge may be used as fertilizer, as noted in section 3.4.3. It may be possible to further dry the sludge and use it in the combustor as fuel.
for the plant, however this would likely require a substantially higher power load for drying, and has not been investigated further here.

5.3 Scenarios

Due to the uncertainties in modelling the GHG intensity of commercial-scale biobutanol production given that the technology is currently at an early stage of development and only operational at pilot scale, a number of scenarios have been investigated. These are detailed in the following sections.

5.3.1 Energy supply scenarios

The commercial biobutanol plant has a substantial electricity and heat energy demand, and there are a number of options for energy supply to the plant. Whilst in the pilot plant all heat and power needs are satisfied by grid electricity, this would be highly unlikely in a commercial-scale plant, and alternative options must be examined here. In a commercial plant, the decision of how to provide heat and power is likely to depend on a number of factors including the local availability and price of electricity, heat and other fuels; the electricity and heat demand profile of the plant; and the required balance between capex and opex costs. It should be noted that these energy supply scenarios only apply to the commercial-scale plant: in the pilot plant all heat and power needs are supplied by grid electricity.

In this commercial plant model, four energy supply scenarios have been tested, labelled A to D. All four options fulfil the heat demand of the plant, as purchase of steam requires co-location with an industrial steam producer, which is not necessarily possible. Each scenario also fulfils some or all of the plant electricity demand, with the remainder of the power demand fulfilled by grid electricity if required.

Option A: Combined heat and power from by-products

In ligno-cellulosic butanol production, there is a substantial by-product stream of recalcitrant biomass, which is composed largely of lignin and undigested sugars (see deliverable 2.6 for full details). This stream has a relatively high calorific value, and can be combusted to provide heat and power to the plant. Biogas is also produced in the anaerobic digestion plant, which can be used as a source of energy in the plant.

In heat and power option A, the recalcitrant biomass and biogas are burned in a boiler to generate steam. This is used to provide all the heat required by the plant. Remaining steam is used to generate electricity in a steam turbine, and the rest of the electricity required in the process is provided by the grid.

Humbird (2011) estimated the thermal conversion efficiency of a boiler combusting wet solids and biogas, to be roughly 80%. The thermal boiler conversion efficiency of a moving bed boiler is typically 70 – 85% (LHV basis) with the lower efficiencies applicable when the biomass has high moisture content and there is no heat recovery system on the boilers (ETI, 2017). For this plant, thermal efficiency of biomass conversion to steam is assumed to be 80%. The amount of power that can be generated from the biomass is very sensitive to the moisture content of the biomass. When it exits the filtration step, the recalcitrant biomass is at around 50% moisture, but use of waste heat is likely able to dry this to around 40% moisture content (Sosa-Arnao et al., 2006).

Electricity production from steam was assumed to be 0.31MJ\textsubscript{electricity}/MJ\textsubscript{steam} based on industry data. The efficiency of this step is limited by the small size of the equipment – high efficiency turbines such as those based on ultra-critical steam are unlikely to be possible at this scale. It should be noted that this set-up is a worst-case-scenario in terms of heat integration of the plant, assuming that all steam required by the plant is at high temperature and pressure, and therefore cannot be used to generate electricity first. In reality, steam would likely be used in the turbine to generate electricity, and then re-used in the plant at lower temperature and pressure to provide process heat. This conservative assumption is challenged, and an improved scenario suggested, in the ‘Low Heat and Power Demand Scenario’ (section 5.3.2).
Option B: Gas boiler + steam turbine CHP

Heat and power option B uses natural gas to fuel the boiler instead of biomass (Option A). The gas boiler generates steam to cover the heat demand of the plant at 85% efficiency, with electricity generated via a steam turbine to cover the whole electricity demand of the plant.

As with option A, the overall plant efficiency is conservative, assuming no steam re-use in the plant.

Option C: Gas Boiler + imported electricity

Option C aims to investigate the impact of generating solely process heat on-site from a gas boiler at an efficiency of 85%, while all electricity into the plant would come from the grid.

Option D: Gas turbine

Option D models a gas turbine CHP operating at a net electrical efficiency of 28% and thermal efficiency of 47% (LHV basis). With these efficiencies fixed, it is sized to meet the steam demand of the plant. In order to supply the heat to the plant, excess electricity is generated, which is exported to the grid.

5.3.2 Plant performance scenarios

Because of the large scale-up from pilot-scale to commercial-scale, there is substantial uncertainty in the theoretical commercial-scale ButaNexT mass and energy balance, for example in accounting for improved efficiency due to larger scale equipment, and in terms of the yield improvements that could be achieved in a fully optimised process. In order to explore the likely range of GHG emissions of butanol produced in a commercial plant, it is therefore important to explore a number of different scenarios around plant performance.

Low heat and power demand

It is likely that some thermal energy can be recovered and reused in order to lower the overall heat demand of the process, for example by re-using low-grade heat in distillation, which does not require very high temperature or pressure steam. It was estimated by discussion with process engineers that a heat energy reduction of 20% could be achieved in large thermochemical plants such as the commercial-scale ButaNexT plant by heat integration across the process. Therefore in this ‘low heat and power demand’ scenario the heat demand is 20% lower compared to the baseline.

Due to the wide range of process set-up and equipment types that could be used in the commercial biobutanol plant, there is also substantial uncertainty around the electricity demand that is used as a baseline in this study. Novel equipment and more optimised plant operation could realistically decrease the electricity demand. In this ‘low heat and power demand’ scenario, the electricity demand is assumed to be 10% lower than the base case.

High conversion efficiency

The high conversion efficiency scenario was developed in order to understand the impact of further improving yields of sugars from biomass, yields of ABE from sugars, and increasing the proportion of butanol produced relative to acetone and ethanol. The difference in these parameters between the baseline and the ‘high conversion’ scenario is outlined in Table 7. This high conversion efficiency scenario was considered by the consortium to be optimistic, but achievable if the process was fully optimised at commercial scale.
Table 7: Changed parameters in high conversion efficiency scenario

<table>
<thead>
<tr>
<th></th>
<th>Baseline scenario</th>
<th>High conversion scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sugars yield (kg sugars/kg biomass (wet))</td>
<td>0.41</td>
<td>0.55</td>
</tr>
<tr>
<td>ABE yield (kg ABE/kg sugars)</td>
<td>0.3</td>
<td>0.35</td>
</tr>
<tr>
<td>Ratio between products (butanol:acetone:ethanol)</td>
<td>70:27:3</td>
<td>78:20:2</td>
</tr>
</tbody>
</table>

These improvements outlined under section 5.3.2 are known as ‘plant performance scenarios. They are combined with all of the possible ‘energy supply scenarios’ to create 16 possible unique scenarios, outlined in Table 8.

Table 8: Summary of energy supply scenarios and plant performance scenarios

<table>
<thead>
<tr>
<th>Plant performance scenario</th>
<th>Heat and power scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Baseline</td>
<td>A1 (biomass boiler + steam turbine)</td>
</tr>
<tr>
<td>2 Low heat and power demand</td>
<td>A2</td>
</tr>
<tr>
<td>3 High conversion efficiency</td>
<td>A3</td>
</tr>
<tr>
<td>4 Low heat and power demand, and high conversion efficiency</td>
<td>A4</td>
</tr>
</tbody>
</table>

5.3.3 Electricity emission factor scenarios

As noted in section 3.4.2 the emission factor of grid electricity varies substantially between different European countries. Therefore a sensitivity analysis was performed to assess the impact of using grid electricity of France (51 gCO₂eq./kWh), the Netherlands (606 gCO₂eq./kWh) and Poland (999 gCO₂eq./kWh), compared to the European average (447 gCO₂eq./kWh). These countries were chosen as they were identified as having substantial feedstock supply potential in deliverable D6.1, and they represent a range of GHG intensity for grid electricity across Europe: France is one of the lowest with a high share of nuclear power, and Poland is one of the highest as it has a high share of coal power.

5.3.4 CO₂ capture and sequestration scenario

Fermentation produces a relatively pure CO₂ stream which could in theory be captured and re-used or sequestered. As this is biogenic CO₂ this would represent a net CO₂ sequestration, or a negative GHG impact on the overall biobutanol GHG intensity. Currently several 1st generation ethanol plants in Europe capture CO₂ and use it for example in the fizzy drinks industry to displace fossil CO₂. Whilst this is strictly carbon capture and re-use, not carbon capture and sequestration, they are in some cases able to claim a ‘GHG credit’ for displacing fossil CO₂ which would otherwise have been used in this application. In this study carbon sequestration is assumed.

In the CO₂ sequestration scenario examined in this study, some additional power is required in order to capture it. Based on the CO₂ capture process in ethanol plants, this is assumed to be: 900MJ/tonne CO₂ sequestered. 90% of the CO₂ produced is assumed to be captured and sequestered. This is very much a
theoretical scenario, as little information was available on the purity of the CO\textsubscript{2} stream from the ABE fermentation process, how the electricity demand for CO\textsubscript{2} capture from ABE fermentation off-gas might compare to CO\textsubscript{2} capture from other processes, what percentage of CO\textsubscript{2} might be able to be sequestered, and the cost impact of doing so. Nevertheless, it aims to illustrate the magnitude of the impact that CO\textsubscript{2} capture and sequestration could have on the overall carbon intensity of the biobutanol.
6 Results
In this section the results of the GHG assessment of biobutanol produced within the pilot plant as part of an acetone, butanol, ethanol (ABE) mixture are presented (section 6.1) and the GHG assessment of biobutanol produced in a conceptual commercial-scale plant are presented in section 6.2.

6.1 Butanol production in pilot plant

6.1.1 Contribution Analysis
The key contributing factors to the GHG emissions of the ABE solvents, when Miscanthus is used as a feedstock and the central emission factor for Miscanthus is used, are: the electricity used in the process, feedstock cultivation, harvesting and transport, and enzymes (Figure 9). The contribution from each of these elements to the overall GHG intensity of biobutanol is 95% electricity, 3% enzymes and 1% feedstock.

![Figure 9 Split of GHG emissions of ABE produced in pilot plant](image)

A breakdown of where the electricity is used within the pilot plant is provided in Figure 10, demonstrating that demand is spread fairly evenly across the different stages of the production process.

![Figure 10 Breakdown of electricity use within biobutanol pilot plant](image)
Figure 11 illustrates the GHG emissions of the ABE solvents produced in the ButaNexT pilot plant, excluding those from electricity in order to provide greater granularity. A feedstock emissions factor of 96.5 gCO₂eq./kg is used, which is reflective of the ‘Miscanthus_medium’ scenario (see also Figure 13). Figure 11 illustrates that when electricity is excluded, over 97% of the emissions result from enzymes and the biomass feedstock. Nutrients, microorganism and the disposal of wastes account for the rest.

When the emissions from electricity supply to the process are added (Figure 12), they dwarf all other emissions, and give a GHG emission factor of the ABE stream that is well above that of the RED comparator (83.8 gCO₂eq./MJ). As noted above, all heat and power is provided to the pilot plant by grid electricity. Because the focus of the pilot plant was on proving production volumes and yields, no effort has been made to reduce or optimise the heat or power demand from the plant. Moreover, electric heating using grid electricity is expensive and GHG-intensive so would not be used at commercial-scale. Therefore whilst the breakdown of emissions from ABE produced in the pilot plant demonstrates that future work should focus on reducing the energy use of the process, the very high overall emission factor given in Figure 12 is not representative of the biobutanol emissions that would be anticipated in a commercial-scale plant.
Figure 12 GHG emissions associated with ABE products produced in ButaNexT pilot plant

This result was obtained using an electricity emissions factor specific to low-voltage electricity from the Spanish grid, as the pilot plant is located in Spain, which has an emission factor of 352 gCO₂eq./kWh. A lower emission factor of the grid, as for example in France or Sweden, could lower this emission factor substantially. However as this assessment is specific to the pilot plant established in Spain, and as the overall result is not representative of commercial biobutanol production, this is not explored further here. For the same reason none of the energy and performance scenarios investigated for the commercial biobutanol plant (sections 5.3 and 5.3.2) are examined in the context of the pilot plant.

6.1.2 Sensitivity: different feedstock types

A sensitivity assessment was carried out in order to analyse the impact of different feedstock GHG emissions on the emissions of biobutanol produced in the pilot plant, using the range of GHG emission values discussed and defined in section 3.4.2 (Figure 13). The emissions from electricity provision are not included within this figure, so that the impact of the changing character of the LC biomass can be seen.
Figure 13 illustrates that GHG emissions of biobutanol from straw and Miscanthus are similar, when calculated according to RED methodology. The straw worst-case scenario is not in-line with RED methodology, and indeed such high GHG emissions can likely be avoided if sustainable straw collection practices are followed (see section 3.4.2). There is a range of possible emission factors associated with Miscanthus cultivation, as commercial cultivation is not currently widespread. Best-practice for cultivation should be followed in order to achieve the low GHG emissions seen in the ‘Miscanthus low’ scenario.

6.2 Commercial-scale butanol production

In this section the results of the GHG assessment of the theoretical commercial-scale biobutanol plant are presented. As described in section 5, the mass and energy balance of the commercial-scale plant is based on the technology used in the pilot plant, but due to the significant difference in scale and technology used, comparison between the GHG intensity of biobutanol produced in the commercial-scale plant (section 6.2) and biobutanol produced in the pilot plant (section 6.1) is not appropriate.

The GHG assessment of biobutanol produced in the conceptual commercial-scale plant is structured around the plant performance scenarios and the heat and power scenarios, as outlined in section 5.3.1 and 5.3.2, and summarized in Table 9.

Table 9 Summary of scenarios

<table>
<thead>
<tr>
<th>Plant performance scenario</th>
<th>Heat and power scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A (biomass boiler + steam turbine)</td>
</tr>
<tr>
<td>1 Baseline</td>
<td>A1</td>
</tr>
<tr>
<td>2 Low heat and power demand</td>
<td>A2</td>
</tr>
<tr>
<td>3 High conversion efficiency</td>
<td>A3</td>
</tr>
<tr>
<td>4 Low heat and power demand, and high conversion efficiency</td>
<td>A4</td>
</tr>
</tbody>
</table>

In section 6.2.1 the key contributing factors to the biobutanol GHG emissions under the ‘Baseline’ plant performance scenario are analysed, across heat and power scenarios A to D. In the following sections 6.2.2 to 6.2.4 plant performance scenarios 2, 3 and 4 are also examined, with a summary provided in section 6.2.5. Sensitivity analysis on the electricity emissions factor is provided in section 6.2.6. Finally,
an additional scenario examining the impact of CO₂ capture in the biobutanol plant on the GHG emissions is presented in section 6.2.7.

6.2.1 Plant performance scenario 1: Baseline
Under the baseline plant performance scenario a number of different heat and power provision scenarios were investigated, as outlined in section 5.3. The breakdown of GHG emissions for scenarios A1, B1, C1 and D1 (Table 9) is provided in Figure 14.

Figure 14 GHG emissions of butanol, under plant performance scenario 1: baseline. Dashed line refers to fossil fuel comparator (Ref. European Commission, 2009)

These results demonstrate that for the commercial-scale GHG assessment, as for the pilot-scale GHG assessment, the majority of the GHG emissions come from the provision of heat and power to the plant, the enzymes and feedstock collection and transport. In the results presented in Figure 14, and across all other scenarios examined for the commercial-scale biobutanol plant (sections 6.2.2 to 6.2.7) the RED-compliant straw GHG emission factor of 54.3 gCO₂eq./kg was used in the calculation. See section 3.4.2 for further discussion of this. In heat and power scenarios B, C and D the recalcitrant biomass and biogas are by-products of the process and have emissions allocated to them. Therefore in these scenarios the contribution from process inputs such as enzymes and feedstock to the biobutanol GHG intensity are smaller compared to scenario A. There is a small negative GHG emissions intensity in scenario D due to exported electricity from the gas turbine CHP.

Across all of the different heat and power provision scenarios presented in Figure 14, the total GHG intensity of biobutanol ranges from 72 gCO₂eq./MJ when lignin and biogas are burned on-site for heat and power, to 128 gCO₂eq./MJ when a gas boiler with steam turbine is used. Compared to the fossil fuel comparator for biofuels, shown as a black line on the graph at 83.8 gCO₂eq./MJ (European Commission, 2009), this represents a GHG saving of 15% in the case of scenario A, and negative GHG emission savings in the case of scenarios B, C and D. Only the scenario with the lignin boiler makes emission savings compared to the comparator. Heat and power scenario B is substantially higher than other scenarios, largely due to the low efficiency of the boiler + steam turbine setup, and consequently large amount of natural gas required by the plant.

6.2.2 Plant performance scenario 2: Low heat and power demand
The plant performance scenario under the assumption of reduced heat and power demand (as outlined in section 5.3.2) was also evaluated across the four different heat and power provision scenarios (Figure 15). In this scenario the breakdown of GHG emissions under each heat and power provision scenario is similar to that in the baseline scenario, but the total life-cycle GHG emissions are lower than fossil gasoline.
or diesel for three out of the four heat and power scenarios. The GHG emissions intensity of butanol is 13-18% lower than in the baseline scenario.

Figure 15  GHG emissions of butanol, under plant performance scenario 2: low heat and power demand. Dashed line refers to fossil fuel comparator (Ref. European Commission, 2009)

Under the low heat and power demand scenario, emissions range from 58 gCO$_2$eq./MJ when heat and power are provided by on-site combustion of waste biomass (heat and power scenario A) to 112 gCO$_2$eq.MJ when heat and power are provided by gas boiler + CHP (heat and power scenario B). The emissions saving compared to the fossil fuel comparator is 30% for heat and power scenario A, 7% for scenario C, 12% for scenario D, and negative GHG emission savings for scenario B. In this scenario, the exported electricity in heat and power scenario D (gas turbine CHP) is smaller, even though there is a decreased electricity demand from the plant. This is because the modelled capacity of the gas CHP unit is sized on the heat demand for the plant, which was reduced by a great amount than the electricity demand in this scenario.

6.2.3 Plant performance scenario 3: High conversion efficiency
The GHG emissions of the commercial-scale butanol under the higher conversion efficiency scenario, as described in section 5.3.2, are given in Figure 16. Life-cycle GHG emissions are 25-35% lower than in the baseline scenario.
Under the high conversion efficiency scenario, emissions range from 46 gCO₂eq./MJ when heat and power are provided by on-site combustion of waste biomass (heat and power scenario A) to 96 gCO₂eq./MJ when heat and power are provided by gas boiler + CHP (heat and power scenario B). The emissions saving compared to the fossil fuel comparator is 45% for heat and power scenario A, 19% for scenario C, 23% for scenario D, and negative GHG emission savings for scenario B.

6.2.4 Plant performance scenario 4: Low heat and power demand and high conversion efficiency

When both low heat and power demand, and high conversion efficiency are combined, the GHG emissions are substantially lower compared to the base plant performance scenario (Figure 17). Life-cycle GHG emissions are significantly lower than fossil gasoline or diesel for three out of the four heat and power scenarios. The lowest GHG emission factor of biobutanol under this scenario is when there is on-site combustion of lignin and biogas with CHP, in which case the biobutanol GHG intensity is 37.8 gCO₂eq./MJ.
When both high conversion efficiency and low heat and power demand are modelled together (Figure 17), emissions range from 38 gCO₂eq./MJ when heat and power are provided by on-site combustion of waste biomass (heat and power scenario A) to 84 gCO₂eq./MJ when heat and power are provided by gas boiler + CHP (heat and power scenario B). The emissions saving compared to the fossil fuel comparator is 55% for heat and power scenario A, 30% for scenario C, 33% for scenario D, and no GHG emission savings for scenario B.

6.2.5 Plant performance scenarios summary

The overall GHG emissions of butanol across all of the plant performance scenarios and heat and power scenarios, which were presented in Figure 14 to Figure 17, are summarised in Table 10. The colours indicate whether in that scenario biobutanol makes no GHG saving compared to the fossil fuel comparator (red) some GHG saving compared to the fossil fuel comparator (amber) or achieves a 50% GHG saving compared to the fossil fuels comparator (green).

Table 10 Summary of GHG emissions across different plant performance scenarios and heat and power scenarios (values in gCO₂eq./MJ butanol)

<table>
<thead>
<tr>
<th>Plant performance scenario</th>
<th>Heat and power scenario</th>
<th>A (biomass boiler + steam turbine)</th>
<th>B (gas boiler + steam turbine)</th>
<th>C (gas boiler + imported electricity)</th>
<th>D (gas turbine CHP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Baseline</td>
<td>A1</td>
<td>71.6</td>
<td>B1</td>
<td>C1</td>
<td>D1</td>
</tr>
<tr>
<td></td>
<td>A2</td>
<td>58.4</td>
<td>B2</td>
<td>C2</td>
<td>D2</td>
</tr>
<tr>
<td>2 Low heat and power demand</td>
<td>A3</td>
<td>46.2</td>
<td>B3</td>
<td>C3</td>
<td>D3</td>
</tr>
<tr>
<td></td>
<td>A4</td>
<td>37.8</td>
<td>B4</td>
<td>C4</td>
<td>D4</td>
</tr>
<tr>
<td>3 High conversion efficiency</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>4 Low heat and power demand, and high conversion efficiency</td>
<td>A4</td>
<td>37.8</td>
<td>B4</td>
<td>C4</td>
<td>D4</td>
</tr>
</tbody>
</table>

Table 10 illustrates that from a GHG point of view, the most optimal heat and power provision scenario is on-site combustion of the biomass which is a by-product of the process.

This demonstrates that reducing the heat and power demand by 20% and 10% respectively can reduce the overall GHG emissions of the plant by 18%, and improving the efficiency of fermentation can reduce the GHG emissions by 35% compared to the baseline. When both of these improvements are implemented together the GHG emissions reduce by up to 47% compared to the baseline. Under the scenario where heat and power demand are reduced, and conversion efficiency is high, the lignocellulosic biobutanol has a GHG emissions intensity of 37.8 gCO₂eq./MJ, which equates to an emissions saving of 55% compared to the RED fossil fuel comparator. A 55% saving meets the current threshold for biofuels produced in plants which started operation before October 2015, and is close to meeting the 60% target for biofuels which were produced in plants in operation after October 2015.

6.2.6 Scenario: country-specific electricity emission factors

As noted in section 5.3.3 the electricity emission factor across European countries can vary substantially, therefore it is important to understand the impact that this could have on the overall plant GHG emissions. For the heat and power scenario where heat and power is provided on-site by lignin combustion and a large amount of electricity is imported to the plant, the emission factor of the electricity substantially impacts the overall plant GHG emissions, as illustrated in Figure 18. This suggests that locating the plant in a country with a low grid electricity emissions factor could be an important consideration in reducing the overall GHG intensity of the biobutanol. However in scenarios where the electricity is generated on-site
from a gas CHP, the emissions factor of the electricity grid has no impact on the overall plant GHG emissions.

As illustrated in Figure 18, under scenario A4 total GHG emissions of biobutanol range from 22 gCO₂eq./MJ if electricity from the French grid is used, to 60 gCO₂eq./MJ if electricity from the Polish grid is used, corresponding to an emission saving of 73% and 28% respectively compared to the fossil fuel comparator.

Figure 18 Variation of overall butanol GHG emissions with electricity emissions factor (for scenario A4 as defined above). Dashed line refers to fossil fuel comparator (Ref. European Commission, 2009)

6.2.7 Scenario: CO₂ capture and sequestration

A scenario was investigated which included CO₂ capture, as outlined in section 5.3.4. In order to understand the ‘best-case’ outcome from the plant, CO₂ capture was imposed on the optimum scenario A4 (see Table 9). Although there is a small increase in emissions due the additional electricity required for CO₂ capture, there is also a large credit for sequestered CO₂, which gives an overall net CO₂ intensity of -8 gCO₂eq./MJ compared with 38 gCO₂eq./MJ for scenario A4 without CO₂ capture (Figure 19). The overall GHG emissions intensity is negative because the amount of CO₂ captured is greater than the CO₂ released during the biobutanol production process. However it should be emphasised that this is an exploratory scenario, with CO₂ capture technologies from ligno-cellulosic butanol fermentation broth yet to be proven at any scale.

Figure 19 GHG emissions of butanol, scenario A4 with and without CO₂ capture. Dashed line refers to fossil fuel comparator (Ref. European Commission, 2009)
6.3 Comparison of butanol with other fuels

6.3.1 GHG emissions of biobutanol assessed by other studies

There are few existing studies of the GHG emissions associated with biobutanol production. Montaño (2009) carried out an LCA of butanol production from wheat straw, although limited information is available on the data which underpins this assessment, and results are only presented in terms of ‘normalised’ impacts, so are not comparable to the results obtained from the ButaNexT study. Pereira (2015) and Brita (2017) also carry out LCA assessments of biobutanol. However in both studies the results are not presented in a way which enables comparison with the results of the ButaNexT study. Wu et al. (2007) was the only source found which provided a useful comparison figure. Wu et al. carried out a GHG assessment of corn-based biobutanol, concluding that the emissions intensity would be 62gCO₂eq./MJ_bibutanol. This is within the range of results presented across the different scenarios in this study, and 63% higher than the lowest-GHG emission scenario explored here. This is in-line with the trend shown by bioethanol, where ligno-cellulosic fuel can achieve lower GHG emissions than the same fuel produced from crops. However additional evidence would be required to determine whether this trend in general holds true for biobutanol.

6.3.2 GHG emissions of biobutanol compared to fossil butanol

The focus of this study so far has been on biobutanol production for use in the transport sector. The methodology used to calculate the GHG emissions of the biobutanol is that laid out in the Renewable Energy Directive for biofuels used in transport, and the GHG saving reported in section 6.2 was given compared to the fossil fuel comparator for biofuels, which is based on fossil diesel and gasoline. Nevertheless, biobutanol could also be used as a chemical feedstock, in which case it would likely replace fossil butanol. Therefore in this section a comparison of the GHG emissions of ButaNexT biobutanol with fossil butanol is provided. The GHG emissions of fossil butanol were taken from the Ecoinvent database for n-butanol produced by hydroformylation of propylene, calculated according to the ReCiPe methodology to be 3.1 kgCO₂eq./kg (93 gCO₂eq./MJ). It should be noted that this only comprises the production of n-butanol, not the embodied carbon within the fossil butanol.

A comparison between ButaNexT biobutanol and fossil butanol is given in Figure 20, comprising scenarios A1 to A4 from this study (see Table 9). The GHG emissions saving compared to fossil butanol ranges from 23% for scenario A1 (baseline plant performance, with lignin CHP for heat and power) to 59% for scenario A4 (lower heat and power demand and high conversion efficiency, with lignin CHP for heat and power). If the carbon embodied in the butanol were released to the atmosphere at the end-of-life of the chemical, this saving would be even higher, as the embodied carbon in fossil butanol is fossil carbon, whereas in biobutanol the carbon is biogenic so does not contribute to global warming.

![Figure 20 GHG emissions of ButaNexT biobutanol, across scenarios A1 to A4, compared to fossil butanol. Data labels show GHG saving compared to fossil butanol](image-url)
It should be noted that unlike the RED methodology for transport fuels, there is no harmonized methodology for calculating the GHG emissions of chemical feedstocks such as fossil butanol. Therefore there are likely to be some methodological differences between the ButaNexT study and the figure provided here for fossil butanol from EcoInvent. For example the transport distance of butanol to a chemical plant may be higher than when it is used as a transport fuel, as demand for chemicals tends to be concentrated in certain large chemical plants whereas demand for transport fuel is more distributed. Different methodologies and assumptions around production method could result in a different figure for the GHG emissions of fossil butanol, and hence for the saving. Patel et al. (2006) for example state that the GHG intensity of fossil butanol is 58 gCO\(_2\)eq./MJ, which clearly would give biobutanol a significantly lower GHG saving, compared to those given in Figure 20. This highlights the importance of a harmonized GHG methodology when comparisons are made between GHG intensities of products.

6.3.3 GHG emissions of biobutanol compared to ethanol

Typical values for the GHG emissions associated with corn ethanol production are given in the RED. For ethanol from wheat with a natural gas boiler this is 46.1 gCO\(_2\)eq./MJ and for ethanol from wheat with a natural gas CHP this is 39.4 gCO\(_2\)eq./MJ. This provides a GHG saving compared to the fossil fuel comparator of 45% and 53% respectively.

Typical values are also given in the RED for ethanol produced from wood and wheat straw. These are based on the values given in the JEC Well-to-Wheels report, although there are some small differences between the two sources. The values reported in the JEC well-to-wheels report are illustrated in Figure 21. As for the values calculated in this study for biobutanol, the fuel production, and feedstock contribute the overwhelming proportion of the GHG emissions, however the GHG emissions of ligno-cellulosic ethanol reported here are substantially lower than those calculated in this study for biobutanol. Whilst the figures from the Well-to-Wheels study are based on old sources, and processes operating only at demonstration-scale, figures available from the UK Renewable Transport Fuel Obligation for the GHG emissions of LC ethanol actually sold into the UK transport market in 2016-17 lie within a similar range (RTFO, 2018). These figures range from 13 gCO\(_2\)eq./MJ for ethanol produced from straw to 25 gCO\(_2\)eq./MJ for ethanol produced from short rotation coppice.

The GHG emissions of biobutanol, as calculated in this study for scenarios A1, A2, A3 and A4, are compared to crop-based ethanol and ligno-cellulosic ethanol in Figure 22. This illustrates that the most ambitious scenario for LC biobutanol (scenario A4) has similar GHG emissions to crop-based ethanol on
a per MJ basis. This is an encouraging result, but illustrates that improvements to the process are still required to get to the low GHG emission factors seen for LC ethanol.

![Figure 22](image-url) **GHG emissions of biobutanol compared to crop-based and LC ethanol. Dashed line refers to RED fossil fuel comparator, and data labels show % GHG saving**

The higher GHG emissions of ligno-cellulosic butanol compared to ligno-cellulosic ethanol seem to be due significantly to:

- Low yields of butanol compared to ethanol
- High energy use modelled in this study

In the following sections these metrics, which have a substantial impact on the overall GHG emissions of the commercial-scale biobutanol, are examined in more detail. A comparison is given with other ligno-cellulosic butanol processes that are reported in the literature, or with ligno-cellulosic ethanol plants, in order to provide further insight into the results provided in sections 6.2 and 6.3.

### 6.3.4 Overall fuel yield

In the baseline mass and energy balance, the overall fuel yield is 0.12 kg ABE products / kg biomass\textsuperscript{wet} or 0.09 kg butanol / kg biomass\textsuperscript{wet}. In the ‘high conversion efficiency’ scenario (section 5.3.2) the overall butanol yield is 0.15 kg butanol / kg biomass\textsuperscript{wet}.

Yields of lignocellulosic ethanol have been reported to be 0.21 kg / kg biomass\textsuperscript{wet} (Wooley, 1999), 0.28 kg ethanol / kg biomass\textsuperscript{wet} (Humbird, 2011), and between 0.19 and 0.23 kg ethanol / kg biomass\textsuperscript{wet} depending on the pre-treatment method adopted (Wang, 2013).

Ligno-cellulosic biobutanol production has not been widely studied to date, but some recent papers model yields of 0.07kg butanol / kg biomass\textsuperscript{wet} (Jang, 2018), 0.1 kg butanol / kg biomass\textsuperscript{wet} (Baral, 2016), 0.13 kg butanol / kg biomass\textsuperscript{wet} (Tao et al. 2014).

Therefore, the baseline yield modelled in this study is within the range seen in the literature for ligno-cellulosic n-butanol production, and the ‘high conversion efficiency’ scenario models a slightly higher overall yield than seen in other sources. Yields of ligno-cellulosic butanol are substantially lower than yields of ligno-cellulosic ethanol, which is unavoidable to some extent as acetone and ethanol are produced alongside butanol, whilst ethanol alone can be produced in fermentation. The lower yield of butanol production may also stem from the earlier stage of development of butanol fermentation technologies.
It is likely that the low yields of the biobutanol process compared to ligno-cellulosic ethanol explain the high contribution from feedstock and enzymes to the overall biobutanol GHG intensity. It is not the case that these inputs themselves have a substantially higher GHG intensity than when used in LC bioethanol plants. Indeed Hong et al. (2013) review the GHG intensity of enzymes used in previous ligno-cellulosic ethanol LCA studies, and also carry out their own modelling of the GHG impacts associated with enzymes, which give results substantially higher than the enzyme emission factor used in this study. They do however note that on-site production of enzymes is likely to have a lower GHG impact compared to off-site production of enzymes, due to the addition of preservatives, more purification, and transport required for off-site enzyme production. Hence in biobutanol production there may be opportunity to further reduce the enzyme emissions factor through on-site production.

Therefore increasing the overall yield of biobutanol from the feedstock is likely to be key in further reducing the GHG emissions of ligno-cellulosic biobutanol towards the low figures seen for ligno-cellulosic bioethanol.

6.3.5 Heat and power use

The heat and power demand from each section of the plant under the baseline scenario is summarised in Figure 23.

As heat and power use is very specific to the technology used in the plant and the engineering of the plant itself, direct comparisons with other systems should be treated with caution. Montano (2009) presents a theoretical LC butanol process where the heat demand is 0.93 MWh\text{heat}/tonne feedstock\text{wet} and 0.29 MWh\text{elec}/tonne feedstock\text{wet} into the plant. This is not dissimilar to that modelled in this study: 1.04 MWh\text{heat}/tonne biomass and 0.52 MWh\text{elec}/tonne biomass.

Compared to an LC ethanol plant (Humbird, 2011) the electricity use (MWh / tonne biomass) basis is around 4 times higher in the ButaNext commercial plant, and the heat use is around 2 times higher. However this also reflects the different technology and yields obtained from LC ethanol production. For example Tao et al. (2014) emphasise the substantially higher energy requirement when separating out the 3 solvents form the ABE process compared to the process for separating ethanol from fermentation products.

Given the substantial contribution from heat and power provision to the overall GHG emissions, the higher heat and power demand of biobutanol compared to ligno-cellulosic ethanol contributes to the higher GHG emissions of ligno-cellulosic ethanol compared to ligno-cellulosic butanol. This also illustrates that improving process efficiency and reducing heat and power demand within the plant should be a focus of future work as the technology is scaled-up.
7 Conclusions

This study assesses the GHG emissions of biobutanol produced in an operating pilot-scale plant and of biobutanol that could be produced in a theoretical commercial-scale plant, using the RED methodology. The mass and energy balance of the pilot plant was obtained from operational plant data. The modelled commercial-scale plant was based on the technology currently operating in the pilot plant, but at much larger scale, with a feedstock capacity of 450 tonnes/annum of straw at a moisture content of 12%. The mass and energy balance of the commercial-scale plant was developed in collaboration with the consortium partners to reflect the process conditions that could likely be achieved at commercial-scale.

The GHG intensity of biobutanol produced in the pilot plant is very high, and comprised mostly of emissions from electricity, which is used to provide both heat and power to the pilot plant. Reducing the energy-use of the production process, and providing that energy efficiently and from a low-carbon source should therefore be a key aim when scaling up the technology from pilot scale.

In the commercial-scale plant, a wide range of scenarios around likely yields and energy provision to the plant were modelled. The majority of GHG emissions across all scenarios come from the heat and power provision to the process, enzymes, and feedstock collection, processing and transport. Comparison of the GHG emissions across a number of heat and power provision scenarios was carried out, considering on-site combustion of by-product biomass, gas boiler with CHP, gas boiler with electricity from the grid, and gas turbine CHP. Across these scenarios, the lowest GHG emissions can be achieved when the by-product biomass is combusted on-site to provide heat and power to the process. A number of scenarios for improved plant performance were also investigated: lower heat and power demand and high conversion efficiency of the process. Respectively these two scenarios reduce GHG emissions of biobutanol by 13 – 18% to compared to the baseline, and by 25 – 25% compared to the baseline. When both low heat and power demand and high conversion efficiency occur together, and heat and power is provided by on-site biomass combustion, biobutanol has a GHG emissions intensity of 38 gCO₂eq./MJ. This is equivalent to a GHG saving of 55% compared to the RED fossil fuel comparator, approaching the 60% GHG saving threshold that is required for biofuels produced in new plants under the RED. This assumes a power demand of 11.4 MJ/kgbiotanol, a heat demand of 20.1 MJ/kgbiotanol, and overall butanol yield of 0.15 kgbiotanol/kgwet biomass can be achieved. These emissions are predominantly due to grid electricity, enzymes and feedstock collection, processing and transport, and could therefore be further mitigated by increasing butanol yield, reducing the energy demand of the process, and using more renewable or low-carbon electricity. Moreover, CO₂ capture was investigated, and was shown to substantially reduce biobutanol GHG emissions, however this technology is currently unproven in biobutanol production.

Under all scenarios modelled in this study, apart from those with CO₂ capture, commercial ligno-cellulosic biobutanol production has higher GHG emissions than ligno-cellulosic ethanol. This is largely due to its lower overall yield and high heat and power demand. Comparisons with bioethanol production and insights gained through this study indicate some key areas of future work to further reduce emissions, including but not limited to:

- Reduce heat and power demand of biobutanol production, for example through improved process integration to enable heat recovery and re-use, and improvements to equipment.
- Investigate the technical and economic impacts of capturing and selling the hydrogen produced in the fermentation process in order to displace fossil hydrogen and further reduce the GHG intensity of the process.
- Drying biomass sludge produced in waste water treatment using waste heat so that it can also be combusted in the boiler.
- Exploring the possibility to capture and sequester CO₂ from the process.
- Improving overall conversion efficiency, so that inputs are lower per unit mass of output.
- Reducing the use of enzymes in biobutanol production process, and reducing GHG emissions from the production of enzymes, potentially through on-site enzyme production.
• Working with biomass producers to make sure that LC biomass with low GHG factor is sourced, for example through low-carbon Miscanthus cultivation methods, or supply chain optimization to reduce transport distances.

The key limitations of this analysis relate to the uncertainties in modelling the commercial-scale biobutanol plant. The technology is currently at pilot-scale, so many assumptions were made in scaling-up to commercial-scale. The technologies that would be used, and the likely performance of those technologies, was based on the existing pilot-plant and literature data from other ligno-cellulosic processes, but these may be adapted and improved as LC biobutanol technology is scaled up in practice. There is therefore a wide uncertainty range around the commercial-scale mass and energy balance. Other uncertainties resulted from the lack of granularity in the location of the plant, as electricity and feedstock GHG emissions could change significantly depending on the plant location and the feedstock supply chain.

Further work on this topic could aim to improve the accuracy of the modelling of the plant energy demand, and investigate in more detail trade-offs between process choices, such as yield vs. productivity of fermentation. This would likely require more detailed data from a stable operating demonstration-scale plant, and detailed engineering work on ligno-cellulosic processing scale-up.
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