

# CIRCULAIR



## Public report: Assessment framework for CIRCULAIR process

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### Abstract

CIRCULAIR investigates the conversion of manure and straw into sustainable fuels for aviation and shipping. The core process, hydrothermal liquefaction (HTL), is in particular suited for wet feedstock. Alongside a viscous biocrude, HTL yields a water phase containing soluble organics, effluent gasses and a solid phase. CIRCULAIR intends to produce fuels with a high yield of kerosene from the HTL biocrude. Furthermore, all product phases will be utilised via various processes. This report describes the initial version of the methodological framework for the system analyses of this highly integrated fuel pathway. The framework serves as basis for the process modelling and the evaluation of environmental, economic and socio-economic performance parameters during the further course of the CIRCULAIR project.

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## Glossary

Acronym	Signification
AEL	Alkaline Water Electrolysis
APOS	Allocation at the Point of Substitution
BHL	Bauhaus Luftfahrt e. V.
CAPEX	Capital Expenses
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization
CF	Capacity Factor
CO <sub>2</sub> -Eq.	Carbon Dioxide Equivalent
EL	Electrolyser
EU	European Union
GHG	Greenhouse Gas
GWP	Global Warming Potential
HTL	Hydrothermal Liquefaction
IO	Input-Output
LCA	Life-Cycle Assessment
LHV	Lower Heating Value
MtJ	Methanol-to-Jet
OPEX	Operational Expenses
PC	Production Costs
PEM	Proton Exchange Membrane
PtL	Power-to-Liquid
PtM	Power-to-Methanol
PtX	Power-to-X
R&D	Research and Development
RIA	Research and Innovation Action
SOEC	Solid Oxide Electrolysis Cell
TEA	Techno-Economic Analysis
TLCC	Total Life Cycle Costs
TRL	Technology Readiness Level
VFA	Volatile Fatty Acid
WO	Wet Oxidation

# 1. Executive summary

CIRCULAIR is a collaborative Research and Innovation Action funded by the European Union that investigates the conversion of abundant agricultural residues (manure, straw) into sustainable fuels for aviation and shipping, via hydrothermal liquefaction (HTL) and coupling to green H<sub>2</sub> generation. The project has started in January 2023 and has a duration of four years. This report establishes a methodological framework that will serve as a basis for the system analyses within the CIRCULAIR project.

The holistic approach of CIRCULAIR foresees the utilisation of all HTL product phases. In particular, a high yield of jet fuel product is targeted and biomass resource utilisation will be maximised by developing suitable valorisation schemes for all relevant side streams.

As a starting point for later process modelling a baseline configuration is defined. This baseline configuration envisages a hub and spoke approach, where several HTL plants feed biocrude to a centralised upgrading facility. In consequence, subsystem technologies and baseline plant layouts have to be defined to establish process models for a representative HTL plant site and the central upgrading site. The results of the process modelling will be used to assess the CIRCULAIR approach in a holistic way, taking techno-economic, environmental and social considerations into account. For this purpose, suitable criteria and metrics have been selected to determine key performance parameters. This will allow for trade-off analyses with respect to different evaluation criteria, and the derivation of recommendations and a roadmap at a later stage of the project.

## 2. Introduction

CIRCULAIR is a collaborative research and innovation action (RIA) that is funded by the European Union (EU)<sup>1</sup>. The project started in January 2023 and will run for four years. The consortium has issued a press release<sup>2</sup> that introduces the scope of the project, the roles of the consortium partners and the expected innovations. The short introduction to the CIRCULAIR project in the following Sections 1.1 and 1.2 is based on this press release, Section 1.3 introduces more specifically the scope of this public report. Further information on the progress of the project implementation and results will be made available via the project website<sup>3</sup> over the course of the CIRCULAIR project.

### 1.1 Key Objectives and ambition

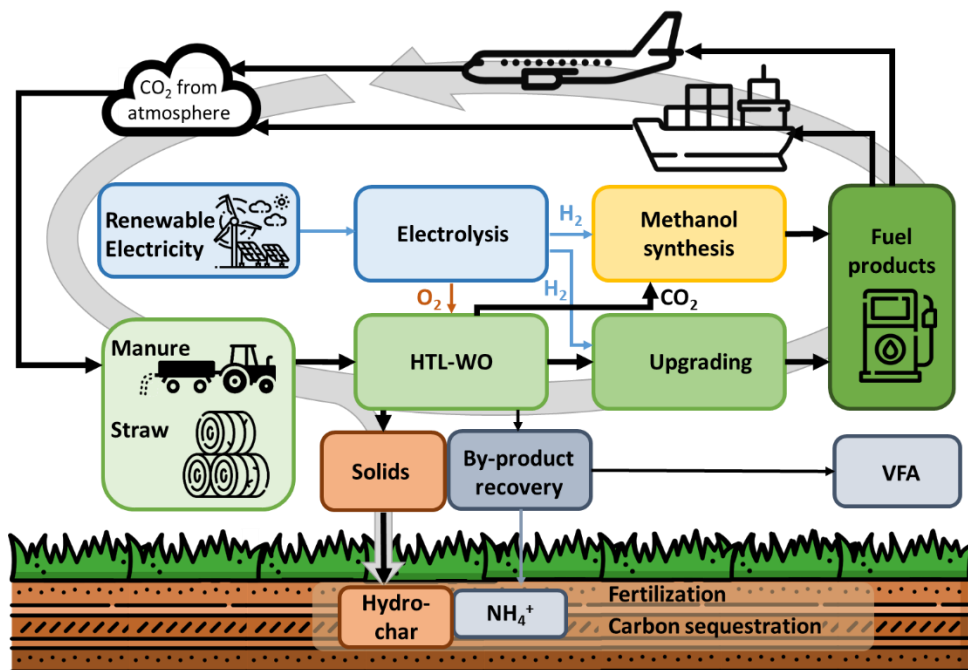


Figure 1: Sketch of the CIRCULAIR concept. The central conversion step is hydrothermal liquefaction (HTL) coupled to a wet oxidation (WO) of the HTL process water. All product phases of HTL conversion are utilized. Coupling with green H<sub>2</sub> enables almost complete carbon to product conversion.

Figure 1 sketches the basic approach of CIRCULAIR. Hydrothermal liquefaction (HTL) is the central biomass conversion process and abundant agricultural residues (manure, straw) are chosen as feedstock due to availability considerations. Compared to other advanced biofuel

<sup>1</sup> <https://cordis.europa.eu/project/id/101083944>

<sup>2</sup> Available via: [https://www.l-up.com/wp-content/uploads/2023/02/CIRCULAIR\\_press\\_release\\_20230222.pdf](https://www.l-up.com/wp-content/uploads/2023/02/CIRCULAIR_press_release_20230222.pdf)

<sup>3</sup> [www.project-circulair.eu](http://www.project-circulair.eu)

technologies, HTL may especially have a competitive advantage for the treatment of wet feedstock such as manures. However, the treatment of the HTL process water has been identified as a key challenge in the commercialisation of HTL pathways [1]. Practical solutions for HTL process water treatment are identified for the conversion of sewage sludge<sup>4</sup> and dry feedstock<sup>5</sup>, but these approaches are unapplicable for manure conversion. One of the main innovations of CIRCULAIR is the coupling of HTL with wet oxidation (WO) of the HTL process water. Thereby, the HTL process water is cleaned-up and the external process heat demand for HTL conversion can be greatly reduced. Ideally, thermo-neutral operation is achieved, such that external process heat is unrequired. Further important innovations relate to the upgrading of HTL biocrudes to final fuel products with a high share of kerosene that fulfils jet fuel specifications. Thereby the approval process of HTL jet fuel for civil aviation is prepared. The holistic approach of CIRCULAIR foresees the utilisation of all HTL product phases. In particular, biomass resource utilisation will be maximised by developing suitable valorisation schemes for all relevant side streams. The HTL process water after WO can still contain significant amounts of organic species with a high share of volatile fatty acids (VFA). The recovery of VFA from this process water will be investigated. Furthermore, effluent gases from HTL conversion and from WO of HTL process waters contain a high share of CO<sub>2</sub>. Here, coupling with green H<sub>2</sub> is investigated to utilise this carbon stream for methanol synthesis. Finally, a solid phase is evolved. CIRCULAIR will fill a knowledge gap regarding the use of HTL chars for soil application, potentially creating a negative contribution to the carbon footprint.

CIRCULAIR builds in important parts on the results of its precursor HyFlexFuel<sup>6</sup>, an EU Horizon 2020 project, which delivered ground breaking research and innovations in HTL fuel production.

## 1.2 Consortium

The CIRCULAIR consortium consists of ten partners from six European countries. The implementation activities have a strong regional focus in Denmark. The partners Aarhus University (Denmark) and Circlia Nordic (Denmark) develop the HTL conversion at pilot scale. Aalborg University (Denmark) and Topsoe (Denmark) concentrate on refining intermediate

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<sup>4</sup> In case of sewage sludge HTL process water may be recycled to the front end of the wastewater treatment plant, this approach is e.g., investigated in the Sludge2Fuel project: <https://www.sludge2fuel.dk>

<sup>5</sup> In case of dry feedstock, the HTL process water can be recycled to prepare the feed slurry for HTL conversion (typical feed slurries have a dry matter content of about 20%).

<sup>6</sup> HyFlexFuel website: [www.hyflexfuel.eu](http://www.hyflexfuel.eu)

biocrudes from HTL with a high share of jet fuel in the final product. RISE (Sweden) investigates an alternative upgrading process for HTL biocrude using slurry hydro-treatment. The analysis of the produced jet fuel is ensured by the skills and capabilities of Research and Development (R&D) laboratories of Eni (Italy). Universidad Complutense de Madrid (Spain) will recover volatile fatty acids and ammonium from aqueous side streams and separate CO<sub>2</sub> of sufficient purity for methanol synthesis. Universität Hohenheim (Germany) investigates the utilisation of HTLchars for soil amendment in agriculture.

Bauhaus Luftfahrt (Germany) analyses the future performance of the fuel pathway in terms of economic, social and environmental parameters and acts as project coordinator of CIRCULAIR. L-up (France) supports project coordination and leads communication and dissemination activities.

### 1.3 Assessment framework for system analyses within CIRCULAIR

The main purpose of the present public report is the definition of an assessment framework for the system analyses on the advanced biomass conversion process that is sketched in Figure 1. The project is funded by the EU under the Destination *Sustainable, secure and competitive energy supply* within *Cluster 5: Climate, Energy and Mobility* of the *Horizon Europe Work Programme 2021-2022*<sup>7</sup>. This Destination aims at *“Research and Innovation actions [that] will help to make the energy supply side cleaner, more secure, and competitive by boosting cost performance and reliability of a broad portfolio of renewable energy solutions, in line with societal needs and preferences.”*

CIRCULAIR contributes to the aims of this Destination by further developing technologies for the production of jet fuel from abundant agricultural residues by a highly integrated HTL approach up to a maturity level of Technology Readiness Level (TRL) 4-5<sup>8</sup>. At this maturity level, individual process steps are still under development at the laboratories of the respective project partners. System analyses are applied to confirm (or refute) that the proposed fuel production pathway has the potential to indeed become cleaner and more competitive than competing alternatives in the future. Such confirmation is based on the evaluation of key performance indicators of the fuel pathway from life cycle assessment (LCA), socio-economic and techno-economic analyses (TEA). These analyses require a derivation of physical parameters like material and energy input and output data. To estimate

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<sup>7</sup> [https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/wp-call/2021-2022/wp-8-climate-energy-and-mobility\\_horizon-2021-2022\\_en.pdf](https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/wp-call/2021-2022/wp-8-climate-energy-and-mobility_horizon-2021-2022_en.pdf)

<sup>8</sup> On a scale from TRL 1 to 9, Definition TRL 4: Technology validated in a lab; TRL5: Technology validated in an industrially relevant environment.

these process parameters, models of individual process steps need to be established and integrated to describe the entire process chain of a future full-scale production facility.

In particular, the results from system analysis are important to assess, if the following main objectives of the CIRCULAIR project are achievable:

- Cost effective biofuel production.
- Nearly complete utilisation of the carbon in the biomass feedstock.
- Carbon negative contribution to fuel production by soil amendment using HTL solids.

Furthermore, wider impact, resulting e.g., from pollution reduction from changes in manure handling practice or socio-economic benefits of HTL value chains in rural environments will be analysed. The evaluation of key performance parameters will allow a comparison of the proposed biorefinery concept to fossil fuel production and competing biomass conversion pathways.

Further important aspects of system analyses relate to the development of the fuel path itself. Proper system analyses allow to derive key drivers of economic and environmental performance, such that further research and development efforts can be guided by identifying the critical levers that optimise the process configuration.

The present public report marks the starting point of the system analyses work within CIRCULAIR by defining an initial assessment framework. In Section 2, a baseline configuration is defined as basis for the process modelling. This includes a definition of the context in terms of the selection of suitable regions for feedstock and electricity supply, the chosen hub and spoke approach, as well as the basic description of the HTL and upgrading plant site.

Furthermore, a discussion of design choices and systemic considerations is included. Section 3 defines criteria and performance metrics that will be applied for the evaluation of the baseline plant design using sustainable, social and economic impact analyses.

It is important to note, that the established methodological framework defines a necessary starting point to establish appropriate process models. During the course of the further work, the methodological framework will be refined and, where necessary, adapted as results from the project implementation, initial modelling results and external insights become available.

## 2 Baseline case and design choices

CIRCULAIR investigates a highly integrated fuel production concept with multiple input streams and multiple products. An important aspect of the assessment framework is the definition of a baseline configuration for the initial process modelling work. The baseline configuration envisages a hub and spoke approach. A notable consequence of this choice is that HTL conversion and biocrude upgrading take place at separated locations. Details on this approach and the resulting baseline plant definitions will be given in the following Section 2.1. Furthermore, the regional context of the baseline configuration is defined in Section 2.2. Finally, important variations of the baseline design choices are discussed in Section 2.3.

### 2.1 The CIRCULAIR baseline configuration

#### 2.1.1 Hub and spoke approach for HTL biocrude production and upgrading

Manure and mixtures of manure with straw have been chosen as feedstock, mainly for two reasons: first, these feedstock are abundant in the agricultural context and secondly, previous work has shown a potential benefit in biocrude yield of the co-liquefaction of manure and straw [2]. The feedstock needs to be gathered in sufficient quantities in the vicinity of each individual HTL conversion plant.

Selecting the appropriate plant capacity for the CIRCULAIR baseline case will be subject to the further investigations within the project. This selection will depend on feedstock availability at the chosen baseline locations (see Section 2.2.1) and techno-economic parameters that define economies of scale. HTL biocrude is a transportable intermediate product and prior work in the EU-H2020 project HyFlexFuel indicates that thermal integration of HTL conversion with upgrading processes is of minor techno-economic relevance [3]. Therefore, a hub and spoke approach, as indicated in Figure 2, is chosen as baseline configuration within CIRCULAIR, that is: several HTL plants feed biocrude to a centralised upgrading facility.

The advantage of the hub and spoke approach is that excessive transportation networks for manure are avoided<sup>9</sup>, and that the upgrading facility can benefit from economies of scale. One consequence of separating HTL conversion and biocrude upgrading is that green H<sub>2</sub> needs to be supplied at both locations (for methanol synthesis and for hydrotreatment). Either H<sub>2</sub> is produced in one location and transported to both the HTL and upgrading plant site, or, as

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<sup>9</sup> The high-water content of manure results in significantly larger weight and volume compared to the corresponding amount of biocrude.

chosen in the baseline case, on-site green H<sub>2</sub> generation is performed at both the decentralised HTL plants and the central upgrading facilities. Furthermore, the complexity for the system modelling is significantly increased, as a large number of HTL plants are needed to feed the central upgrading facility. In the proposed modelling approach this complexity is reduced by defining a single representative baseline HTL plant capacity. It is assumed that a certain number of identical plants feed the upgrading facility<sup>10</sup>. Economies of scale for the HTL plant sites and overall feedstock density in the area of interest will define the number of individual HTL plants. The distance to the upgrading plant can be varied, which keeps the HTL biocrude transport network variable. The overall catchment area is location specific and will be defined in a later stage of the project.

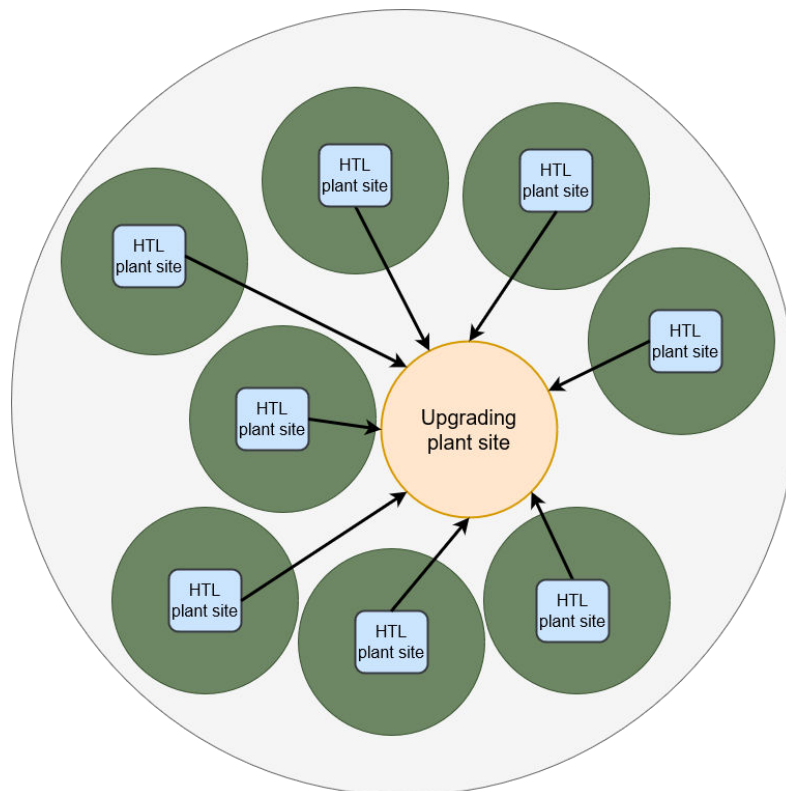


Figure 2: Hub and spoke approach as used in the CIRCULAIR baseline case. Several HTL plants supply biocrude to a central upgrading plant. In a first approach, it is assumed that all HTL plants have the same capacity to keep the modelling effort at a tolerable level. Figure 3 and Figure 4 show configurations for the HTL plant site and the upgrading plant site, respectively.

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<sup>10</sup> In perspective, the HTL reactor is based on a modular approach. Depending on the local feedstock availability, the HTL plant size can be easily adjusted by increasing the number of modules.

### 2.1.2 Baseline process configuration at the HTL sites

Figure 3 depicts the basic building blocks of the baseline process configuration at the HTL plant sites. After collection and transport to the HTL plant site, the feedstock is prepared and fed into the HTL reactor. A continuous HTL reactor operating in the subcritical regime is assumed. Upscaling of the HTL plant is based on the pilot plant at Aarhus University [4]. Conversion of biomass in the HTL reactor yields four main product streams, a so-called biocrude, a HTL process water that contains a significant share of carbon from the feedstock, a CO<sub>2</sub> rich off gas and a solid phase.

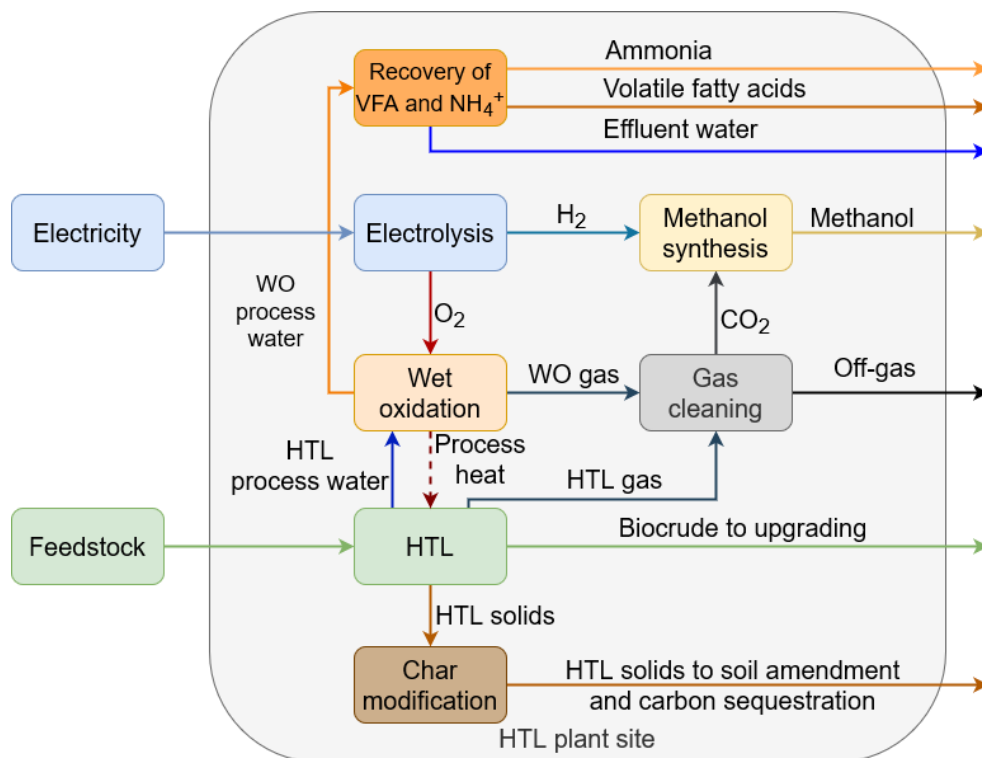


Figure 3: Sketch of the baseline process configuration at the HTL site. HTL plant sites in Figure 2 refer to the whole plant site (large grey box), while HTL (green box) refers to the actual HTL reactor.

The main product at the HTL plant site is biocrude (Figure 3). As discussed before, biocrude is transported to the centralised upgrading facility in order to obtain the desired fuel products. The configuration of the centralised upgrading facility is discussed in the next Section 2.1.3. Treatment of the HTL process water is performed via WO. During WO organic material in the process water is oxidised under heat and pressure using O<sub>2</sub> as oxidising agent [5]. WO is introduced into the CIRCULAIR concept mainly for two reasons: First, to clean-up the process water by reducing the carbon content and second, to provide process heat to the HTL reactor from the exothermal WO process. Initial tests have shown that carbon containing species in

the HTL process water are mainly transformed to CO<sub>2</sub>. The process water after WO can still contain VFAs and ammonium ions, both species are recovered from the process water. The gaseous stream from WO is combined with the HTL gas phase, both streams contain a high share of CO<sub>2</sub>. Subsequent cleaning of the combined gas phase produces a pure CO<sub>2</sub> stream that is combined with H<sub>2</sub> for methanol synthesis. The H<sub>2</sub> stream is generated from water and electricity via water electrolysis. Oxygen that is evolved as a co-product can be used for WO. The fourth HTL product stream is the HTL solid phase. In the baseline case, modification of the HTL solid phase for the purpose of soil amendment and carbon sequestration will be investigated.

### 2.1.3 Centralised Upgrading plant site

As indicated in Figure 2, a centralised upgrading plant is envisaged for the hydrotreatment of the HTL biocrudes produced in several individual HTL plants. Figure 4 presents the building blocks of the baseline process configuration at the upgrading plant site. In line with the project objectives, it is the aim to produce a high share of kerosene, which fulfils jet fuel specifications. At first, biocrude is pre-treated to remove inorganic impurities before being fed to a hydrotreatment step, such that the upgraded product consists almost entirely of hydrocarbons. This upgraded product already contains a significant amount of kerosene, the main lever to further increase the kerosene yield is hydrocracking of upgrading products with higher boiling point than kerosene. The H<sub>2</sub> demand for hydrotreating and hydrocracking is again met by an electrolyser at the upgrading plant site. In the initial baseline case, fixed bed reactors will be assumed for hydrotreating and hydrocracking. The CIRCULAIR project implementation also investigates slurry upgrading as an alternative option for hydrotreatment. The baseline assumption of fixed bed reactors may be reconsidered depending on project results.

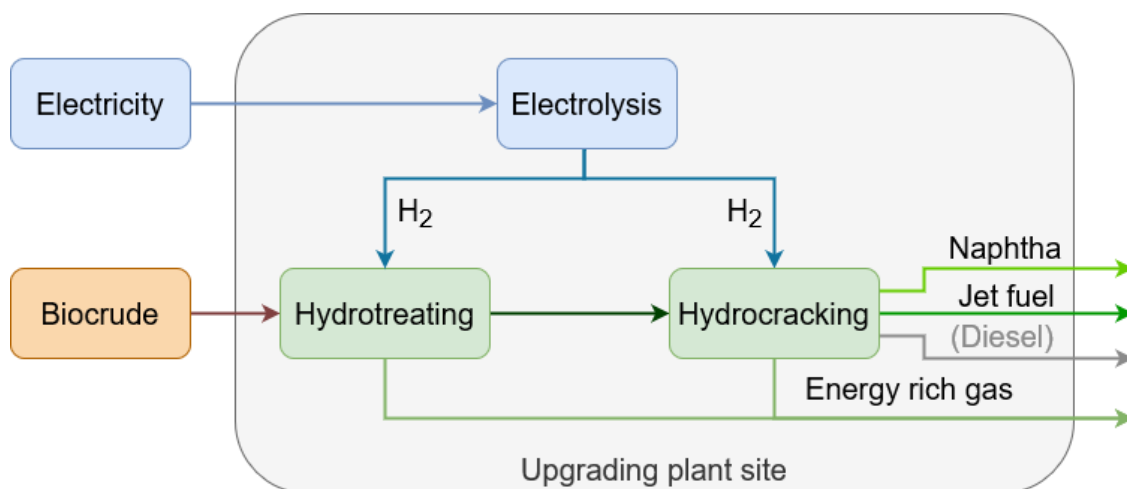


Figure 4: Sketch of the process baseline configuration at the upgrading plant site.

## 2.2 Feedstock supply: Baseline locations and coupling with green H<sub>2</sub>

The baseline configuration of the CIRCULAIR concept (see prior Section 2.1) requires a regional context where agricultural residues and renewable electricity is available. It is expected that biogenic feedstock availability as well as the conditions for green H<sub>2</sub> generation play an important role for the economic and environmental performance. It is therefore important to select representative baseline locations for evaluation.

### 2.2.1 Potential availability of agricultural residues

The potential availability of agricultural residues was studied in detail during the EU funded HyFlexFuel project<sup>11</sup>. Manures and straws were identified as the most abundant agricultural residues in the EU. Figure 5 shows HyFlexFuel results for maximum theoretical biomass potentials of cattle excretions (left) and cereal straw (right), respectively. Several regions across Europe show high potential feedstock density. The Central Denmark Region is chosen as regional context for the initial evaluation of the CIRCULAIR baseline configuration, as good availability of both manure and straw for HTL conversion coincide with favourable conditions for green H<sub>2</sub> generation from wind energy (see Section 2.2.2). Figure 5 highlights further preference regions for biogenic feedstock supply. A small number of additional locations across Europe will be chosen for evaluation at a later stage of the project.

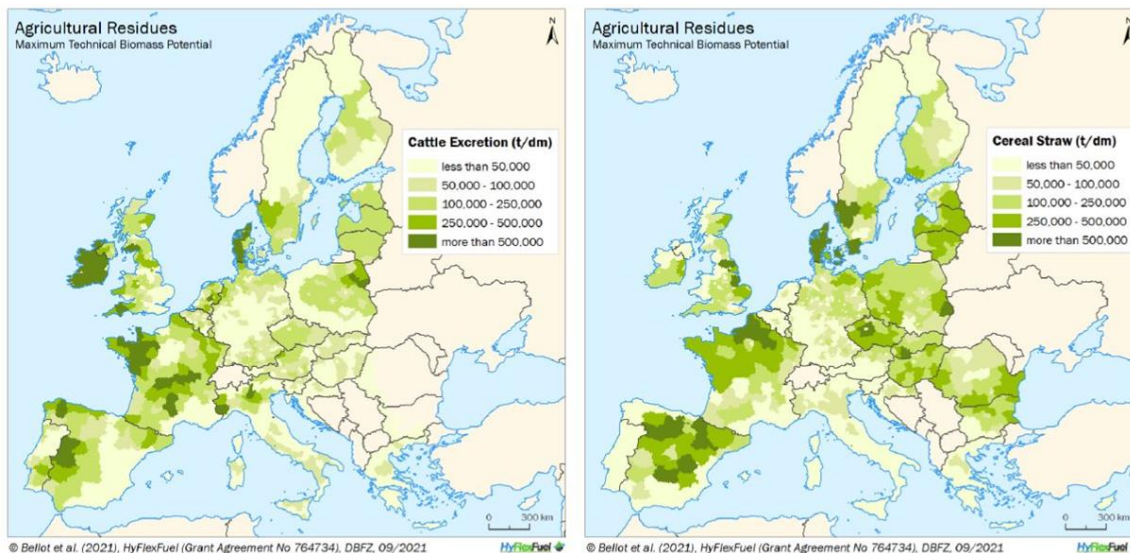


Figure 5: HyFlexFuel results for the maximum theoretical potential of cattle excretions (left) and cereal straw (right)<sup>12</sup>.

<sup>11</sup> [www.hyflexfuel.eu](http://www.hyflexfuel.eu), Feedstock availability was studied by Deutsches Biomasseforschungszentrum (DBFZ)

<sup>12</sup> Results provided by DBFZ within the HyFlexFuel final workshop; online available at [https://www.hyflexfuel.eu/wp-content/uploads/11\\_2021-09-24\\_HFF\\_Final\\_Workshop\\_DBFZ\\_v1\\_Bellot\\_FINAL.pdf](https://www.hyflexfuel.eu/wp-content/uploads/11_2021-09-24_HFF_Final_Workshop_DBFZ_v1_Bellot_FINAL.pdf)

## 2.2.2 Green H<sub>2</sub> generation from renewable electricity

The CIRCULAIR baseline configuration foresees the coupling of advanced biofuel and green H<sub>2</sub> production. Green H<sub>2</sub> is mainly used for two purposes, for methanol synthesis in combination with CO<sub>2</sub> streams from HTL and WO at the HTL plan site (see Figure 3) and as a source of refinery H<sub>2</sub> at the centralised upgrading facility (see Figure 4). It is a well-established finding, that the cost and Greenhouse Gas (GHG) emissions associated with H<sub>2</sub> generation play a key role in Power-to-X (PtX) schemes [6, 7], consequently the Central Denmark Region is chosen as regional context for the initial evaluation of the CIRCULAIR baseline configuration (compare to Section 2.2.1) as it is well suited for competitive H<sub>2</sub> generation from wind energy. Figure 6 shows average wind speeds and solar irradiation across Europe. The fluctuating nature of wind and solar energy induces a strong dependence of the capacity factors (CFs) of electricity generation and water electrolysis. Time resolved power profiles<sup>13</sup> will serve as a basis for the evaluation of the CIRCULAIR baseline configuration. Alkaline electrolysis (AEL) or proton exchange membrane electrolysis (PEM) will be chosen for the baseline case due to their ability for load following operation and their high technological maturity<sup>14</sup>. H<sub>2</sub> storage in form of pressurised tanks is chosen as a baseline approach to decouple fluctuating renewable electricity generation from the continuous operation of the HTL plant. However, various options to couple HTL conversion with H<sub>2</sub> from intermittent renewable electricity generation may be investigated in the course of the project.

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<sup>13</sup> Derived from <https://www.renewables.ninja/> or similar sources

<sup>14</sup> Note that the CIRCULAIR implementation employs an existing solid oxide electrolyser that operates at high-temperature. High-temperature electrolysis has specific advantages, especially in terms of energy conversion efficiency. Research and development of electrolysers is beyond the scope of CIRCULAIR, therefore more widely available low-temperature electrolysis is chosen.

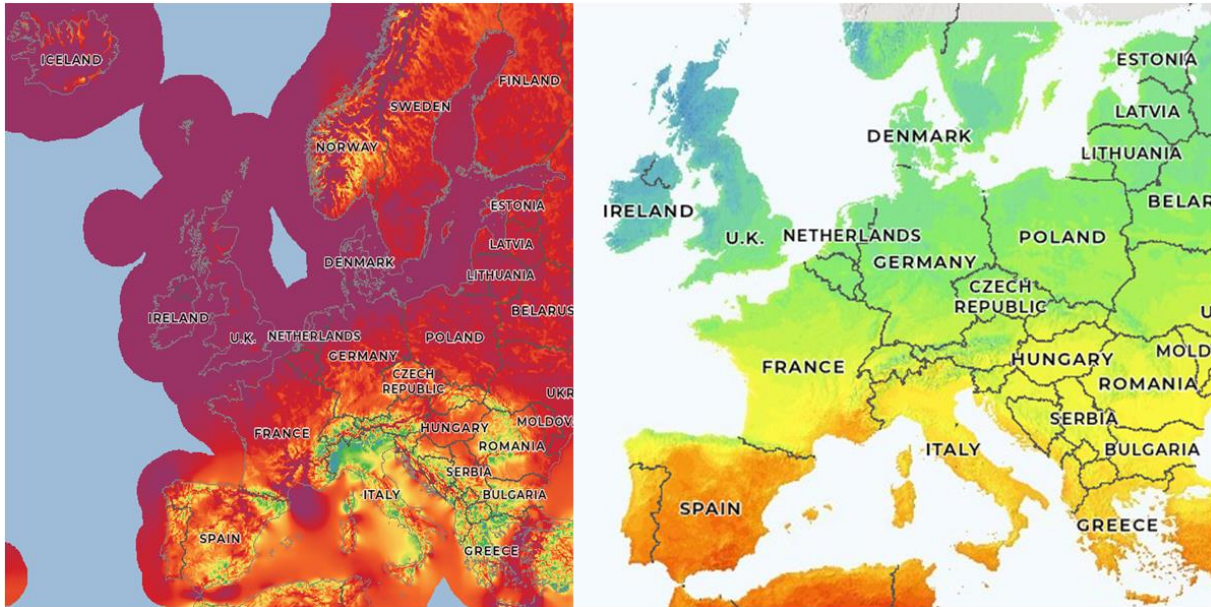


Figure 6: Left: Average wind speeds in Europe [8]. Purple shows the highest wind speeds, blue shows the lowest wind speeds. Right: Solar irradiation in Europe [9]. Red shows the highest solar irradiation, blue shows the lowest solar irradiation.

## 2.3 Technological options and alternative design choices

The preceding sections of Section 2 define a baseline configuration for the initial process modelling in CIRCULAIR. This definition requires baseline choices for several subcomponent technologies. It also narrows down the design space by choosing a specific configuration for an integration of the individual subcomponents. Such a reduction in design space is necessary for more detailed process modelling, the following Section 2.3.1 discusses technology and design choices and introduces alternative options for consideration at a later stage of the project. Section 0 becomes more specific on distinct options to create negative contributions to the global warming potential (GWP) of the CIRCULAIR pathway. The reference year in which HTL fuel production is considered is set to 2030.

### 2.3.1 Technology choices and alternative configurations

Table 1 identifies technology and design choices for selected process steps<sup>15</sup>. The initial modelling will be based on the baseline choices. The investigation of some alternative options is foreseen for the experimental implementation of the CIRCULAIR project (e.g., co-processing of manures and straw, slurry upgrading of HTL biocrude, alternative applications for HTL solids treatment). A further set of alternative options will be analysed on a system

<sup>15</sup> No alternative options are foreseen for HTL conversion, HTL process water treatment by WO, gas cleaning and recovery options for  $\text{NH}_4^+$  and VFA. HTL conversion is essential. Alternative options for WO, gas cleaning  $\text{NH}_4^+$  and VFA recovery will only be investigated if insights from the implementation require reconsideration.

analysis basis either to establish important reference cases (grid electricity, conventional H<sub>2</sub> generation<sup>16</sup>) or to investigate the option of additional jet fuel production via Methanol-to-Jet conversion (MtJ). Table 1 also lists further potential options that were identified as potentially important variations during the preparation of this public report, the investigation of these options is likely, but final decisions will be made at a later stage of the project.

Table 1: Baseline choices and important alternative options. Baseline choices correspond to the initial choice for process modelling. Alternative options for investigation identify variations that need to be considered, while the investigation of further potential options will be defined at a later stage of the project.

Subsystem	Baseline choice	Alternative options for investigation	Further potential options
Electricity supply	Wind	Grid electricity	PV, Wind/PV hybrid
Electrolysis	Low temp. electrolysis (AEL or PEM)	-	SOEC
H <sub>2</sub> supply	On site electrolysis	Steam reforming of natural gas <sup>16</sup>	Green H <sub>2</sub> pipeline network
Feedstock	Cattle manure	Cattle manure – wheat straw mixtures	Further types of manure and lignocellulosic residues
HTL solids	Soil amendment & carbon sequestration	Use as sorbent material	-
Biocrude upgrading	Fixed bed hydrotreatment	Slurry hydrotreatment	Use of HTL biocrude as marine fuel or fuel oil
CO <sub>2</sub> utilization	Power-to-Methanol	Methanol-to-Jet	CO <sub>2</sub> sequestration

<sup>16</sup> Only foreseen as H<sub>2</sub> source for biocrude upgrading (not meaningful as a H<sub>2</sub> source for methanol synthesis using effluent CO<sub>2</sub> from HTL plant sites)

### 2.3.2 Options to generate negative contributions to the GHG balance

One important objective of the CIRCULAIR project is the investigation of overall negative contributions to the GWP. The CIRCULAIR concept provides three main options to generate negative emissions. These are:

- Application of HTL solids to soils.
- A change in manure handling compared to the current practice.
- Potential sequestration of CO<sub>2</sub> from HTL and WO.

Only the utilisation of HTL solids for carbon sequestration and soil amendment is a central aspect of the experimental implementation of the CIRCULAIR project (see Section 1.1). Carbon sequestration may be achieved by fixing carbon from the feedstock in the soil, the long-term stability of this carbon fixation and the respective negative emission potential will be part of the analysis within the project. Furthermore, soil improvement and fertilising effect may reduce the climate impact of the overall process.

The second way of creating negative emissions could be achieved by an alternative manure handling strategy. Right now, manure is used in biogas plants, which are also an alternative to long-time storage or stored for longer periods, due to restrictions concerning its use as fertiliser, which is only allowed before plant growth phases. During these storage periods, significant amounts of GHGs are released. These GHG emissions could be reduced when using manure timely in an application such as fuel production via HTL. In this case, GHG emissions are avoided in the agricultural sector. In contrast to carbon sequestration, there is no physical GHG or carbon sink; however, the additional benefit of GHG emission avoidance may be attributed as a negative contribution to the balance of HTL fuel production. For communication and dissemination of results it will be important to clearly distinguish physical GHG or carbon sinks from negative contributions to the GHG balance of HTL fuel production that arise from emission avoidance in another sector (see Section 3.2.4).

The potential sequestration of CO<sub>2</sub> streams that result from HTL and WO is another way to generate negative contributions to the GHG balance. The baseline configuration (Figure 3) utilises the CO<sub>2</sub> streams for the synthesis of methanol, in order to increase the biomass resource utilisation for fuel production. On the other hand, CO<sub>2</sub> could also be used to create negative emission in so-called carbon capture and storage (CCS) scenarios. This option will only be addressed cursory in CIRCULAIR, i.e., no modelling of CCS is planned, but a rough quantification based on literature may be included.

## 3 Sustainable, social and economic impact analyses in CIRCULAIR

The main effort of the system analysis work in CIRCULAIR is dedicated to the development of tailored process models that describe all relevant parameters of a full-scale fuel production facility, and consecutive derivation of key performance parameters via environmental, techno-economic and socio-economic assessments. The preceding Section 2 described the context for the modelling by defining a baseline configuration. Section 3.1 defines the modelling framework that will be implemented in CIRCULAIR, while Section 3.2 defines the main purpose of the modelling framework in form of assessment criteria and metrics for evaluation.

### 3.1 Modelling framework

The high-level structure of the modelling framework is outlined in Figure 7. The system modelling is subdivided in three main process modelling efforts with different scope and different level of detail. High TRL processes such as electrolysis or methanol synthesis will mainly be modelled based on external references. Insights and experimental results from the CIRCULAIR implementation will be adopted for processes that are further developed within the project<sup>17</sup>. The system modelling will then provide key process parameters, such as energy and mass balances, for the further process assessment via LCA, TEA and socio-economic analyses.

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<sup>17</sup> Where necessary, results will be extrapolated to describe a full-scale facility.

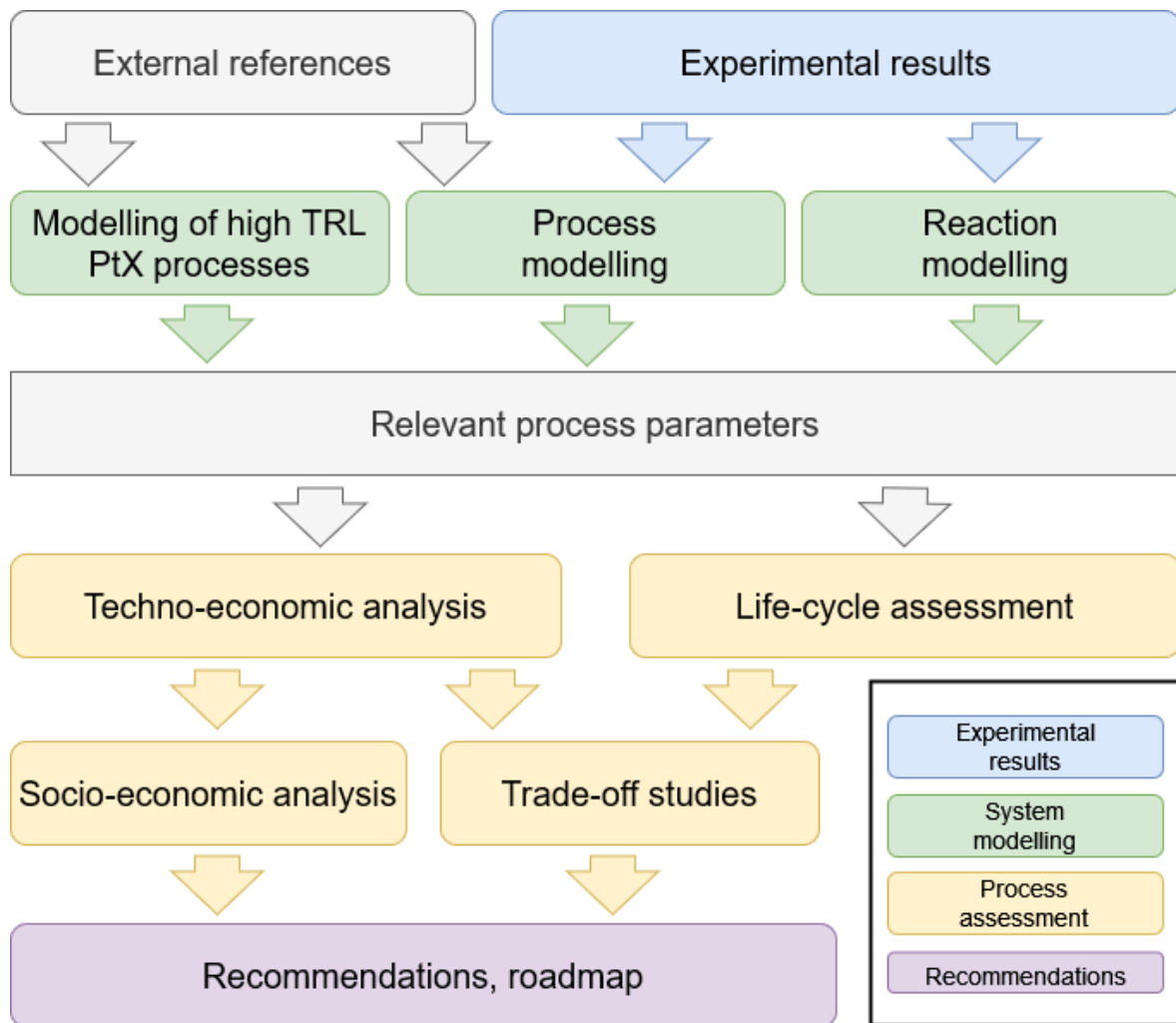


Figure 7: Outline of the modelling framework established in CIRCULAIR.

### 3.1.1 System modelling

The integrated process scheme of CIRCULAIR requires modelling of various subsystems and their interaction. Individual subsystems will be modelled at different level of detail. The focus will be on the modelling of HTL conversion based on a HTL reaction network. This work will be based on an existing in-depth model that has been established in the EU project HyFlexFuel [3, 10]. This existing model will be further improved and adapted to the conversion of manure and straw taking the results from CIRCULAIR experimental campaigns into account. Furthermore, numerical system models of all CIRCULAIR sub-processes will be developed based on experimental results obtained in CIRCULAIR. Where appropriate, this work will be based on prior models from the HyFlexFuel project [3, 10]. The process modelling will also cover the integration of all subsystems into an entire process chain on an industrially relevant scale. Hereby, a focus will be set on modelling of the thermal integration of HTL with WO of the HTL process water. Some subsystems, such as water electrolysis or methanol synthesis have already achieved a high level of technological maturity and are

therefore not subject of the research and innovation effort in CIRCULAIR<sup>18</sup>. These high TRL subsystems will be modelled at reduced level of detail based on literature and external references. Furthermore, the generation of additional jet fuel via methanol-to-jet conversion, which is not part of the CIRCULAIR implementation, will be modelled, again at reduced level of detail and based on external references. The main result from this system modelling is the quantification of overall mass and energy streams, as well as product compositions.

### 3.1.2 System analyses

In a next step, the relevant parameters from the process model are fed into the respective evaluation methods to determine key performance indicators. In the CIRCULAIR project, the main evaluation methods used to characterise the fuel production pathway are LCA, TEA and socio-economic analysis.

For the LCA, a strong emphasis will be put on the evaluation of the GWP and in particular on the evaluation of the potential to generate negative contributions to the GWP. In every LCA, a functional unit, as well as system boundaries have to be defined. In the CIRCULAIR project, the functional unit is defined as 1 MJ<sub>jet fuel</sub> and the investigated system is defined as well-to-tank.

The TEA will be used to determine jet fuel production cost from capital expenses (CAPEX), operational expenses (OPEX).

In case of the socio-economic analysis, the focus will be on evaluating the potential of a fruitful linkage of fuel production with regional economics, which will be measured as a regional job-creation potential. Additionally, the job-creation potential will also be evaluated outside of the region.

Overall, the aim of system analyses is to identify the key drivers of the environmental, economic and socio-economic performance.

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<sup>18</sup> Demonstration of methanol synthesis based on electrolysis H<sub>2</sub> and CO<sub>2</sub> from HTL conversion is part of the planned work, but no technology development of these process steps takes place. The purpose of this demonstration is to show that the CO<sub>2</sub> stream from CIRCULAIR fulfils the requirements for methanol synthesis, e.g., in terms of purity.

### 3.1.3 Allocation methods

The holistic refinery concept of CIRCULAIR results multiple products. A list of CIRCULAIR products is presented in the following:

- Main target product: Jet fuel from HTL biocrude upgrading.
- Main by-products (fuels):
  - Naphtha from HTL biocrude upgrading.
  - Methanol from PtX (CO<sub>2</sub> from WO and HTL offgas).
- Optional and alternative by-products:
  - HTL solids/char for soil amendment.
  - VFA recovered from process water after WO.
  - NH<sub>4</sub><sup>+</sup> recovered from process water.
  - Hydrocarbon rich gas from biocrude upgrading.
  - Methanol derived jet fuel (alternative to methanol as final PtX product).
  - Diesel and fuel oil from HTL biocrude upgrading.
  - Alternative use of HTL solids (e.g., as adsorbent).
  - CO<sub>2</sub> for sequestration (instead of PtX).

In the CIRCULAIR system analysis, the jet fuel fraction from the upgrading of HTL biocrude is defined as the main target product. Consequently, 1 kg or 1 MJ of HTL jet fuel is defined as functional unit for the TEA and LCA baseline case, respectively. The respective quantitative results for the techno-economic and environmental performance of HTL jet fuel production will then depend on the economic value and the environmental burden that is allocated to the different by-products. The proper methodological choice of by-product allocation is important as different allocation keys can be used and will likely lead to different results. Examples include:

- Physical allocation: Based on characteristics like mass, volume, or energy content.
- Economic allocation: Value of product and by-products.

The choice of allocation method is subject to the work on upcoming techno-economic and sustainability assessments in the course of the CIRCULAIR project. For instance, it is anticipated that the allocation method for the methanol by-product can have a significant impact on TEA, but also LCA results. This is due to the expected relevance of the methanol product stream (in relation to the amount of target product). On the other hand, the choice of allocation method may play a reduced role for smaller by-product streams. Since different allocation keys may produce different final results, proper by-product allocation is therefore an iterative process, whereby multiple allocation methods may be applied to show the impact of allocation key selection on the final results.

## 3.2 Assessment criteria and performance metrics

In the following Section, the criteria and metrics that will be used to answer the above established objectives and research questions. As can be seen, the structure of the assessment framework outlined in Section 1.3 is followed here. In addition, requirements specified in the topic description of HORIZON-CL5-2021-D3-02-09 are stated.

### 3.2.1 Requirements specified in topic HORIZON-CL5-2021-D3-02-09

As listed in Table 2, the choices of methods of system analysis, as well as criteria and performance metrics, which will be discussed in detail in the following sub sections, have been made in accordance with the scope of topic “HORIZON-CL5-2021-D3-03-09” under which CIRCULAIR is funded<sup>19</sup>.

Table 2: Requirements specified in topic HORIZON-CL5-2021-D3-02-09.

Scope of topic - general	Method of system analysis
Develop cost-effective solutions [...] in sustainable biofuel production	Techno-economic analysis
[...] along with addressing socio-economic aspects	Socio-economic assessment
Overall GHG emissions should be assessed on the basis of Life Cycle Analysis	Life-cycle assessment
Scope of topic - detailed	Criterion / Performance metric
TRL levels of 4-5 should be reached by the end of the project	Technology Readiness Level
Increase of biomass conversion efficiency	Carbon efficiency
Increase of bioenergy efficiency	Energy conversion efficiency
Increase of Sustainability, including sustainable biomass resource utilisation	<ol style="list-style-type: none"> <li>1. Fertiliser effect (of HTL solids)</li> <li>2. Long-term stability (of HTL solids)</li> <li>3. Sustainability of manure handling</li> <li>4. Global Warming Potential</li> </ol>
Biofuel production should generate negative emissions	Global Warming Potential

<sup>19</sup> <https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/opportunities/topic-details/horizon-cl5-2021-d3-03-09>

### 3.2.2 Process parameters

Important process parameters that will be evaluated during the CIRCULAIR project are part of Table 2. TRL describes the technical maturity of a process. TRL values go from TRL 1 to TRL 9, whereby TRL 1 equals basic research and understanding of the functional principle of a process and TRL 9 attributes demonstration in a commercial, industrial environment. TRL 4 is defined as “Technology validated in a lab” and TRL5 as “Technology validated in an industrially relevant environment”.

Secondly, two different process parameters to measure process efficiencies will be investigated. The first one is the energy conversion efficiency, which is defined as the energy content (LHV) of the fuel divided by energy input (including feedstock and auxiliary inputs). The second one is the carbon efficiency, defined as the quantities of carbon in the products divided by the total carbon present in the feedstock.

### 3.2.3 Life-cycle criteria

The main focus of the LCA in CIRCULAIR is the determination of the GWP. Within the determination of the GWP, two main aspects are anticipated to channel the analysis. First, it will be important to determine the impact of different design choices on the results of the baseline configuration. Secondly, as already discussed in Section 0, different options to generate negative contributions to the GHG balance play an important role in the analysis. In this regard, it is crucial to define criteria and performance metrics. These are:

- Fertiliser quality: describing how much HTL char is needed to achieve the same biomass yield as when using conventional fertiliser.
- Long-term stability: the long-term stability of HTL solids as soil amendment, i.e., the GHG emissions over a long period of time are not known yet.
- Current manure handling is known to have large GHG emissions, which potentially can be reduced by an alternative manure handling strategy, i.e., reducing storage time.

The effect of a reduced storage time on the GHG emissions will be evaluated.

Based on the GWP, the GHG emission reduction potential, i.e., the GHG emissions compared to those of the conventional jet fuel production can be deduced. Criteria and metrics for assessment of the environmental performance are shown in Table 3.

Table 3: Criteria and metrics for assessment of environmental performance.

Criterion	Performance metric	KPI type	Unit of measure
Fertilizer equivalence	Amount of HTL char to replace conventional fertilizer	Process step	%
Long-term stability of HTL char	GHG emissions	Process step	[g <sub>CO2eq</sub> /MJ <sub>jet fuel</sub> ]
Long-term stability of HTL char	Fixed carbon	Process step	[g <sub>fixed carbon</sub> /kg <sub>solids</sub> ]
Sustainability of manure handling	GHG emissions	Process step	[g <sub>CO2eq</sub> /MJ <sub>jet fuel</sub> ]
Global warming potential	GHG emissions	Entire process chain	[g <sub>CO2eq</sub> /MJ <sub>jet fuel</sub> ]
GHG emission reduction potential	Relative GHG emission reduction	Entire process chain	[-]

### 3.2.4 Techno-economic criteria

TEA studies have already concluded that HTL-based fuel production using residues is promising in terms of production costs, as there was no cost item identified that contributes excessively to the total costs [10, 11].

However, in the case of CIRCULAIR, specific questions arise that need to be answered from an economic perspective. An important aspect here is the process integration of HTL with WO, upgrading and the use of green H<sub>2</sub>. The process has to be designed efficiently and cost-effectively, taking into account the technical requirements. For this purpose, different plant configurations are considered and evaluated to see how they affect the fuel production costs. The economic analysis also considers the effect of scaling. The HTL plant size depends largely on how much feedstock is available. In the design of the biocrude upgrading plant, the economy of scale plays an essential role. The size of the upgrading plant and the transport distance are determined from an economic point of view and thus contribute to the more detailed definition of the baseline case over the course of the project (compare Section 2.1.3). In order to adequately assess the economics of the CIRCULAIR process, various techno-economic metrics are applied. To derive the total cost of products from plant, various cost items pertaining to the plant and its operation must be estimated. CAPEX is incurred for the acquisition of buildings, machinery, equipment, piping, service facilities, land, and other

resources necessary for the fuel production. OPEX are distinguished between direct, i.e., what is paid for the equipment that is actually supplied, and indirect cost components, i.e., for services that are required for the installation and use of the plant, such as engineering, legal costs, and construction costs. Table 4 shows selected parameters that are considered in more detail in the TEA.

Table 4: Selected techno-economic criteria and performance metrics.

Criterion	Performance metric	KPI type	Unit of measure
Economic competitiveness	CAPEX	Entire process chain	[€]
Economic competitiveness	OPEX	Entire process chain	[€/year]
Economic competitiveness	Production cost (PC)	Entire process chain	[€/MJ <sub>jet fuel</sub> ]

### 3.2.5 Socio-economic criteria

Job-creation is one of the most important socio-economic benefits of green-investment actions. To determine the social impacts of an HTL plant, its job-creation potential will be identified. This is not limited regionally (direct job-creation), but also indirect job-creation outside of the region of the plant will be evaluated. To execute this estimation, input-output (IO) tables will be employed. IO tables permit the assessment of both industry-specific and country-specific effects of investments. IO tables have seen frequent usage to determine demand increase and job-creation; because of the ready availability of public IO data, and because of it being a transparent, replicable methodology. Recent years have seen multiple publications that use IO tables to demonstrate the socio-economic benefits of investments in renewable energy generation.

### 3.2.6 Trade-off analyses

The baseline configuration aims at high biomass resource utilization and a high yield of jet fuel product as a starting point, in accordance with the overall objectives of the CIRCULAIR implementation. Trade-off analyses are foreseen at a later stage, for instance, it is anticipated that maximising resource utilisation may lead to different design configurations than minimising production costs. The definition of the trade-off studies will take place at a later stage, once first results from process modelling and performance analyses became available.

## 4 Conclusions and Outlook

CIRCULAIR investigates advanced biofuel production via hydrothermal liquefaction in an agricultural context, using manure and straw as feedstock. A hub and spoke approach are envisaged, in which several HTL plants gather the feedstock in a certain region and transform it into biocrude. The HTL biocrude will be transported to a centralised upgrading plant in order to yield fuel products. An important bottleneck of HTL applications, the treatment of the HTL process water, will be tackled by wet oxidation. Besides a clean-up of the process water, this also allows heat integration with the HTL reactor. Both HTL conversion and wet oxidation produce substantial amounts of carbon dioxide, which can be cleaned and used in PtX schemes for further fuel production. In the CIRCULAIR baseline case, the synthesis of methanol is envisioned. Furthermore, VFAs and ammonium are recovered from the process water after WO, and soil amendment using solids from HTL conversion is investigated.

Due to the highly integrated way the CIRCULAIR concept is set up, a huge number of design choices are potentially interesting, and several alternative options may be investigated. Section 2 defines a baseline configuration and initial design choices. Thereby, the design space is narrowed down, which is necessary to define a manageable framework for process modelling. In particular,

- A hub and spoke approach are chosen, in consequence two separate baseline designs are defined for the HTL plant site and the centralised biocrude upgrading site.
- An initial set of technology choices is defined for the respective baseline plant sites.
- The Central Denmark Region is chosen as regional context for initial evaluation. This region is preferential for agricultural residue supply and green H<sub>2</sub> production from wind energy.

This baseline configuration and subsystem technology choices establish the context of the initial process modelling in CIRCULAIR. Furthermore, alternative technology and design options were defined for investigation at a later stage of the project, this includes:

- Alternatives that are subject of investigation within the workplan of CIRCULAIR (alternative upgrading scheme, alternative use of solids, further upgrading of methanol product to jet fuel).
- Important reference cases that serve as comparator system for the CIRCULAIR baseline approach, such as the use of grid electricity for electrolysis or conventional H<sub>2</sub> generation from natural gas for biocrude upgrading.
- Further options to generate negative contributions to the GWP of fuel production.

Section 3 describes the initial concept for the process modelling and system analyses. The modelling approach foresees:

- a detailed description of core conversion processes that are experimentally investigated in CIRCULAIR, in particular an in-depth modelling of the HTL conversion;
- literature based modelling of high TRL PtX processes at reduced level of detail;
- system models that integrate the individual subsystems at the respective plant sites, with emphasize on thermal integration at the HTL plant site.

In order to evaluate the CIRCULAIR concept with respect to its objectives from a techno-economic, a life-cycle and a socio-economic perspective, suitable criteria and metrics have been identified and selected in accordance with the process chains and research questions. Important considerations relate to allocation methods, given the multi-input and multi-product nature of the CIRCULAIR process, and to the accounting of negative contributions to the GWP. The quantification of economic and environmental performance parameters will allow for the implementation of trade-off analyses at a later stage of the project<sup>20</sup>. In the final stage of the project key recommendations as well as a roadmap towards commercial exploitation will be derived from the results of the system analyses.

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<sup>20</sup> The baseline configuration aims at high biomass resource utilisation and a high yield of jet fuel product as a starting point in accordance with the high-level overall objectives of CIRCULAIR.

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