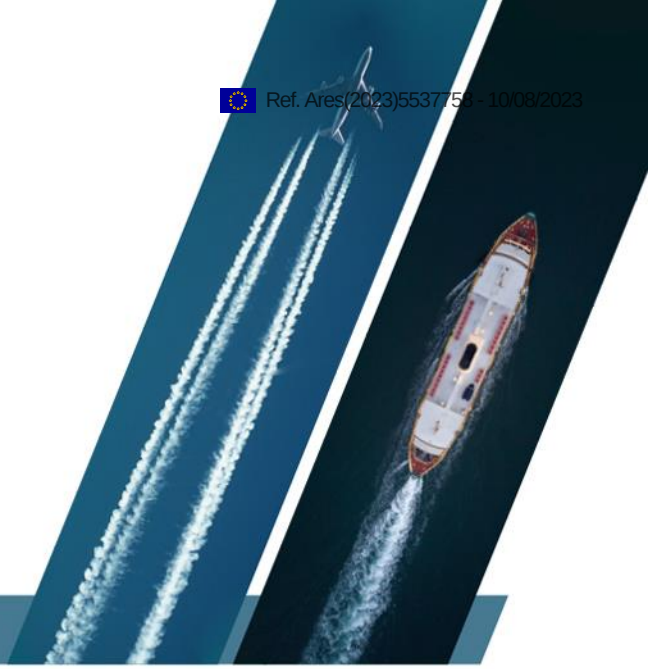
BioSFerA
Biofuel for biotravels



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Abbreviations

BtL	Biomass-to-Liquid
TAGs	Triglycerides
DFBG	Dual Fluidized Bed Gasification
CAPEX	Capital Expenditures
HRSG	Heat Recovery Steam Generator
WP	Work Package
PSA	Pressure Swing Adsorption
ATR	Autothermal Reforming
CGE	Cold Gas Efficiency
WGS	Water-Gas Shift
CU	Carbon Utilization
EFE	Energetic Fuel Efficiency
SAF	Sustainable Aviation Fuel
HEFA	Hydroprocessed Esters & Fatty Acids

Contents

1 Executive Summary

Building on the Biomass-to-Liquid (BtL) process chain, introduced in Deliverable D2.5, this report aims at further specifying, reforming, and optimizing the major aspects and the resulting Heat & Mass balances of the process layout, thus laying the foundation for further scale-up ambitions and socio-economic studies in the BioSFerA project. By using the latest input from WP3, WP4, WP5, and WP6, CERTH updated and modified the process layout and model in continuous communication with the involved partners.

Section 3 contains the updated description of each part (thermochemical, biotechnological, thermocatalytic) of the BioSFerA process chain as well as the elected configuration for the integrated concept. In section 4, the attention is given on the process adaptions and optimizations that ensure the model alignment with the up to now experimental findings. In section 5, using the updated process model, full-scale (200 MWth) simulations are performed and the generated stream results along with the energy/carbon balances are presented. Moreover, a commentary is provided regarding the correlation of the estimated performance and the initial project targets. Section 6 refers to the benchmarking of the proposed scheme with other established BtL technologies. Section 7 provides a summary of the most important points of the current document as well as the way forward.

The elected optimized configuration and the exported Heat & Mass balances constitute a remarkable milestone of the project that will serve its apt evaluation and further scale-up endeavors.

2 Introduction

The BioSFerA concept was initially introduced in Deliverable D2.5 'Full process basic definition' [1] (Figure 1). The overall process can be separated into three distinct parts: the thermochemical part, the biotechnological part and the thermocatalytic part. The thermochemical part is based on the Dual Fluidized Bed Gasification (DFBG) unit, followed by a catalytic reformer and a proper syngas conditioning (contaminants reduction). The biotechnological part contains the double stage syngas fermentation (syngas → acetic acid → lipids) and the subsequent lipids purification system. Finally, the thermocatalytic part refers to the hydrotreatment activities that are applied for the conversion of the obtained lipids (TAGs) into drop-in liquid fuels.

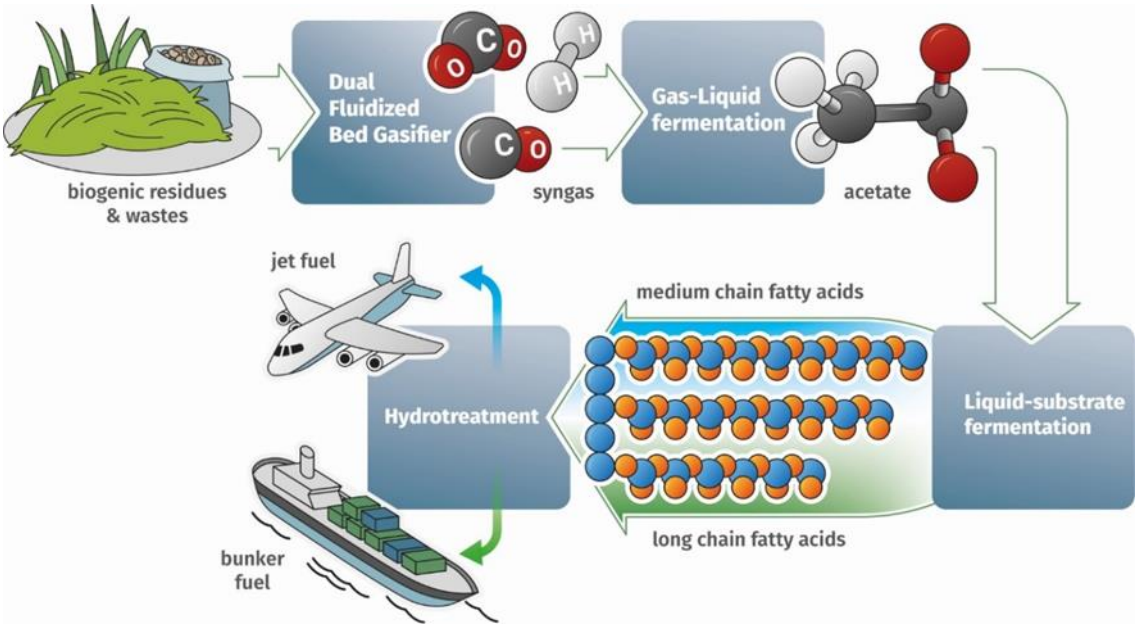

Figure 1. The BioSFerA concept [1]

The extensive experimental tests, that have taken place during the last period, allowed the re-evaluation of the technologies involved, the determination of their optimal operational framework, as well as the efficient integration of the individual components in the developed Biomass-to-Liquid (BtL) scheme.

3 Description of the BioSFerA concept

3.1 Thermochemical part

The conversion of the biomass feedstock into syngas is carried out with the DFBG technology. The aimed feedstock flexibility has been proved with the completion of Deliverable D3.1 'Bench-scale gasification tests at TRL4' [2]. The DFBG system consists of two interconnected CFB[1] (Circulating Fluidized Bed) reactors, the gasifier (fuel reactor) and the oxidizer (air reactor). The steam that enters the gasifier is generated via thermal utilization of hot syngas, while the flue gases from the oxidizer are used for the pre-heating of the air that enters the air reactor. Both hot streams (i.e. syngas & flue gas) may be available for further thermal exploitation in a Heat Recovery Steam Generator (HRSG). (Figure 2)

The gasification reactions take place in the gasifier, while the produced char, other residues (i.e. ash), and part of the bed material are transported to the oxidizer where they react with the oxidizing medium (i.e. air) to produce heat. The (hotter) bed material returns to the gasifier, serving as the heating medium for the endothermic steam gasification reactions. The produced raw syngas is filtered at the exit temperature of the gasifier and subsequently is catalytically reformed. The remarkable content of light hydrocarbons along with the non-negligible tars production indicate the need of catalytic reforming in the downstream process of BtL applications in order to avoid tar-related operational problems and enhance the H_2, CO syngas content. The autothermal reformer (ATR) is heated by partial syngas combustion with air, and in addition, the reforming reactions consume steam and/or CO_2.

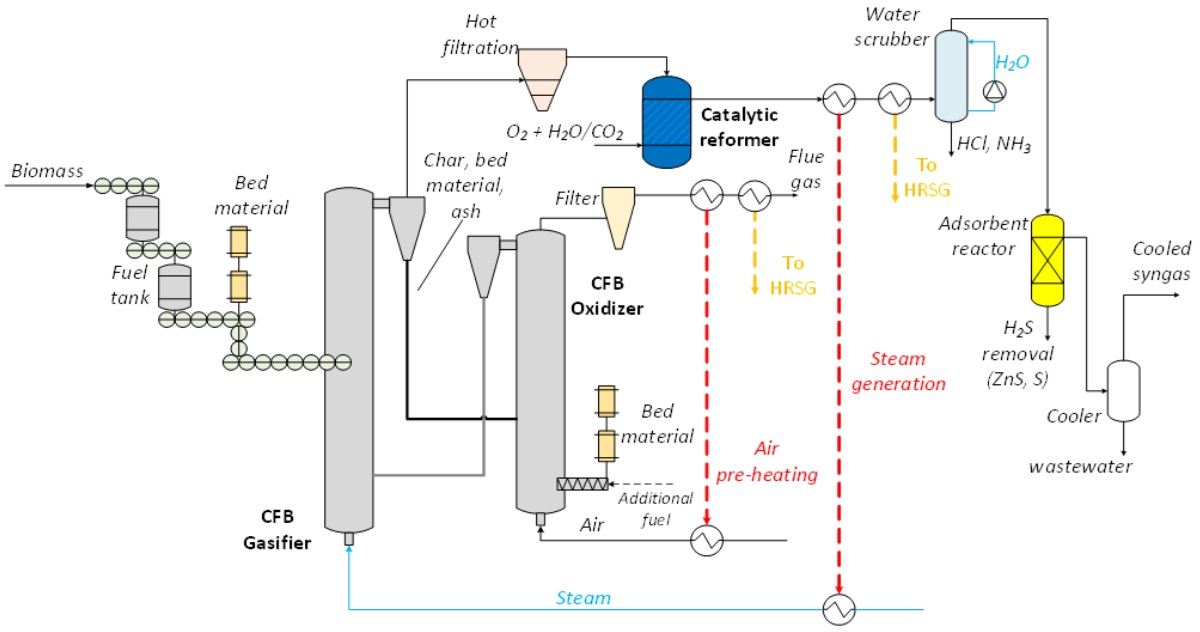

Figure 2. Thermochemical part of the BioSFerA value chain [1], [3]

[1] The DFBG configuration with two CFB reactors is recommended as the most suitable for large scale applications in terms of technical feasibility and has been adopted from VTT for the DFBG pilot plant as well [24]

The primary function of the catalytic reformer may be to convert tars and hydrocarbon gases to H_2 and CO, but it can also be modified to attain several targets relating to the syngas purification requirements for the subsequent fermentation process. For example, the reformer can be designed to largely decompose ammonia (NH_3) or hydrogen cyanide (HCN), and especially the latter which has turned out to be a major contaminant causing deactivation of the fermentation bacteria. The BioSFerA gas treatment unit, as initially proposed by VTT and introduced in Deliverable D2.5, consists of a water scrubber for the removal of hydrochloric acid (HCl) and an adsorbent reactor that utilizes metal oxides (e.g. Zn) and activated carbons (AC) for partial removal of sulfur compounds (H_2S, COS). Beyond that, depending on the target purity level, additional scrubbers and adsorbents (i.e. guard beds) can be implemented for the efficient removal of the undesired syngas contaminants.

The described gas cleaning unit was successfully tested during the first pilot test campaigns that were carried out recently in Finland (WP4 - VTT facilities). In particular, the obtained highly purified syngas was able to fulfill the gas fermentation requirements and sufficient syngas consumption from the microorganisms was observed. The applied gas cleaning scheme is already milder than the exhausting gas cleaning techniques (e.g. amines, Rectisol, etc.) required for chemical fuel synthesis applications (e.g. Fischer –Tropsch), but pilot tests with 'dirtier' syngas are still planned within BioSFerA project for further cost reductions related to gas cleaning demands (WP4). The pilot test activities were ongoing when this deliverable was being prepared and for that reason, any advancement concerning the further reduction of the required gas cleaning steps was not included in Task 6.2. Any suggested amendment in the presented gas cleaning chain will be financially evaluated in Deliverable D7.1 'BioSFerA Techno-Economical Assessment'.

The main operating conditions for the thermochemical part at industrial scale, as derived from the up to now experimental/pilot activities of VTT are presented in Table 1.

Table 1. Main operating conditions for the thermochemical part of the BioSFerA concept

Parameter	Input
Pressure (bar)	1.5
Gasifier temperature (°C)	780
Oxidizer temperature (°C)	880
Steam-to-biomass ratio (kg/kg dry,ash free)	0.7
Steam pre-heating temperature (°C)	350
Air pre-heating temperature (°C)	400
Reformer (ATR) temperature (°C)	900
Steam-to-carbon ratio (ATR) (mol/mol)	1.5
Pressure drop in the gasifier (bar)	0.2
Pressure drop in the reformer (bar)	0.2

3.2 Biotechnological part

In the first step of the biotechnological part of the process, the interaction of syngas with the acetogenic bacteria under anaerobic conditions leads to acetic acid production. For the syngas fermentation stage, after the extended experimental testing, *Moorella thermoacetica DSM 2955* was selected as the most efficient acetate producer strain [4]. The operating temperature is set around 55 °C, since the optimal temperature range for these strains is 55-60 °C [5]. The operating pressure of the reactor was

considered to be 5 bar in order to achieve higher solubility of the reacting gases. Two critical factors, that highly influence the fermentation kinetics and consequently the acetate productivity, are the gas solubility and the ratios of CO_2/CO/H_2. The unconverted syngas components (off-gas) can be either recycled back to the fermenter or utilized elsewhere in the plant (see section 3.4). The broth containing the produced acetate in low concentration is extracted in continuous way, and the liquid volume is kept constant by adding fresh culture medium. A cell recycling system (hollow fiber membrane) is required to keep the cells in the fermenter while extracting the liquid effluent. The procedure of acetate production in a continuous mode is illustrated in Figure 3 (left).

The second fermentation step refers to the production of TAGs via aerobic fermentation of the diluted acetic acid stream. Taking into account the experimental trials of WP3, *Yarrowia lipolytica*[2] is the yeast strain that has been selected to be involved in the liquid substrate fermentation of acetate [6], [7]. The diluted acetate effluent stream from the syngas fermentation enters the aerobic fermenter, where the targeted TAGs are formed as intracellular products in the presence of oxygen, additional nutrients, salts and the oleaginous yeast (*Y. lipolytica*). A cell recycle system (hollow fiber membrane) can be installed to recirculate the cellular biomass in the bioreactor while extracting the spent effluent. At the same time, a gaseous CO_2-rich stream is produced and leaves the bioreactor from the top. The continuous acetate fermentation process is schematically shown in Figure 3 (right).

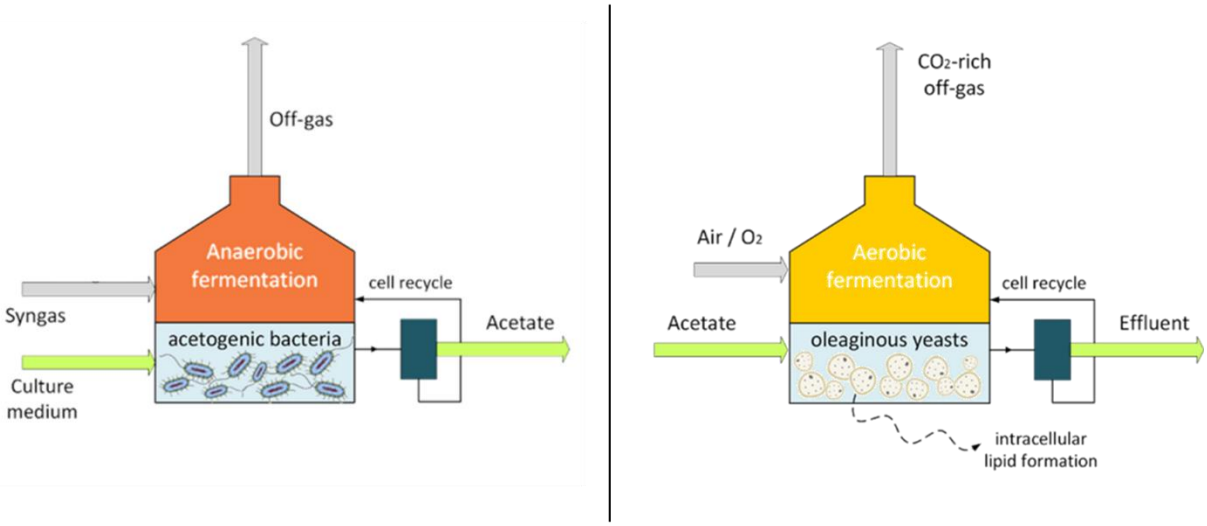

Figure 3. Syngas fermentation (left) and acetate fermentation (right) in a continuous mode [1], [3]

Lipids extraction from the oleaginous yeasts is an important step before hydrotreatment. As oleaginous yeasts present in the fermentation broth store lipids in intracellular forms, extraction is required to obtain TAGs. Cell disruptions alongside lipid extraction steps are critical for large-scale biofuel production in terms of cost adequacy. Mechanical disruption requires energy inputs such as shear forces, electrical pulses, waves or heat. Mechanical processes generally provide high products recovery yields with good management and scalability, but they are energy intensive. Among the options actually available, there are novel technologies with considerably lower power consumptions such as steam explosion, centrifugation and membrane separation considering different process parameters and extraction

[2] A genetically modified strain of *Yarrowia lipolytica*, able to accumulate high amount of lipids

procedures. Within BioSFerA project, based on the insights gained in Deliverable D3.6 ‘Lab scale downstream processing for TAGs recovery and purification using conventional and novel strategies’, a scalable DSP (downstream processing) train was defined for the efficient lipids recovery from the fermentation broth (Figure 4).

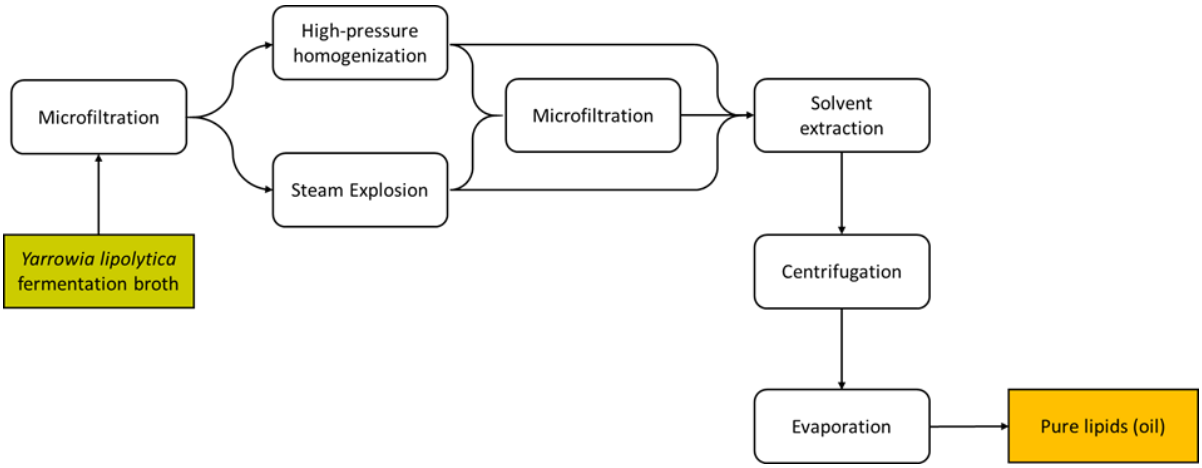

Figure 4. Proposed DSP train for lipids purification [8]

Steam explosion is an innovative method with reduced environmental impact, lower costs and energy demand, compared to other techniques that are widely used. In steam explosion, raw material exposed to steam at 180-240 °C for several minutes and then subjected to depressurization to ambient conditions. This generates an explosion that causes cell-wall disruption. In context in which heat flows are available as downstream of other processes, and so steam could be generated at low cost (such as the BioSFerA concept), steam explosion should be considered as potential technology for cellular biomass fractionation with high yields of recovery. The relevant experimental activities of WP3 revealed that steam explosion should be performed at low pressure and temperature (about 5 bar and 150 °C) in order to avoid the TAGs disruption. Microfiltration/Centrifugation have been positively evaluated for their ability to separate oil from the broth deriving from steam explosion. The solvent extraction step should be further investigated because of the difficulties associated with the formation of emulsions.

The choice between using the high-pressure homogenization or steam explosion for the cell-breaking stage for future scale up of the DSP process should be made following some technical and economic considerations. Before solvent extraction, a microfiltration step can be included to remove the cell debris and to increase lipids concentration. A detailed investigation of the investment costs and the energy consumptions can be part of BioSFerA Task 6.3 ‘Process layout and cost engineering’ as well as Task 7.1 ‘Techno-economic assessment’.

The main operating conditions for the biotechnological part at industrial scale, as derived from the up to now experimental/pilot activities of BBEPP, CARTIF, CSIC, and ENVIPARK are presented in Table 2.

Table 2. Main operating conditions for the biotechnological part of the BioSFerA concept

Parameter	Input
Gas Fermentation Pressure (bar)	5
Gas Fermentation Temperature (°C)	55
Liquid Fermentation Pressure (bar)	1
Liquid Fermentation Temperature (°C)	28
Steam Pressure for Steam Explosion (bar)	5
Steam Temperature for Steam Explosion (°C)	150

3.3 Thermocatalytic part

The final section of the BioSFerA value chain includes the upgrading of microbial oil into drop-in aviation and marine biofuel. The core of the thermocatalytic part of the concept is the hydrotreatment unit where the consecutive hydrogenation, deoxygenation, isomerization and fractionation procedures of the purified TAGs take place. Common catalysts for this process are Pt, Ni or other metals based on Al_2O_3.

In particular, the saturated fatty acids are converted to straight long-chain alkanes by hydrodeoxygenation and decarboxylation, co-producing propane, methane, water, CO, and CO_2. The deoxygenated straight chain paraffins are selectively hydrocracked or isomerized yielding highly branched alkanes. The resulted organic product is a mixture of straight and branched C_nH_{2n+2} that can be suitably used as drop-in liquid fuel. Fractionation is necessary to separate the jet from marine fraction.

The envisaged configuration for the hydrotreatment unit is presented in Figure 5.

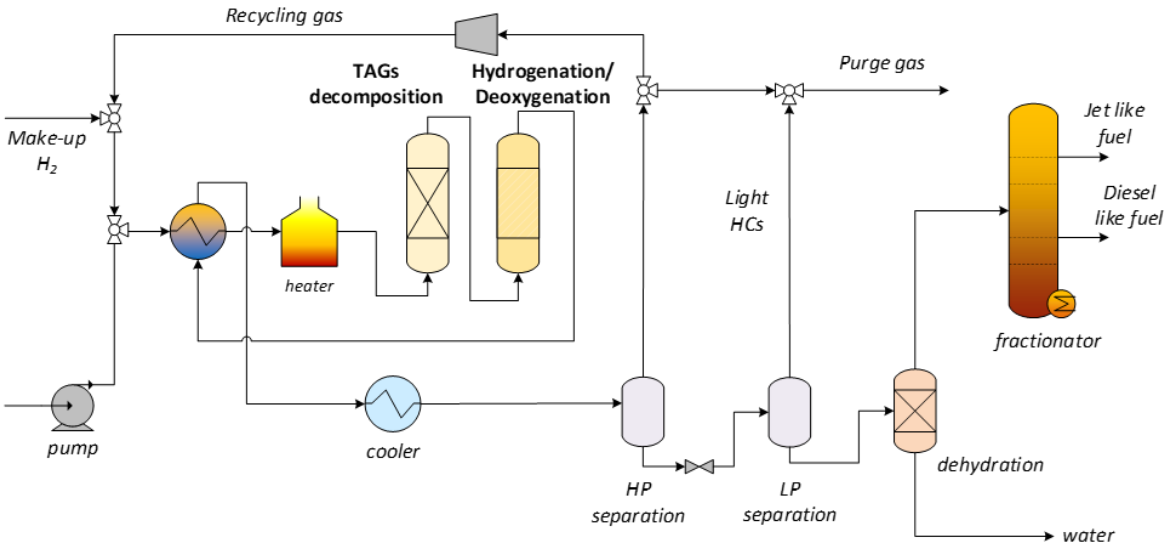

Figure 5. Hydrotreatment of the BioSFerA value chain [1], [3]

The main operating conditions for the thermocatalytic part at industrial scale, as derived from the up to now experimental/pilot activities of CERTH and KPRT are presented in Table 3.

Table 3. Main operating conditions for the thermocatalytic part of the BioSFerA concept

Parameter	Input
Reactor pressure (bar)	100
Reactor temperature (°C)	370
Hydrogen-to-TAGs ratio (kg/kg)	0.05

3.4 BioSFerA integrated Biomass-to-Liquid (BtL) process chain

Taking into account the extensive conceptualization and design considerations of Deliverable D2.5 'Full process basic definition' as well as the findings from the experimental activities of each sub-process, the integrated BioSFerA process chain was updated targeting to the greatest possible performance and cost efficiency. The elected (optimized) configuration of the integrated BioSFerA value chain is illustrated in Figure 6.

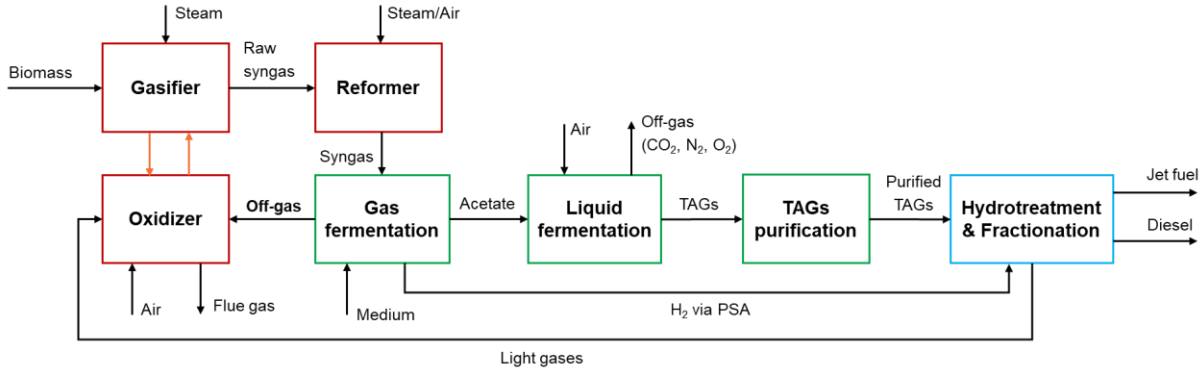

Figure 6. Block Flow of the integrated BioSFerA concept

The major aspects of the integrated concept are:

- Utilization of the off-gas (unreacted gas) of the anaerobic fermentation (gas fermentation) in the oxidizer of the DFBG unit → higher gasification efficiency, avoidance of technical barriers related to internal gas recycle in the bioreactor (i.e. inerts/contaminants accumulation)

- Internal hydrogen extraction (and supply to the hydrotreatment unit) from the off-gas of the anaerobic fermentation via PSA (Pressure Swing Adsorption) → avoidance of such an energy/cost-consuming unit like an electrolyzer

- Air-driven autothermal reforming of syngas hydrocarbons instead of oxygen-driven, since in the absence of gas recycle in the bioreactor, some nitrogen content in the reformed gas would not be a critical problem → avoidance of operational costs related to external purchase of industrial oxygen

A more detailed schematic of the suggested Biomass-to-Liquid (BtL) process chain, originating from the latest input from all project partners is given in Figure 7. Based on this layout, the main stream results as well as the process heat and mass balances are calculated (see section 5).

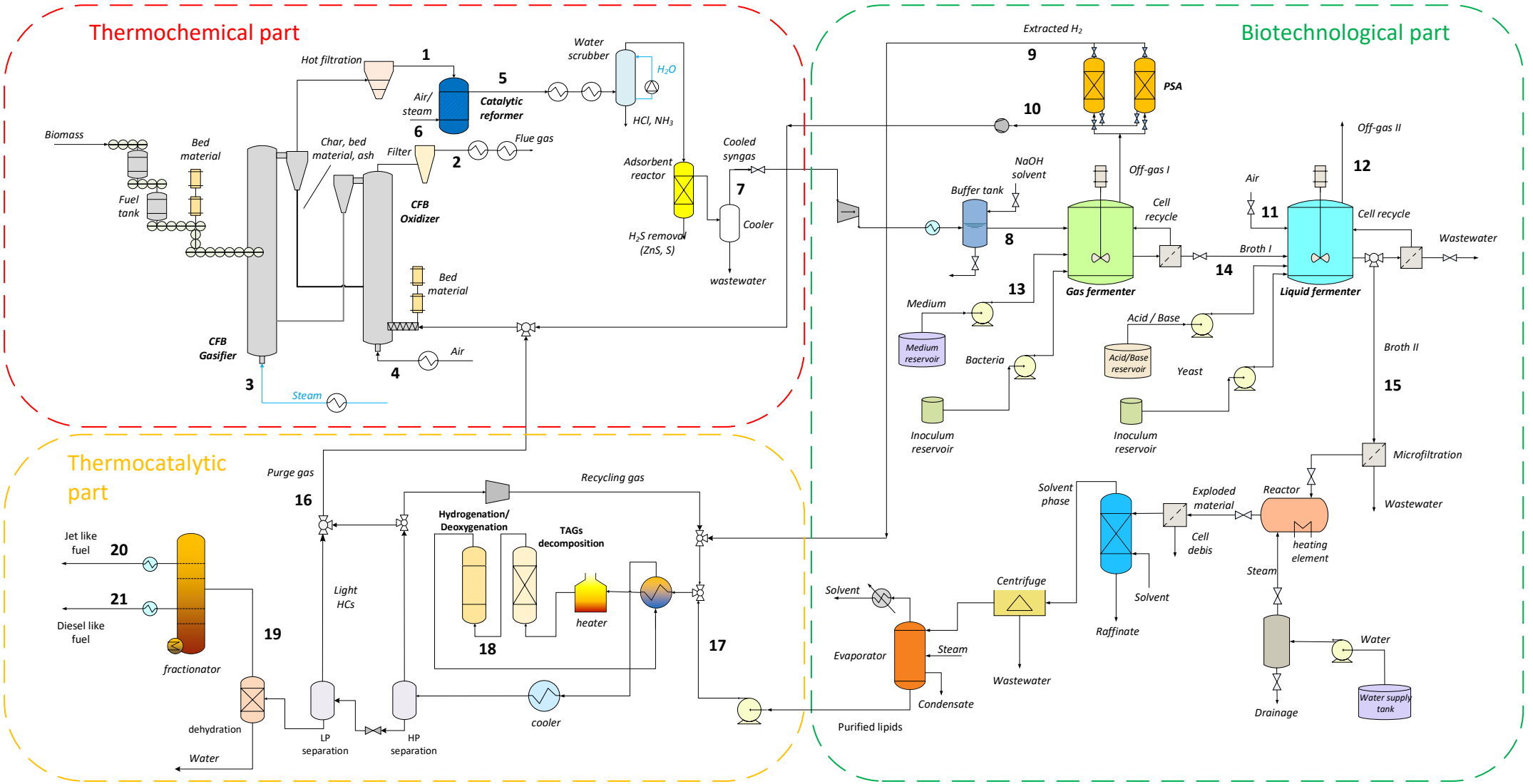

Figure 7. Process Flow Diagram (PFD) for the BioSFerA BtL process chain

4 Optimization of model parameters and model adaptations

The model development for the full-scale (200 MWth)[3] BioSFerA concept was largely based on the design considerations of Deliverable D2.5 'Full process basic definition'. Every performed experimental activity up to this point was taken into account for the validation of the process as well as the optimization of the model. This section refers to the main interventions (optimization measures) that were carried out in order to enhance the fidelity of the model and the effectiveness of the concept design.

4.1 Dual Fluidized Bed Gasification (DFBG)

The DFBG upscaling was investigated in Task 6.1 'Model development of the gasification process' [9]. In particular, SHI FW generated an initial design for the full-scale unit (Figure 8) and, after calibrating their comprehensive DFBG model according to actual DFBG pilot runs (200 kWth) performed by VTT, proceeded with full-scale (100 MWth) calculations. An estimate on the dimensioning of the illustrated design will be included in Deliverable D6.3 'Process layout and cost engineering of the BioSFerA biorefinery plant'.

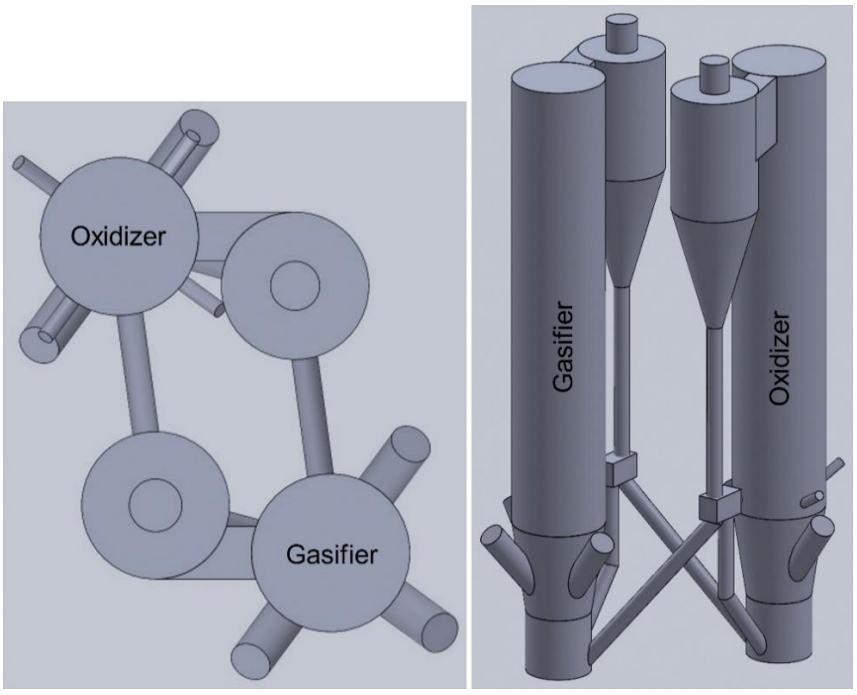

Figure 8. Initial design of the full-scale unit [9]

The DFBG upscaling considerations as well as the full-scale simulation results by SHI FW were utilized by CERTH in order to assess the reliability of the 200 MWth DFBG model that serves the calculation of

[3] A potential plant scale of 200 MWth has been selected for the full-scale BioSFerA process simulations. The feedstock availability for a plant of this size has been secured (WP2). Moreover, also other past BtL projects (CLARA, COMSYN, FLEXCHX) assume a plant of 200 MWth to support their techno-economic analysis. This fact will also facilitate the benchmarking with other similar gasification based technologies.

the overall Heat & Mass balances in the present document. Thus, Figure 9 presents the correlation between the actual pilot runs (200 kWth) by VTT, the 100 MWth simulations by SHI-FW, and the 200 MWth simulations by CERTH. The focus is given on the main syngas species (H_2, CO, CO_2, CH_4). In all cases, autothermal DFBG operation was considered (no external fuel, 1% inherent heat losses).

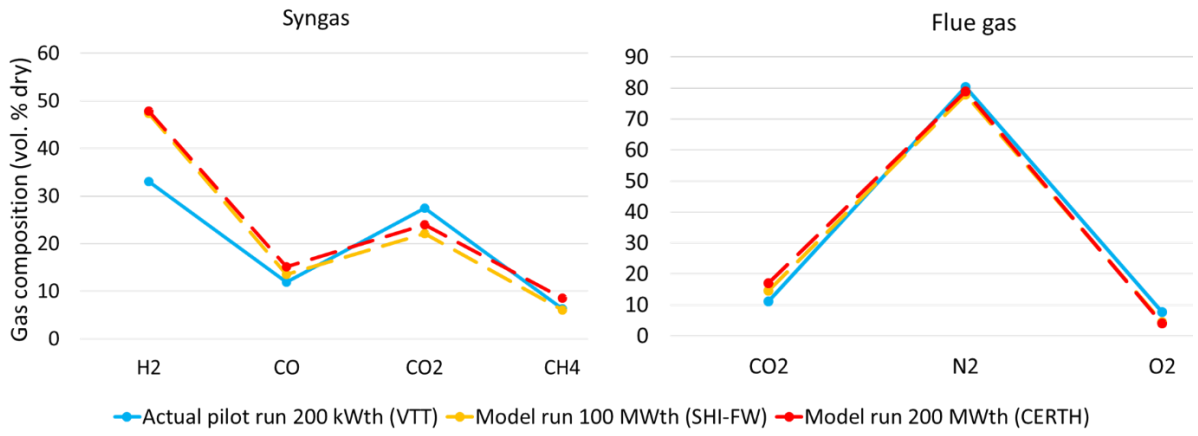

Figure 9. Validation of the 200 MWth DFBG model

It is observed that the 200 MWth 'syngas curve' (red) matches well with the corresponding 100 MWth syngas composition (orange) simulated by SHI FW. The discrepancies between the simulated commercial applications and the actual pilot runs (blue) are mainly due to the increased nitrogen content (~20%)[4] of the produced gas during the pilot tests. On the contrary, the share of purge nitrogen in potential commercial applications is smaller and the produced syngas is of higher quality. As expected, the flue gases composition is almost identical for all three cases. In summary, the 200 MWth DFBG model seems to be in good agreement with the SHI FW predictions (100 MWth) regarding the operation of a commercial DFBG system, and both large-scale simulation results follow in a logical way the actual experimental results (pilot tests). Thus, it can be considered as a reliable tool for the full-scale process simulations of the BioSFerA concept.

4.2 Syngas fermentation (Anaerobic gas fermentation)

The optimization of the gas fermentation model was based on data extracted from the WP3 and WP4 tests as well as on literature studies for similar industrial processes (e.g. gas fermentation for ethanol production).

To represent the growth of the acetogenic bacteria (*Moorella thermoacetica*) taking place in the reactor (RStoic), Reactions (1) & (2) were added. It was assumed that ammonia (NH_3) is the nitrogen source during growth. The elemental formula for the bacteria was considered to be $CH_{1.75}O_{0.5}N_{0.25}$ [10].

$$2\,CO + 0.25\,NH_3 + 0.5\,H_2O \rightarrow CH_{1.75}O_{0.5}N_{0.25} + CO_2 \quad (1)$$

[4] Due to the inherent constraints of a pilot configuration, some air is introduced in the gasifier during the DFBG pilot tests in order to ensure stable performance. This leads to increased percentage of N_2 in the produced gas. This is not the case in potential commercial DFBG units, where almost nitrogen-free syngas is attainable.

$$CO_2 + 2\,H_2 + 0.25\,NH_3 \rightarrow CH_{1.75}O_{0.5}N_{0.25} + 1.5\,H_2O \quad (2)$$

The acetic acid production was simulated by Reactions (3) & (4). Based on literature and the fermentation tests conducted in WP3, which have demonstrated that *M. thermoacetica* does not generate any by-products, no by-product formation was considered in the model.

$$4\,CO + 2\,H_2O \rightarrow CH_3COOH + 2\,CO_2 \quad (3)$$

$$2\,CO_2 + 4\,H_2 \rightarrow CH_3COOH + 2\,H_2O \quad (4)$$

The conversion rates for Reactions (1) - (4) can be seen in Table 4.

Table 4. Conversion rates for syngas fermentation.

Parameter	Input
Conversion of CO in Reaction (1)	0.05
Conversion of H_2 in Reaction (2)	0.05
Conversion of CO in Reaction (3)	0.95
Conversion of H_2 in Reaction (4)	0.95

A high gas utilization was assumed since in large-scale reactors, the increased surface area, the enhanced mixing, the reduced concentration gradients and the optimal process design allow for efficient gas transfer. Specifically, after reviewing literature on gas fermentation for ethanol production [11], [12], a 90% utilization percentage for CO and an 80% utilization percentage for H_2 were selected. Therefore, the low quantity of unreacted syngas in the off-gases of the fermenter eliminates the need for installing a gas recycle system. Consequently, this eliminates associated operational risks and costs, such as the accumulation of impurities and inert gases, as well as the compression of larger gas volumes. Thus, it was decided to utilize this quantity of unreacted gas in the oxidizer of the DFBG unit (combustion). This is expected to enhance the carbon conversion in the gasifier and subsequently improve the quality of the produced syngas.

4.3 Acetic acid fermentation (Aerobic liquid fermentation)

To optimize the liquid fermentation model, a similar approach was adopted, wherein data was collected from the WP3 and WP4 liquid fermentation tests, as well as from relevant literature studies on microbial oil production.

The fermentation broth from the gas fermenter containing 30 g/L acetic acid is sent directly to the liquid fermenter. The results obtained from the WP3 and WP4 fermentation tests indicated that the oleaginous yeast can grow effectively on the broth deriving from the gas fermenter, without the necessity of any purification steps.

The liquid fermentation was divided into two phases: the growth phase and the lipid production phase. Reaction (5) was added for biomass formation. It was assumed that ammonia (NH_3) is the nitrogen source during growth. The elemental formula for the yeast was considered to be $CH_{1.66}O_{0.54}N_{0.14}$.

$$CH_3COOH + 0.908\ O_2 + 0.147\ NH_3 \rightarrow 1.05\ CH_{1.66}O_{0.54}N_{0.14} + 0.95\ CO_2 + 1.349\ H_2O \quad (5)$$

Reactions (6) - (9) describe the intracellular lipid production phase. Triolein ($C_{57}H_{104}O_6$), tripalmitin ($C_{51}H_{98}O_6$), trilinolein ($C_{57}H_{98}O_6$) and tristearin ($C_{57}H_{110}O_6$) were selected as the representative TAGs produced during this phase.

$$59\ CH_3COOH + 38\ O_2 \rightarrow\ C_{57}H_{104}O_6 +\ 61\ CO_2 +\ 66\ H_2O \quad (6)$$

$$50.11\ CH_3COOH + 27.72\ O_2 \rightarrow\ C_{51}H_{98}O_6 +\ 49.22\ CO_2 +\ 51.22\ H_2O \quad (7)$$

$$62\ CH_3COOH + 45.5\ O_2 \rightarrow\ C_{57}H_{98}O_6 +\ 67\ CO_2 +\ 75\ H_2O \quad (8)$$

$$56\ CH_3COOH + 30.5\ O_2 \rightarrow\ C_{57}H_{110}O_6 +\ 55\ CO_2 +\ 57\ H_2O \quad (9)$$

The conversion rates for Reactions (5) - (9) are gathered in Table 5. The TAGs representation and conversion rates have been set in a way to be consistent with the fatty acid distribution extracted during the WP3 experimental tests (Figure 10).

Table 5. Conversion rates for acetate fermentation.

Parameter	Input
Conversion of CH_3COOH in Reaction (5)	0.1
Conversion of CH_3COOH in Reaction (6)	0.428
Conversion of CH_3COOH in Reaction (7)	0.211
Conversion of CH_3COOH in Reaction (8)	0.126
Conversion of CH_3COOH in Reaction (9)	0.135

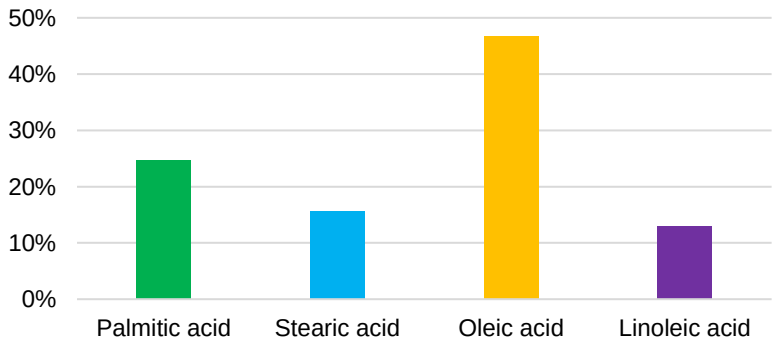

Figure 10. Fatty acid distribution (simulation output).

The air supply flow rate for the two phases was regulated by the oxygen concentration in the off-gases, as measured during the lab tests of WP3. Specifically, according to the lab results, the oxygen content in the off-gases is 16% and 18% during the growth and lipid accumulation phase, respectively.

The simulation results of the two-step fermentation process (gas fermentation & liquid fermentation) were compared and found to be consistent with the results obtained from the continuous fermentation tests conducted by BBEPP, which indicates the reliability and validity of the simulation model.

4.4 Influence of acetic acid & TAG productivity on residence time and working volume of gas and liquid fermentation

In order to gain a clearer understanding of the design requirements and specifications of the two-stage fermentation unit, a sensitivity analysis was performed. The analysis was based on the 200 MW_{th} simulations and focused on examining how the productivity of AA and TAGs affects the residence time, the total working volume, and the number of reactors in gas and liquid fermentation, respectively.

In the sensitivity analysis conducted for the gas fermentation, the gas utilization percentages and the reaction conversions were held constant at the aforementioned values (see Section 4.2). The AA titer was also fixed at 30 g/L. The results can be seen at Figure 11, Figure 12 and Figure 13.

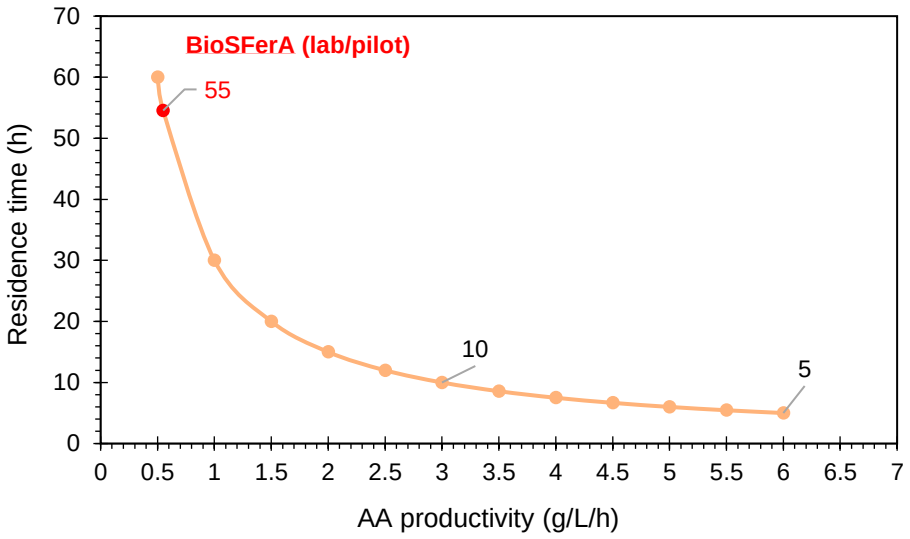

Figure 11. Influence of AA productivity on residence time (gas fermentation).

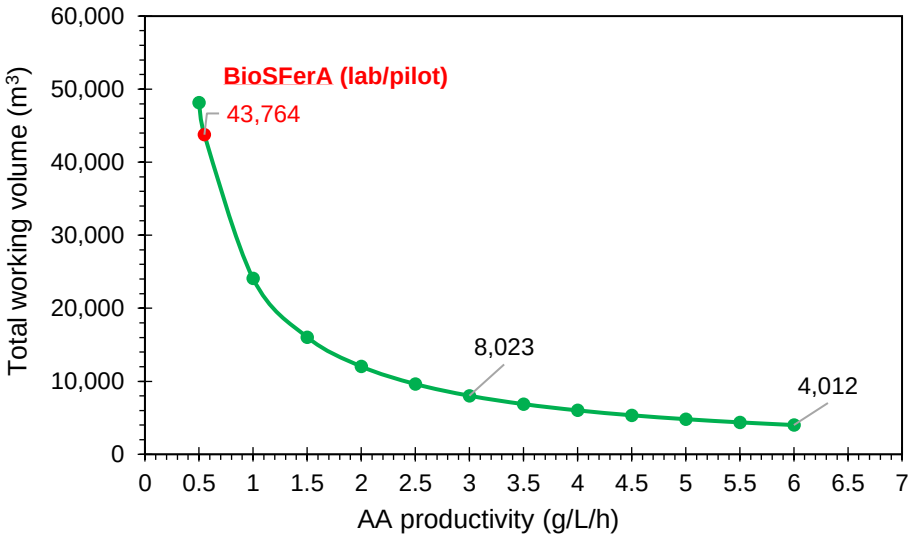

Figure 12. Influence of AA productivity on total working volume (gas fermentation).

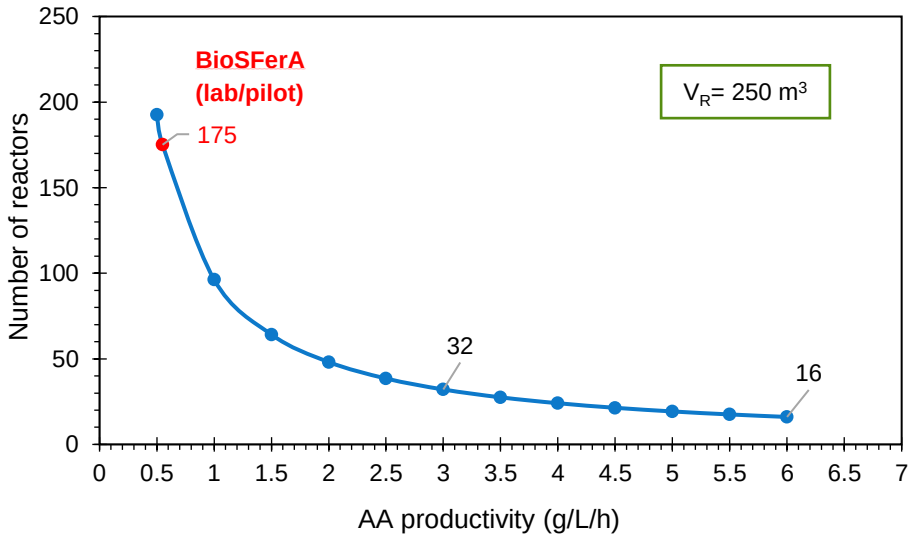

Figure 13. Influence of AA productivity on total number of reactors (gas fermentation).

Similarly, in the sensitivity analysis conducted for the liquid fermentation, the reaction conversions were fixed at the aforementioned values (see Section 4.3) and the AA concentration in the feed was maintained at 30 g/L. Figure 14, Figure 15 and Figure 16 depict the obtained results.

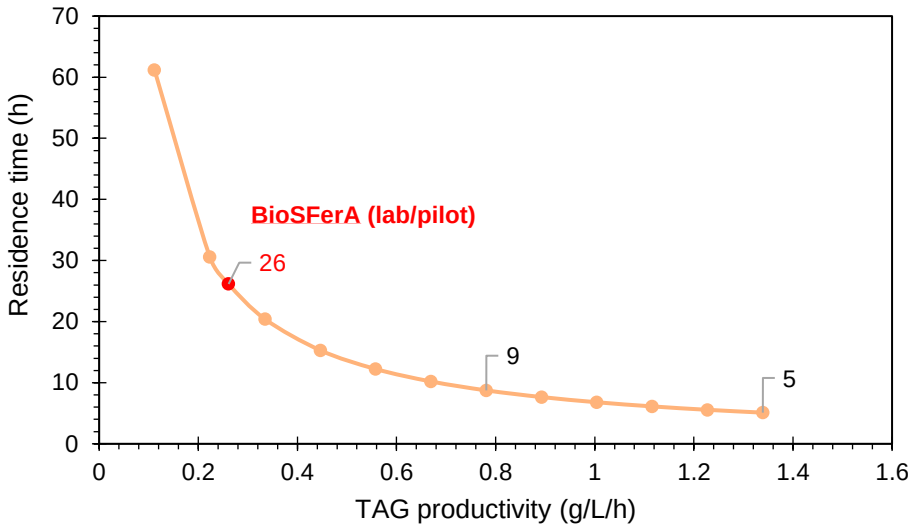

Figure 14. Influence of TAG productivity on residence time (liquid fermentation).

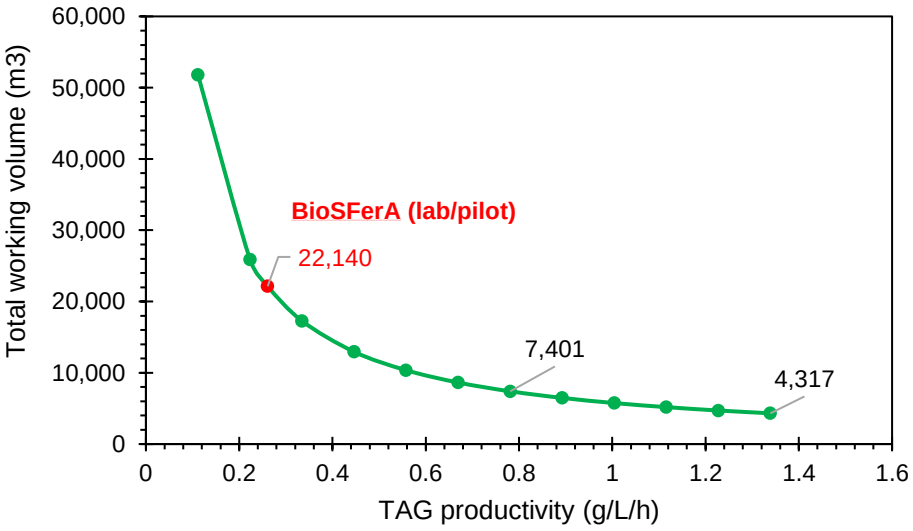

Figure 15. Influence of TAG productivity on total working volume (liquid fermentation).

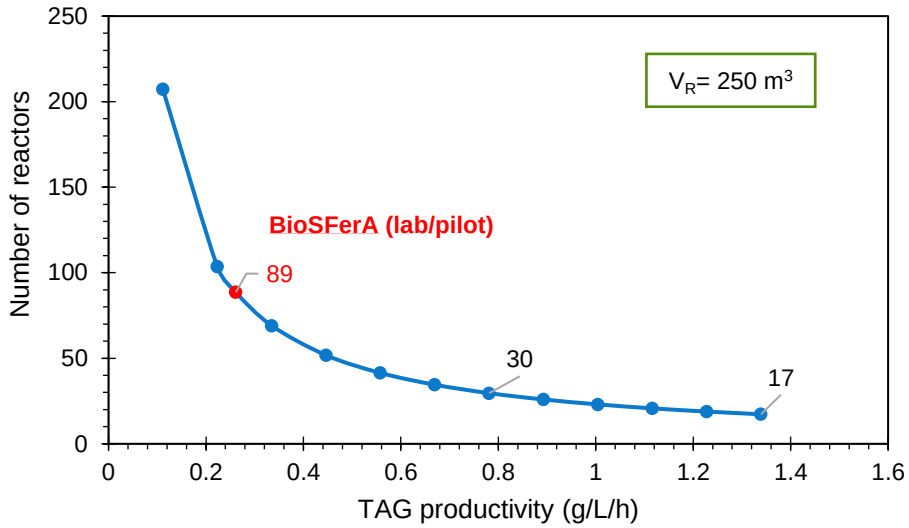

Figure 16. Influence of TAG productivity on total number of reactors (liquid fermentation).

As expected, the BioSFerA productivity targets that refer to the lab/pilot tests (AA productivity: 0.55 g/L/h & TAG productivity: 0.26 g/L/h) are still far from meeting the demands of commercial-scale applications. Such low productivities would lead to excessively long residence times and subsequently unfeasible working volumes and required number of reactors[5] in an industrial setup. Therefore, higher productivity values for AA (>3 g/L/h) and TAGs (>0.8 g/L/h) will be adopted for the scaled-up configuration, aligning with more suitable figures for industrial applications, as supported by relevant literature [13]–[15]. It has to be mentioned that the work carried out within this task related to the industrial layout of the biological part can serve as preliminary input for Task 6.3 'Process layout and cost engineering'.

4.5 TAGs hydrotreatment

For the enhancement of the thermocatalytic part, the model was updated and enriched with data obtained from CERTH's TRL3/4 hydrotreatment tests performed during Task 5.2 'Selection of 2 catalyst and preliminary processing conditions' [16], as well as data extracted from the literature.

More specifically, the operating conditions for the hydrotreatment model were carefully reassessed (see Table 3) and their selection was based on CERTH's experimental activities for the optimum catalytic system selection. Moreover, the final yields of the jet and marine fractions (47% and 53%, respectively) were determined based on the same experimental results.

The paraffinic composition of the two fuel fractions (as detailed in section 5.1, Table 9, streams 20 & 21) was based on relevant literature studies focusing on the production of jet-like and diesel-like fuels from hydrotreated oils [17], [18]. The simulated jet and marine fuels resulted in LHVs of 44.4 MJ/kg and 43.8 MJ/kg, respectively.

[5] To determine the required number of reactors, a standard bioreactor operating volume typically employed in industrial fermentation applications (V_R=250 m^3) was used for the calculations.

Special focus was given on the jet fuel due to its strict specifications that ensure the fuel's safety, performance, and compatibility with aircraft engines. Table 6 provides information on the properties of jet fuel stream deriving from fractionation of the hydrotreated oil, as calculated in Aspen Plus, along with the respective specifications for commercial Jet A-1.

Table 6. Properties of the produced jet fuel (deriving from fractionation) and Jet A-1 specifications (ASTM D1655)

		Simulated Jet	Jet A-1 spec
LHV	MJ/kg	44.4	> 42.80
Density (15 ºC)	kg/m^3	730	775–840
Viscosity (-20 ºC)	mm^2/s	5.45	< 8.0
Flash point	ºC	48.5	> 38.0
Distillation 10%	ºC	170.9	< 205.0
Distillation 100%	ºC	270.7	< 300.0

As can be seen, the obtained jet fuel stream simulates the targeted fuel relatively well with most of its properties meeting the specifications for Jet A-1. This can be considered as a form of validation for the model. However, it has to be pointed out that the simulated jet and diesel streams consist only of normal paraffins. Although these paraffinic fuel fractions form a solid basis for the representation of the targeted drop-in fuels, the actual drop-in fuels usually contain also iso-paraffins, cycloparaffins and aromatics in order to meet the necessary standards for safe and efficient use in jet and diesel engines.

5 Heat & Mass balances

Updated full-scale (200 MWth) process simulations were performed for the BioSFerA integrated BtL process chain. A 200 MWth (mass $flow_{feedstock}$ = 11.24 kg/s, $LHV_{feedstock}$ = 17.79 MJ/kg a.r.) plant with crushed bark[6] as feedstock has been elected as the 'base case scenario'. The main stream results for the case of crushed bark are presented in Table 7, Table 8, and Table 9. The stream results comprise of three tables, as it was decided to include one table for each of the main parts of the BioSFerA concept (i.e. thermochemical part, biotechnological part, thermocatalytic part). All the stream numbers and descriptions refer to the BioSFerA BtL flowsheet presented in section 3.4. Moreover, the Heat & Mass balances of the overall value chain were solved and the overall performance of the concept was assessed via two critical factors:

- Energetic Fuel Efficiency (EFE) is the fraction of the chemical energy in the initial feedstock that is transferred to the final fuels
- Carbon Utilization (CU) is the fraction of carbon in initial feedstock that is converted to the final fuels

5.1 Stream results

Table 7. Stream results for the thermochemical part (BioSFerA 200 MWth full-scale simulations)

Stream No	1 Syngas after filtration	2 Flue gas after filtration	3 Pre-heated steam	4 Pre-heated air	5 Reformed syngas (ATR)	6 Air (ATR)	7 Cooled syngas
Mass flow (kg/s)	16.99	35.86	7.92	25.40	24.19	7.21	19.19
Temp (°C)	780	880	350	400	900	400	15
Press (bar)	1.3	1.1	1.5	1.5	1.1	1.5	1.1
			Composition (vol. %)				
H_2	30.89	-	-	-	32.61	-	41.53
CO	12.79	-	-	-	15.33	-	20.34
CO_2	14.58	14.20	-	-	13.15	-	15.86
H_2O	31.95	8.04	100	-	22.73		1.71
N_2	2.04	73.71	-	79.00	15.38	79.00	19.58
H_2S	178 ppm	-	-	-	127 ppm	-	21 ppm
CH_4	5.26	-	-	-	0.75	-	0.96
NH_3	0.19	-	-	-	273 ppm	-	84 ppm
HCN	12 ppm	-	-	-	-	-	-
COS	10 ppm	-	-	-	7 ppm	-	7 ppm
C_2H_4	1.74	-	-	-	-	-	-
C_6H_6	0.37	-	-	-	27 ppm	-	27 ppm
$C_{10}H_8$	0.17	-	-	-	-	-	-
O_2	-	4.05	-	21.00	-	21.00	-

[6] It was felt that the commercial 'base case scenario' should be based on a feedstock (crushed bark) that has already been successfully tested at DFBG pilot scale. Feedstock properties available at deliverable D2.3 [25].

Starting with the DFBG unit, stream 1 and stream 2 represent the raw syngas that leaves the gasifier and the flue gas that leaves the oxidizer, respectively. Concerning the raw syngas composition, the relatively large steam flow (stream 3) required for DFBG technology leads to extended WGS (Water-Gas Shift) effect and subsequent dominance of H_2 over CO in the produced syngas. The remarkable content of light hydrocarbons (CH_4 & C_2H_4) along with the non-negligible tars production indicate the need of catalytic reforming downstream of the gasifier in order to avoid tar-related operational problems and enhance the H_2, CO syngas content. The flue gas contains primarily the N_2 of the inlet air (stream 4), the CO_2 and H_2O formed from the combustion of char and off-gases (stream 10 & stream 16), and some excess O_2. The reformed syngas (stream 5) contains an affordable percentage of N_2, since the thermal autonomy of the catalytic reformer is secured with some air inlet (stream 6). The purified syngas (after gas cleaning) is further cooled down (water removal) prior compression (stream 7) and then enters the gas fermentation unit.

Table 8. Stream results for the biotechnological part (BioSFerA 200 MWth full-scale simulations)

Stream No	8 Gas prior fermenter	9 Purge H_2	10 Gas fermenter off-gas	11 Air	12 Liquid fermenter off-gas	13 Medium	14 Broth -I	15 Broth-II
Mass flow (kg/s)	19.18	0.10	9.50	109.9	115.2	236.5	245.7	14.07
Temp (°C)	55	15	55	28	28	55	55	28
Press (bar)	5	100	5	1	1	5	5	1
	Composition (vol. %)					**Composition (wt. %)**		
H_2	41.53	100	15.02	-	-	-	-	-
CO	23.34	-	6.56	-	-	-	-	-
CO_2	12.86	-	18.31	-	3.28	-	0.15	0.10
H_2O	1.71	-	2.65	-	3.74	100	96.74	87.05
N_2	19.58	-	54.85	79.00	75.16	-	-	0.10
H_2S	10 ppm	-	44 ppm	-	-	-	-	-
CH_4	0.96	-	2.69	-	-	-	-	-
NH_3	88 ppm	-	330 ppm	-	-	-	-	-
C_6H_6	27 ppm	-	51 ppm	-	-	-	-	-
O_2	-	-	-	21.00	17.81	-	-	-
Acetic acid	-	-	-	-	-	-	3.11	-
Tripalmitin	-	-	-	-	-	-	-	3.15
Triolein	-	-	-	-	-	-	-	5.93
Trilinolein	-	-	-	-	-	-	-	1.65
Tristearin	-	-	-	-	-	-	-	1.99

Fermenter is preceded by a buffer tank with NaOH solvent, which is used periodically in order to avoid potential contaminants accumulation in the treated gas (stream 8). The required hydrogen for the hydrotreatment unit is extracted via PSA (stream 9) from the off-gases (unconverted syngas – stream 10) of the anaerobic fermenter. The culture medium (stream 13) was set as pure water and no nutrients were included. The acetic acid concentration in the effluent stream (stream 14) from the syngas fermentation is around 30 g/L. The liquid fermentation of acetic acid takes place in the presence of air

(stream 11), while the off-gases of the aerobic fermenter (stream 12) contain a remarkable excess O_2 content that prevents their potential direct re-utilization in the anaerobic gas fermenter (bacteria deactivation). The formed TAGs (Tripalmitin, Triolein, Trilinolein, and Tristearin) are collected in the effluent stream from the aerobic fermentation in a concentration of 100 g/L (stream 15).

Table 9. Stream results for the thermocatalytic part (BioSFerA 200 MWth full-scale simulations)

Stream No	16 Light gases	17 Purified TAGs	18 Fatty acids/ propane	19 Jet/Diesel paraffins	20 Jet-like fuel	21 Diesel-like fuel
Mass flow (kg/s)	0.29	1.82	1.92	1.51	0.71	0.80
Temp (°C)	30	50	370	30	30	30
Press (bar)	1	100	100	1	1	1
	Composition (vol. %)	**Composition (wt. %)**				
Tripalmitin	-	24.76	-	-	-	-
Triolein	-	46.63	-	-	-	-
Trilinolein	-	12.99	-	-	-	-
Tristearin	-	15.62	-	-	-	-
Palmitic acid	-	-	22.36	-	-	-
Oleic acid	-	-	42.29	-	-	-
Linoleic acid	-	-	11.78	-	-	-
Stearic acid	-	-	14.17	-	-	-
H_2	78.08	-	4.58	-	-	-
CO	4.59	-	-	-	-	-
CO_2	8.41	-	-	-	-	-
Propane	4.97	-	4.83	-	-	-
Methane	3.95	-	-	-	-	-
C_9H_{20}	-	-	-	4.03	8.52	-
$C_{10}H_{22}$	-	-	-	7.03	14.87	-
$C_{11}H_{24}$	-	-	-	4.36	9.23	-
$C_{12}H_{26}$	-	-	-	3.68	7.78	-
$C_{13}H_{28}$	-	-	-	3.52	7.44	-
$C_{14}H_{30}$	-	-	-	22.92	47.15	1.21
$C_{15}H_{32}$	-	-	-	6.90	3.11	10.29
$C_{16}H_{34}$	-	-	-	6.59	1.90	10.80
$C_{17}H_{36}$	-	-	-	28.34	-	53.74
$C_{18}H_{38}$	-	-	-	12.64	-	23.96

The decomposition of purified TAGs (stream 17) leads to the formation of palmitic acid, oleic acid, linoleic acid, and stearic acid as well as propane (stream 18). The light gases (stream 16) leaving the hydrotreatment reactor, consisting of propane, methane, carbon dioxide, and unconverted hydrogen are partially recycled back to the oxidizer of the DFBG unit (some hydrogen is recovered for re-utilization in the hydrotreatment unit). The dominant species in the final liquid products (stream 19) are C_{14} & C_{17} alkanes. Fractionation is required for the separation of jet-like (stream 20) and diesel-like (stream 21) fractions. The overall liquid fuel mass yield, expressed in kg $_{\text{liquid fuel}}$ / kg $_{\text{crushed bark}}$, is estimated at 0.134.

5.2 Energy and carbon balance

The energy balance of the integrated concept is presented in Figure 17 and the carbon balance in Figure 18.

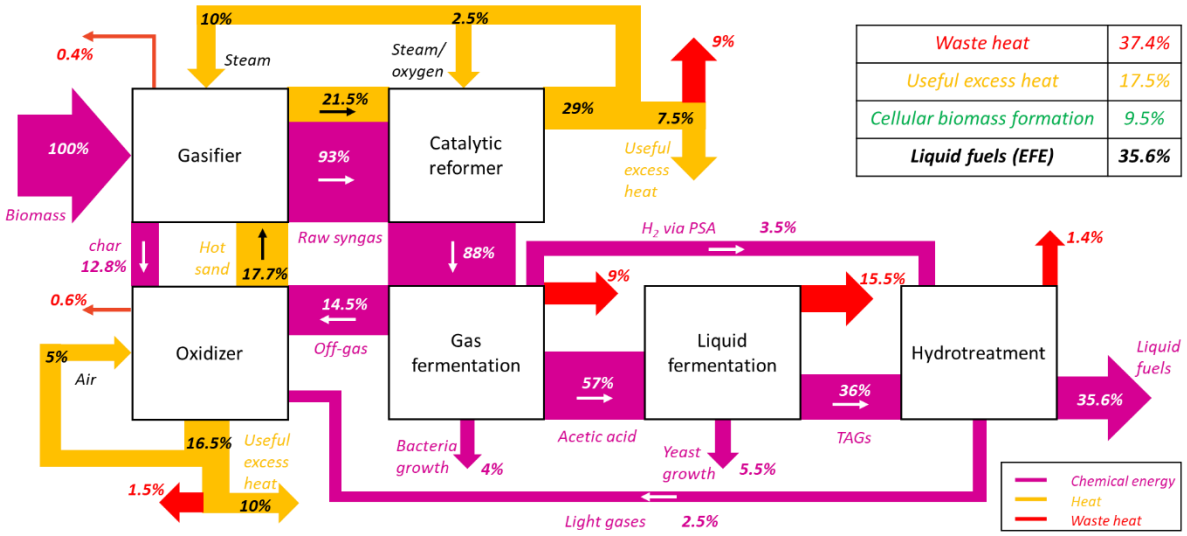

Figure 17. Energy balance of the integrated concept (BioSFerA 200 MWth full-scale simulations)

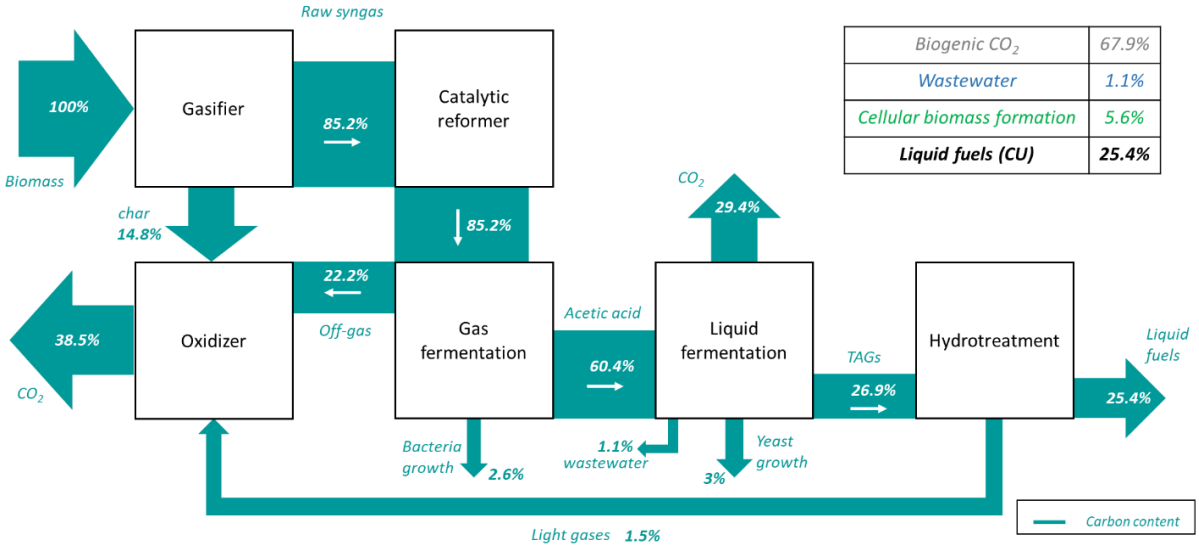

Figure 18. Carbon balance of the integrated concept (BioSFerA 200 MWth full-scale simulations)

The Energetic Fuel Efficiency (EFE) is measured at 35.6%. The main energy losses are observed in the double-stage fermentation, and especially during the aerobic conversion of acetic acid into TAGs. Moreover, a non-negligible amount of the inlet energy (9.5%) seems to be consumed by the microorganisms (bacteria and yeast) for their growth. The re-utilization of the off-gases from the gas fermentation for the thermal assistance of the oxidizer leads to enhanced gasification efficiency. The presence of the DFBG unit (two hot outlet gas streams) ensures a remarkable useful excess heat content (17.5%) that can serve any further thermal requirements of the plant (e.g. steam generation for

TAGs purification) apart from the pre-heating of air and steam. Finally, the electricity requirements of the entire process are estimated at 0.14 kWh_{el} / kWh_{th} of produced biofuel, mainly sourcing from the compression unit prior gas fermentation.

The obtained Carbon Utilization (CU) of the integrated BtL plant has been calculated equal to 25.4%. A large portion of the inlet carbon (67.9%) ends up in the form of CO_2 either in the outlet of the oxidizer or in the outlet of the aerobic fermenter. The rest carbon 'expenses' of the process are minor and consist of the cellular biomass formation (5.6%) as well as the low organic content of wastewaters (1.1%).

5.3 Initial targets and actual performance

The initial targets that had been set for the EFE and the CU of the integrated BioSFerA concept were 40% and 37%, respectively. While the calculated EFE of 35.6% indicates that the initial EFE target (40%) is within reach, the distance between the actual calculated CU of 25.4% and the initial CU target (37%) is remarkable. As discussed in Deliverable D2.5 'Full-process basic definition', the exploitation of the CO_2 generated during liquid fermentation in the gas fermentation and the parallel support of the concept with an electrolyzer, ensure the achievement of the initial targeted metrics. However, the extra required purification[7] of the CO_2 stream prior re-utilization on the one hand, and the inherent high costs of an electrolyzer on the other hand, led to the decision to avoid these possibilities in order to ensure the financial competitiveness and sustainability of the concept (Table 10).

Table 10. Initial BioSFerA targets and estimated actual performance of the integrated concept

Concept	EFE	CU
BioSFerA initial target	40%	37%
Integrated BioSFerA concept (selected)	35.6%	25.4%
Integrated BioSFerA concept enriched with external electrolyzer and purification/ re-utilization of CO_2 off-gas (not selected)	45%*	37%*

* These metrics have already been calculated from D2.5

The avoidance of burdening the design of the process with significant extra capital and operational expenses (electrolyzer, CO_2 purification), in order just to fulfill the initial performance targets of the project at the expense of the financial targets, is a strategic choice of the BioSFerA consortium that is based on two critical factors:

- The already obtained competitiveness of the BioSFerA concept in terms of performance compared to other similar BtL technologies (see section 6)
- The aim of the BioSFerA concept is the establishment of a competitive BtL technology based on mild operating temperatures, low pressures and generally reduced costs. This aspect is expected to be more evident in the techno-economic assessment of the project (Task 7.1)

Nevertheless, some potential alternative BioSFerA configurations that could enhance the process performance, but without assuring the financial viability of the concept, can be found in the Appendix.

[7] The experimental activities of liquid fermentation revealed that a portion of the inlet oxygen remains unconverted and is found among the off-gases of the bioreactor. The presence of oxygen prevents the potential direct re-utilization of the off-gases (CO_2) in the anaerobic gas fermenter, and thus CO_2 purification is required for this purpose

6 Benchmarking with other competitive biofuel technologies

This section aims to conduct a comparative evaluation of the BioSFerA concept in terms of liquid fuels productivity, in relation to other certified biofuel production pathways based on the same type of feedstock (lignocellulose). The focus is primarily on assessing performance indicators such as EFE and CU. Specifically, the selected technologies for comparison are the Fischer-Tropsch synthesis (FT) via gasification of lignocellulosic biomass, the Alcohol-to-Jet (ATJ) via hydrolysis of lignocellulosic biomass and the ATJ via gasification of lignocellulosic biomass (followed by syngas fermentation).

Fischer-Tropsch liquids are produced through bio-based gasification with FT synthesis using lignocellulosic biomass as feedstock. This technology is now just approaching commercialization (TRL 7-8) and has received growing attention since it offers clean and potentially carbon neutral fuels directly usable in the transportation sector. Alcohol-to-Jet is a pathway that produces fuels from sugary, starchy, and lignocellulosic biomass, such as sugarcane, corn grain and switchgrass, via fermentation of sugars or syngas to ethanol or other alcohols. This technology is also at a pre-commercial level (TRL 7-8). The only commercially applied technology (TRL 8-9) for producing SAF is the HEFA pathway, which produces fuels through the hydrogenation of vegetable oils. However, for direct comparison purposes, within this section, only the most advanced technologies utilizing lignocellulosic feedstock are mentioned in order to maintain consistency with the BioSFerA concept. Moreover, due to the feedstock constraints of HEFA technology (limited availability), there are claims that the next decades will be dominated by technologies handling advanced feedstock (biogenic residues/wastes) such as FT, AtJ, and the BioSFerA pathway [19].

An estimation of the performance range of the aforementioned technologies has been carried out, utilizing data sourced from previous studies reported in the literature [20]–[23]. The EFE and CU range for each technology and their comparison with the BioSFerA pathway, can be seen in Figure 19 and Figure 20, respectively.

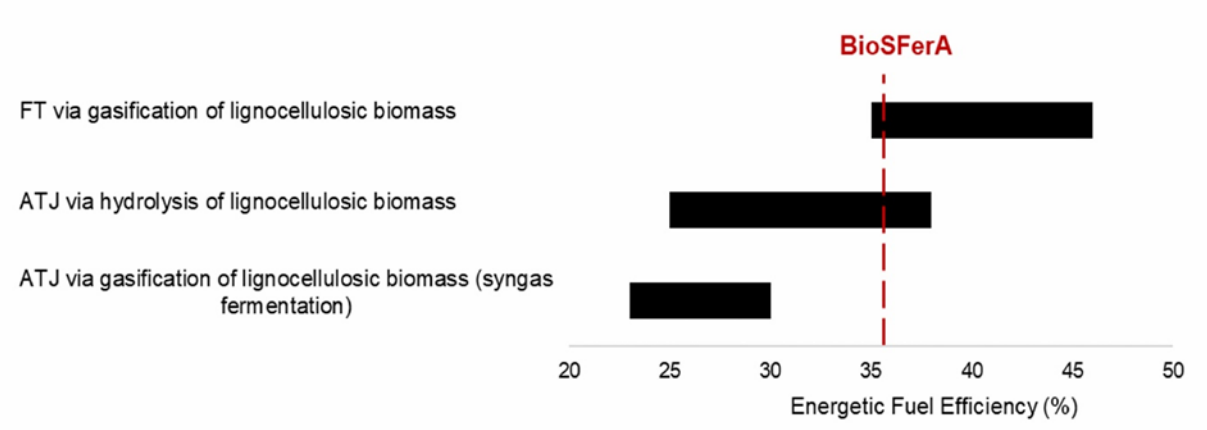

Figure 19. Comparison of the BioSFerA 'base case scenario' with other certified biofuel production pathways in terms of EFE

Figure 20. Comparison of the BioSFerA 'base case scenario' with other certified biofuel production pathways in terms of CU

As can be seen from Figure 19 and Figure 20, biofuel production through the FT route yields higher levels of EFE and CU compared to the ATJ routes and the BioSFerA pathway. This can be attributed to the FT route's inherent advantage of requiring fewer process steps, allowing for the direct conversion of syngas into liquid fuel, while the other routes involve multiple steps to final fuel production resulting, thus, in significant carbon losses. However, it is evident that the BioSFerA pathway demonstrates competitive values in terms of liquid fuel productivity (EFE, CU) when compared to already certified technologies that exploit similar feedstock (i.e. FT, ATJ). The favorable position of BioSFerA lies on its ability to reach decent efficiency levels by avoiding the strict specifications of FT that usually require costly and energy demanding equipment or the several unit operations (pre-treatment, hydrolysis, fermentation, dehydration, oligomerization) of the ATJ route that raise the total production costs. Task 7.1 "Techno-economic assessment" will provide further insights into the economic feasibility of the BioSFerA concept, enabling a more comprehensive and equitable comparison with other well-established biofuel production technologies.

7 Conclusions

In this deliverable, the process layout of the BioSFerA concept, initially defined in Deliverable D2.5, was re-evaluated, was enriched with the insight from the relative experimental work throughout the process chain, and was optimized according to the expertise of the entire consortium on BtL schemes.

The experimental results were utilized for the calibration of the developed models. The configuration for the integrated commercial concept was elected with the aim of technical viability as well as the greatest possible performance/cost balance. Thus, the updated Heat & Mass balances were calculated for a potential 200 MWth BioSFerA concept with crushed bark as feedstock (base case scenario). Some experimental findings (e.g. remarkable oxygen presence in the off-gas of the liquid fermentation) along with some strategic design choices with techno-economic background (i.e. avoidance of electrolyzer) led to slightly lower overall performance compared to the raw initial targets. However, the performed benchmarking of the BioSFerA pathway with other established BtL technologies (Fischer-Tropsch, Alcohol-to-Jet) in terms of performance revealed that the BioSFerA concept could be fully competitive. Moreover, the upcoming techno-economic assessment (Task 7.1) is expected to bring to the fore the advantageous aspects of the BioSFerA concept (e.g mild temperatures, low pressures, no need of CO_2 removal) by enabling sustainable and competitive biofuel production costs.

The presented configuration and the exported Heat & Mass balances will be utilized as input for the upcoming process design/cost engineering (Task 6.3) as well as the horizontal evaluation of the proposed technology (WP7). Finally, the proven feedstock flexibility of the BioSFerA concept ensures the reliable estimation of the Heat & Mass balances of the concept for other types of feedstock from the BioSFerA feedstock inventory (prunings, wheat straw, etc.) as well.

8 References

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9 Appendix

Alternative BioSFerA configurations for further performance enhancement:

- Concept 1

  A potential concept would be to employ a cryogenic CO_2 Compression and Purification Unit (CPU) in order to extract the CO_2 from the liquid fermenter's off-gas and utilize it as a substrate for the gas fermentation process. Via this technique, the gas is compressed, cooled to extremely low temperatures in order to be liquefied and purified to remove impurities and contaminants from the CO_2 gas. An electrolyzer can be used in order to secure the required H_2 for the production of acetic acid from the recycled CO_2, as well as to provide the liquid fermenter with pure O_2 and avoid thus the large volumes of nitrogen in the off-gas (Figure 21).

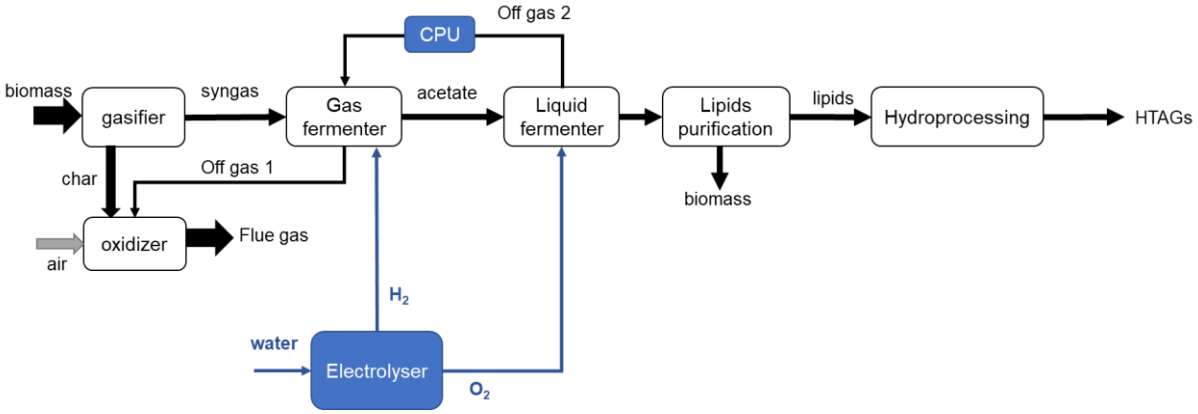

Figure 21. Carbon utilization enhancement through CPU

- Concept 2

  Another idea would be to send the off-gas of the liquid fermenter directly to an algae cultivation system. This concept offers the advantage of eliminating the necessity to separate CO_2 from the off-gas, thereby avoiding the use of costly carbon capture techniques. Algae have the capability to assimilate CO_2 through photosynthesis and convert it into valuable products, like lipids. These lipids can be extracted from the algae and further be processed into jet and diesel-like fuels through hydrotreatment. This concept is depicted in Figure 22.

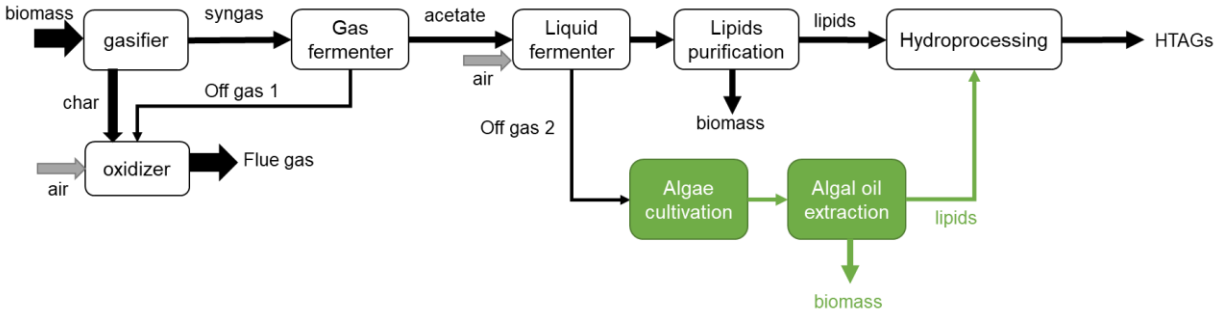

Figure 22. Carbon utilization enhancement through algae cultivation

- Concept 3

  An alternative approach could involve the employment of a Direct Air Capture (DAC) system to capture the CO_2 from the liquid fermenter's off-gas. This technique uses chemical reactions to extract CO_2 from the surrounding gases. This CO_2 can then be redirected back to the gas fermenter to serve as a carbon source for the anaerobic bacteria. An electrolyzer can be employed to obtain the necessary H_2 for producing acetic acid from the recycled CO_2, as well as to secure pure O_2 for the liquid fermentation process. The block flow diagram for this concept can be seen in Figure 23.

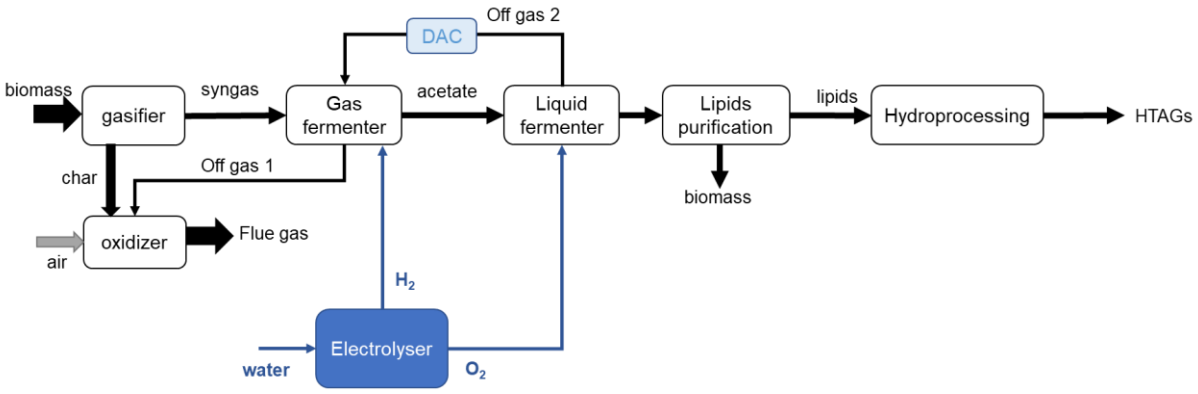

Figure 23. Carbon utilization enhancement through DAC