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ALGAESOL

Sustainable aviation and shipping fuels from microalgae and direct solar BES technologies

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Specifications of process flows and requirements for component models and use cases

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Executive summary

The Horizon Europe project ALGAESOL (Grant Agreement No. 101147112) aims at developing and evaluating several solutions for the sustainable conversion of sunlight into fuels, advancing the state-of-the-art by creating and consolidating new value chains for shipping and aviation fuels based on micro-algae and direct solar renewable fuel technologies.

The current document (Deliverable D1.3 - Specifications of process flows and requirements for component models and use cases), reports the outcomes of WP1-Task T1.3, which defined the specification and assessed the key components of the process for the development of an appropriate model for the overall project system and for the representation of the project use-cases, considering the use of SIMTECH's simulation environments IPSEpro and IPSE GO. Deliverable D1.3 was prepared by SIMTECH in co-creation with the consortium technical partners UdG, LEITAT, NORCE, DTI, and SOCAR (the Use-Cases provider).

The outcomes of task T1.3 reported in this document will be relevant for all tasks related to the numerical models that represent ALGAESOL, for modelling its main system solution, as well as for the simulation work in WP5 (T5.1 and T5.2), for the creation of customized component models in IPSEpro, and for simulating the overall process and for the modelling and showcase of the virtual Use-Cases using IPSE GO, with the main aim to assess the developed ALGAESOL technology with real data of different use-case scenarios of the aviation and shipping applications.

Abbreviations

The abbreviations relevant for WP1-T1.3, used in the ALGAESOL Deliverable D1.3 are listed in the table that follows.

Table 1: Abbreviations used in this document.

Abb.	Description	Abb.	Description
BES	Bio-Electrochemical System	MDK	IPSEpro Model Development Kit
CC	Creative Commons	Mx	Project Month x
DoA	Description of the Action	MSx	Project Milestone x
EC	European Commission	NADES	A natural deep eutectic solvent
EU	European Union	PCx	Process Connection x
GA	Grant Agreement	PFx	Process Flow x
GHG	Green House Gases	PSE	IPSEpro Process Simulation Environment
IP	Intellectual Property	SAF	Sustainable Aviation Fuel
IPSEpro	SIMTECH's Simulation Environment	WP	Work Package
IPSE GO	SIMTECH's Simulation Web-Platform	WPx-Ty.z	Work Package x Task Ty.z

Table of Contents

1. Introduction

ALGAESOL ("Sustainable aviation and shipping fuels from microalgae and direct solar BES technologies") is a publicly funded Horizon Europe project (GA No. 101147112 [1]), that aims to develop and evaluate several solutions for the sustainable conversion of sunlight into fuels. ALGAESOL will advance the current state-of-the-art by creating and consolidating new value chains for shipping and aviation fuels based on micro-algae and direct solar renewable fuel technologies.

The current document composes ALGAESOL Deliverable D1.3, which reports the outcomes of WP1-Task T1.3. Overall, WP1 ("Requirements and specifications for sustainable solar/algal biofuels production") has four objectives: (1) Establish quality requirements and characteristics of the specific target fuels for shipping and aviation to be produced through BES/electrochemical platform; (2) Evaluate the most convenient waste streams to be operated in each BES/electrochemical process considered, and the key parameters to optimize the production to the target set; (3) Define the specification and assess the key components of the process for the development of an appropriate model for the overall project system and for the use-cases; and (4) Define goal and scope to be achieved and define system boundaries for the sustainability analyses.

Task T1.3, led by SIMTECH, counted with the contributions from the technical partners UdG, LEITAT, NORCE, DTI, and SOCAR (the Use-Cases provider). T1.3 was carried out during the first 6 months of the project and dealt with the definition of all relevant specifications for the project system-level modelling procedure and its process models' characteristics to ensure feasible computational effort, when using the simulation tools provided by SIMTECH (IPSEpro & IPSE GO), including compatibility and some necessary adaptability of the showcase simulation web-platform (IPSE GO), to virtually represent the project use-cases in the applications defined for ALGAESOL (Aviation and Shipping). Hence, the required data coming from the energy conversion streams, specified in the parallel WP1 tasks, together with the relevant features, information and requirements of the real use-cases scenarios compose the core part of the outcomes of task T1.3 (reported in D1.3).

Deliverable D1.3 ("Specifications of process flows and requirements for component models and use cases") was produced by SIMTECH, in close collaboration with all ALGAESOL WP1 involved partners. The outcomes of task T1.3 reported in this document will be relevant for all tasks related to the numerical models that represent ALGAESOL, for modelling its main system solution, as well as the simulation work in WP5 (T5.1 and T5.2), for the creation of customized component models in IPSEpro, and for simulating the overall process and for the modelling and showcase of the virtual Use-Cases using IPSE GO, with the main aim to assess the developed ALGAESOL technology with real data of different use-case scenarios of the aviation and shipping applications.

The information provided in this document builds up on the general guideline of the ALGAESOL overall concept, and focuses on its modelling, emphasizing the simulation concept of the project and the adaption of the simulation tools for the design of the project process flows and use-case, considering the boundary conditions imposed by each specific application. In this context, the document provides the general basis to be considered as a guide during the project process modelling and use-cases implementation.

This document is structured in the following way: The Introduction Section (1) includes a brief description of how the simulation is considered in the concept of ALGAESOL; and presents an overview about the IPSEpro simulation environment and the IPSE GO web-platform, which serves as the ALGAESOL use-cases demonstration tool. Section (2) describes the relevant aspects of the specifications and requirements for the implementation of the process models. It gives the overall goals of the simulation procedure, including the identification of the Process Flows for the representation of the ALGAESOL Renewable Fuel Production Paths, and the development of a customized library of component models, ALGAESOL_Lib. Section (3) presents an overview of the ALGAESOL Use-Cases, with information provided by SOCAR. Section (4) summarizes the data required for the use-cases process modelling using IPSE GO, with the description of the four Renewable Fuel Production Paths, including the main input data to implement their process models. Section (5) draws some concluding remarks about the work carried out in task T1.3 and its impact within the ALGAESOL project. Finally, Section (6) lists the references upon which the work done was based.

1.1. Simulation within ALGAESOL

The ALGAESOL project proposes an ambitious and efficient R&I workplan to develop several solutions for the sustainable conversion of sunlight into fuels. To achieve this, the project will advance the current state-of-the-art, while creating and consolidating new value chains for shipping and aviation fuels based on microalgae and direct solar renewable fuel technologies (see Figure 3).

Overall, ALGAESOL will develop direct solar fuel, as well as microalgae, production and purification technologies for making advanced transportation fuels. ALGAESOL will develop energy-efficient purification methods of microalgae biomass and direct solar fuel components and delivery to advanced algae-based fuels and direct solar fuels for aviation and shipping. ALGAESOL will ensure enhanced sustainability of aviation and shipping fuels, taking fully into account circular economy, social, economic and environmental aspects in line with the European Green Deal priorities. In particular, the effects on CAPEX, OPEX, energy efficiency, greenhouse gas (GHG) balance and circularity of materials and process streams will be addressed.

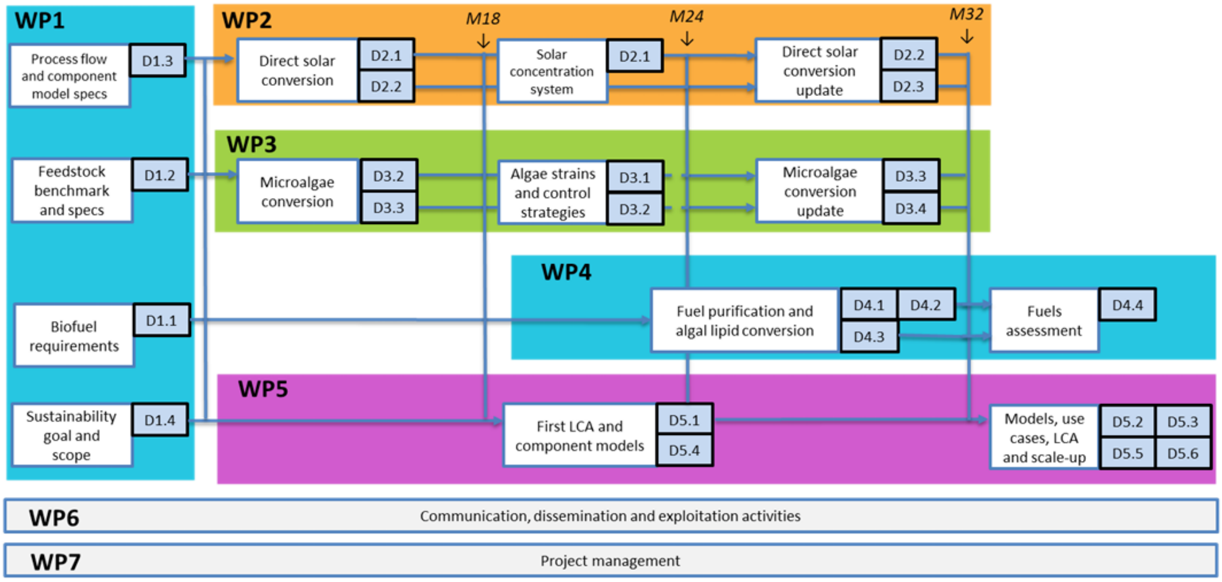


Figure 1: ALGAESOL Work Packages Structure [1].

As shown in Figure 1, WP1 (led by UdG) begins with setting of requirements and specifications in ALGAESOL. It then follows with the development in the two interlinked conversion routes – direct solar (WP2 – led by LEITAT) and microalgae-based (WP3 – led by DTI). Halfway through the project WP4 starts, led by SOCAR, where purification of fuels coming from the previous two WPs takes place, along with algal lipid conversion and testing of the resulting fuels. WP5 (led by SIMTECH) is ongoing throughout the project with component and process modelling, simulations, sustainability assessments and scale-up strategies development. Similarly, WP6 (led by AMIRES) spans the whole duration of the project with communication, dissemination and exploitation activities. WP7 (led by NORCE) is dedicated to project management support throughout the project.

For the production of sustainable and renewable aviation and shipping fuels from sunlight, ALGAESOL has designed a 36-month work plan, composed of 7 Work Packages (see Figure 1), which will allow the consortium to achieve the project's objectives, mainly following two main paths of fuel production, one for direct solar fuel production and the other one via microalgae (see Figure 2 and Figure 3).

ALGAESOL work plan revolves around 4 highly interconnected working pillars: (1) direct solar conversion technologies for renewable fuel, (2) microalgae-based renewable fuel technology development, (3) purification and fuel development, and (4) simulations, sustainability and scale-up strategies.

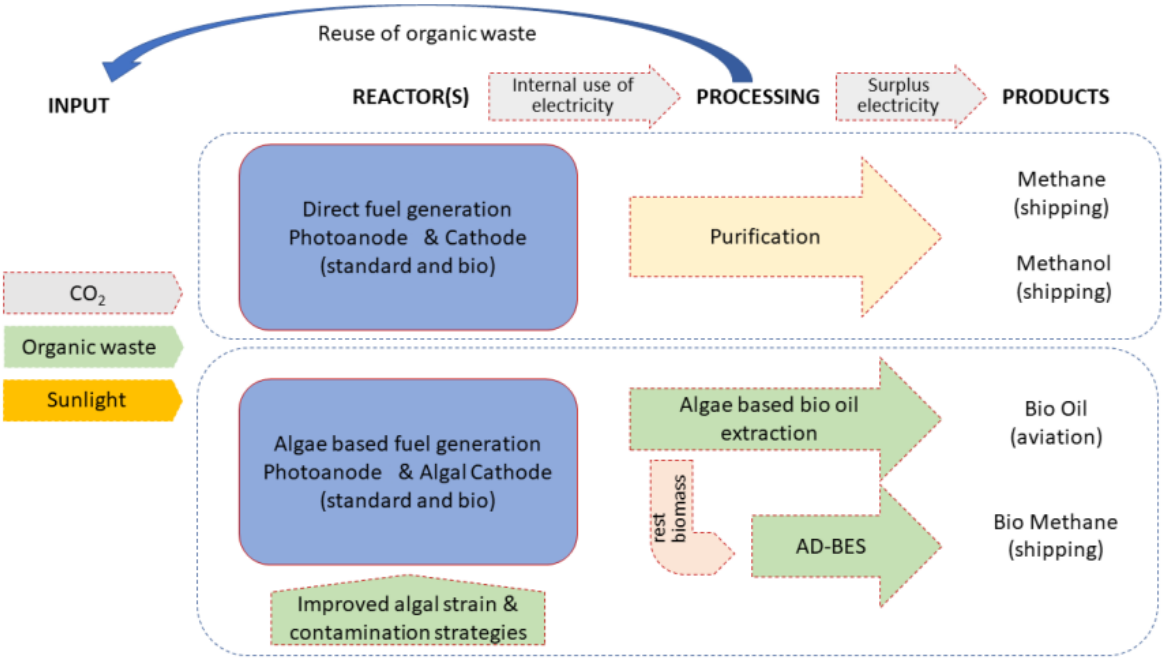


Figure 2: Renewable fuel production paths evaluated in ALGAESOL.

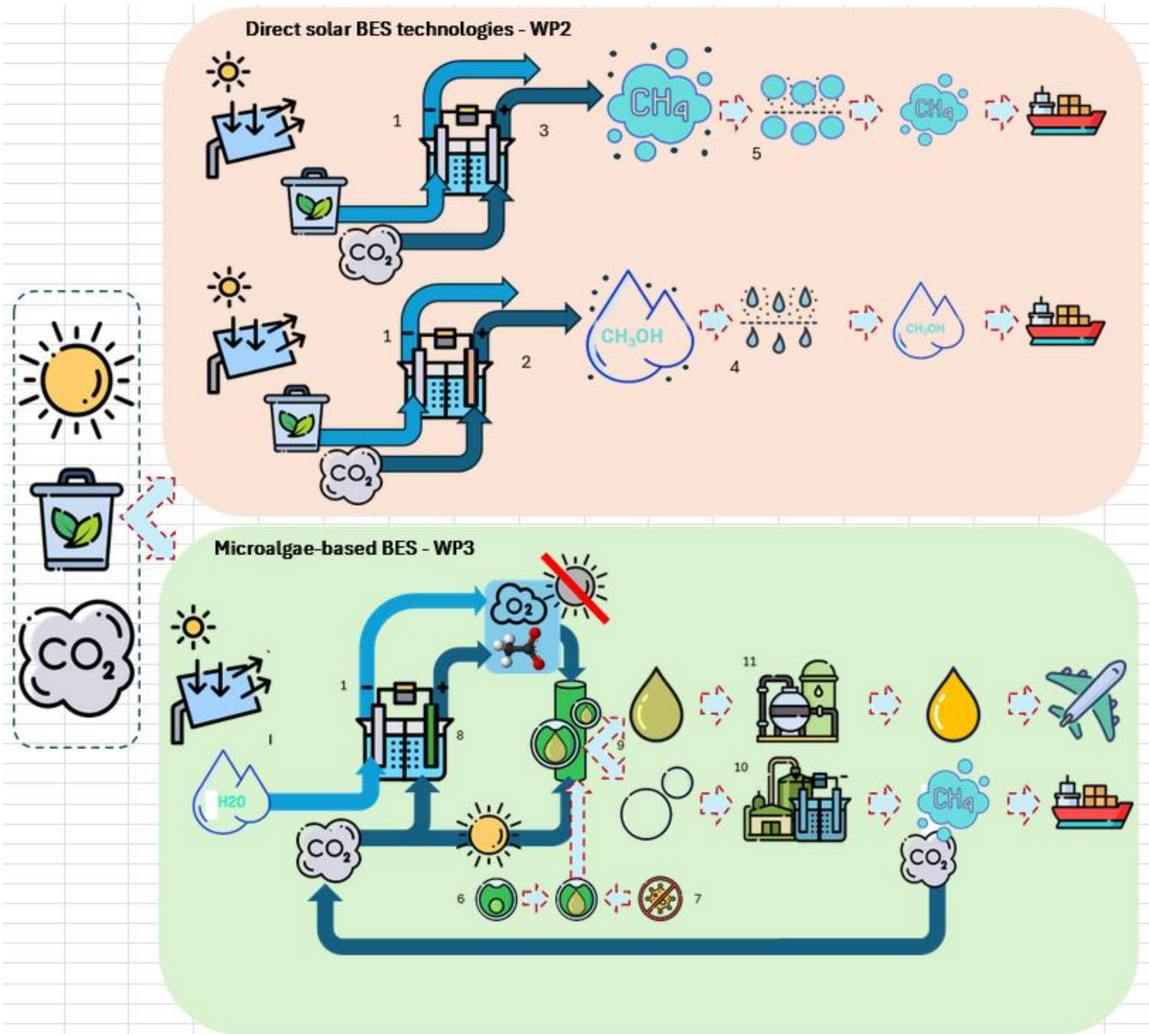


Figure 3: Renewable fuel production paths (Process Flows) evaluated in ALGAESOL.

Table 2 lists the technologies shown in Figure 3 (via their numbers), with their abbreviations and the project partners responsible for their development in ALGAESOL (source: Material from WP1-Task T1.2).

Table 2: Technologies used / developed in ALGAESOL.

Legend	Technology	Abbreviation	Responsible partner
1	Photoanodes	P	LEITAT
2	EC-Metanol	EC/P-EC	LEITAT
3	BES-Methane	BE/P-BE	LEITAT
4	Methanol purification	pMeOH	LEITAT
5	Methane purification	pCH4	LEITAT
6	Microalgae cultivation	MA	NORCE
7	Microalgae pest control	MA-PC	DTI
8	BES-Microalgae	BE-MA/P-BE-MA	UdG
9	Lipid extraction	LE	LEITAT
10	Anaerobic digestion BES	AD-BES	LEITAT
11	Lipid processing	LP	SOCAR

The simulation in ALGAESOL project will validate the project overall concept via the optimized modelling of the process flows indicated in Figure 3, for the two applications of aviation and shipping. The use-cases that will follow from those fuel production streams, will be fully showcase the capability of the project concept in scaled-up scenarios. Therefore, the overall ALGAESOL system will be virtually implemented and optimized using SIMTECH's simulation tools (IPSEpro and IPSE GO).

1.1.1. The IPSEpro Simulation Environment

IPSEpro is an open modelling framework, which handles components' mathematical representations and physical property methods apart from its solver module. Hence, application specific information is maintained in model libraries, completely separate from the core software (see Figure 4), bringing a high degree of flexibility and sustainability to both projects and system maintenance.

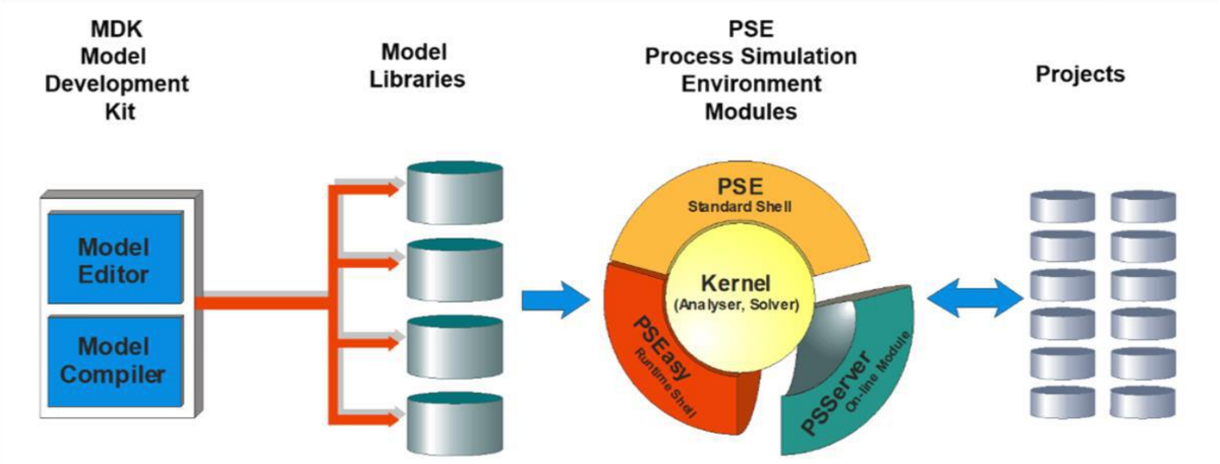


Figure 4: IPSEpro Core System (incl. MDK, PSE, and other IPSEpro Modules (https://www.simtechnology.com/cms/ipsepro/program-modules).

IPSEpro-MDK: Using MDK (Model Development Kit), one can create and modify Model Libraries, and new component-models of existing equipment to populate the Model Library of components that will be used in modelling processes to simulate a scenario or plant configuration.

For using MDK to create component models for a library, information about the parameters and behaviour of the physical components (e.g.: turbines, heat-exchangers, pumps, etc.) are needed, and a user-friendly interface is provided with a built-in intuitive equation-oriented model development language (MDL) and a graphics editor for designing the graphic representation (icon) of the defined component.

IPSEpro-PSE: Using PSE, the user can build process models of the needed plant configuration to be simulated, using the flowsheet environment available in PSE and a Model Library available (or created in a customized way) for his/her project within the chosen/specified application area.

1.1.2. The IPSE GO Web Platform

IPSE GO (https://about.ipsego.app/) is a cloud-based simulation platform, which can be interpreted as an online version of IPSEpro-PSE. The web-based platform IPSE GO uses the capabilities of the process simulation system IPSEpro via the web. IPSE GO was designed to run in all internet browsers, from any device you may wish to work with (computers, mobile devices, etc.) with and intuitive user interface that can handle the complexity of the industrial level within a user-friendly way. IPSE GO offers a highly flexible modelling environment with numerous components from available Model Libraries that allow you to calculate almost any application area in process simulation. A strong advantage of using IPSE GO is the "effortless collaboration" aspect that it offers to all its users. In this respect, sharing IPSE GO projects with coworkers, project partners or students, happens in a fast and easy way within a simple click.

The use of the web-based platform will enable the performance evaluation of the Use-Cases interactively and will be made available to a wider audience of end-users and stakeholders related to the virtual Use-Cases provided. It will allow them to adjust the Use-Cases according to their requirements, using the platform via web browsers. Additionally, the platform users will be able to investigate new testing cases, multiplying the impact of the project's concept validation.

Thus, IPSE GO offers the appropriate simulation environment, providing an excellent basis for the fulfilment of the requirements of the virtual use-cases and thus the objectives of the project.

The modular approach of the component models, interconnected for building simulation projects, guarantees high modularity of the processes simulated in this environment. In addition, this characteristic allows for partial modification of a section or sub-system of the project to adapt it to further users' demands, guaranteeing a high degree of flexibility.

Finally, the graphic interface of its flowsheet, where the different components are represented by small icons and their connections, includes all technical information needed in the model and helps the users to have an overview of the simulated process at a glance. This is quite adequate for showcasing the virtual use-cases and much more attractive and representative than other software, for which models are not graphically represented, but with lines of code.

In ALGAESOL, the final Use-Cases representations in WP5 will be made publicly available online via SIMTECH's web-based platform IPSE GO (illustrated in Figure 5). The IPSE GO platform will be customized for the project to demonstrate the capabilities of the overall project concept, allowing the virtual implementation and performance optimization of the two use-cases for aviation and shipping, which will use the 4 fuel production paths evaluated in the project. It involves the following steps:

- Definition of the required individual component models to be arranged and integrated to represent a system.
- Set up of the Renewable Fuel Paths evaluated in ALGAESOL, and further the Use-Cases for aviation and shipping, on the basis of the pre-defined customized component models.

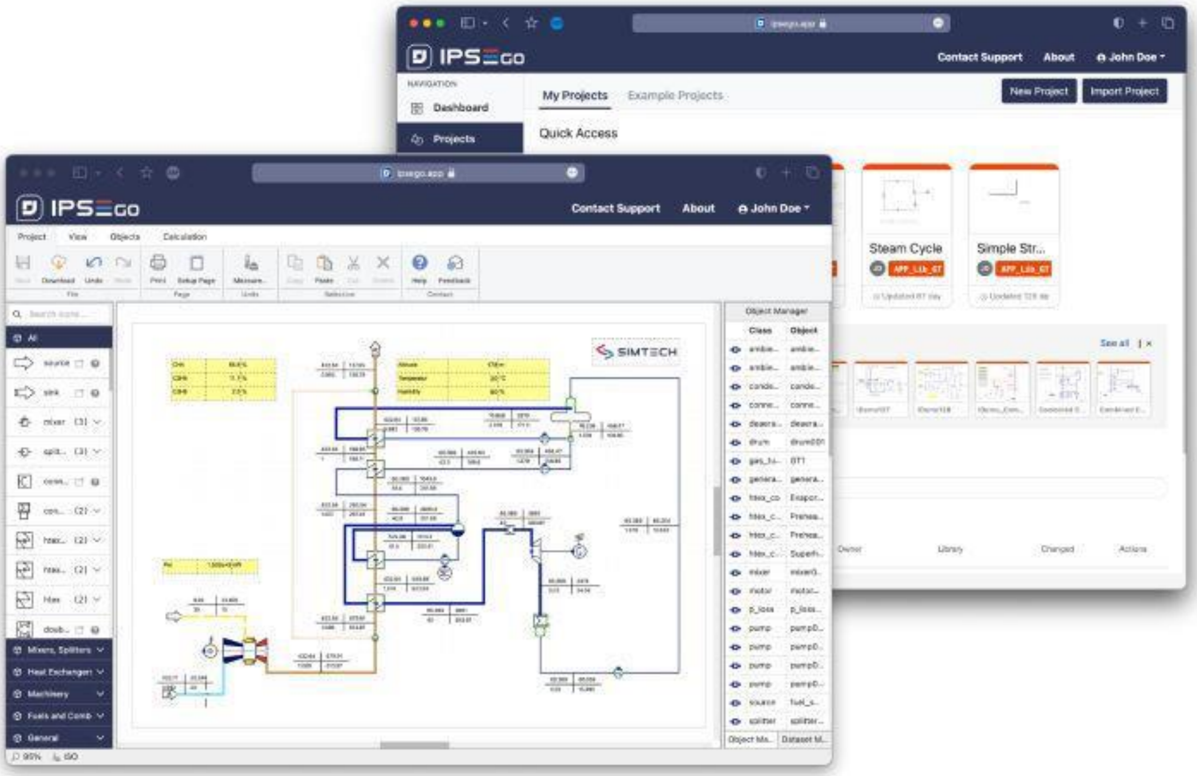


Figure 5: IPSE GO Web-based Platform (https://about.ipsego.app/).

2. Models Specifications & Requirements

This section describes the relevant aspects of the specifications and requirements for the implementation of the ALGAESOL process models, including for instance: feasible computational effort, compatibility between models, and adaptability to the web-platform, modularity and flexibility.

The first step in task T1.3 was to define the application framework of the specifications and requirements to be applied to the models developed within the ALGAESOL project which must be implemented in the simulation platform, in order to ensure the compatibility between both. Complex models developed in the frame of the project whose first aim is to support detailed results for the precise design of the prototypes are not in the application framework of the result of the task due to their present high computational effort and a long time of simulation.

The requirements identified and defined within the development of task T1.3 include:

- **Comprehensive simulation time**: Reduced simulation duration, as maximum in terms of minutes.
- **Modularity:** The Models of components to be developed in ALGAESOL should be programmed following an object-oriented philosophy, making them able to be connected to other component models.
- **Validation:** Models must be validated with experimental results, external bibliography or other validated complex models.
- **Comprehensive computational effort:** The models must be able to be simulated in a normal user computer (RAM 8G, CPU i3) and on the servers for the web-based platform.
- **Description:** Models should include a brief description and, if applied, mention the calculation hypothesis.

In addition, the simulation platform must include a **user-friendly interface**, making it easy to use and understand by all potential users. All the models developed/planned to be developed have been/will be tested in order to ensure the fulfilment of these requirements.

All the above listed aspects can be fulfilled using IPSE GO, which adaptation to the project's requirements enforced improvements on its:

- **Usability:** via user-friendly functions, and enhancements on the graphical usability of the flowsheet, following an intuitive and logical user-based approach.

- **System Design & Robustness:** via Architectural design improvements; More robustness on the standard browser-based flowsheet editor for entering data and displaying results of the simulation; Framework Management revised and improved; Optimization of the Data / User / Session Management feature; and Enhanced calculations response time, carried out on library hosts.

- **Sharing / Portability / Compatibility / Security:** via Full-Capability to Exchange Projects with IPSEpro (desktop simulation environment version), so that projects can be further worked online and vice-versa. Easy and fast sharing of process and component models among project partners, as projects are stored on web servers. Enhanced overall security within the platform for data, user and projects / sessions management.

Moreover, the IPSE GO features described and illustrated in the sequel ensure that the basic defined requirements are achieved. The features are: (1) Integration between IPSEpro and IPSE GO projects (Figure 6) ; (2) Multi-platform Modern Editor (Figure 7); (3) Collaboration & Sharing Feature (Figure 8); as well as features relative to (4) Access Rights and Security (Figure 9).

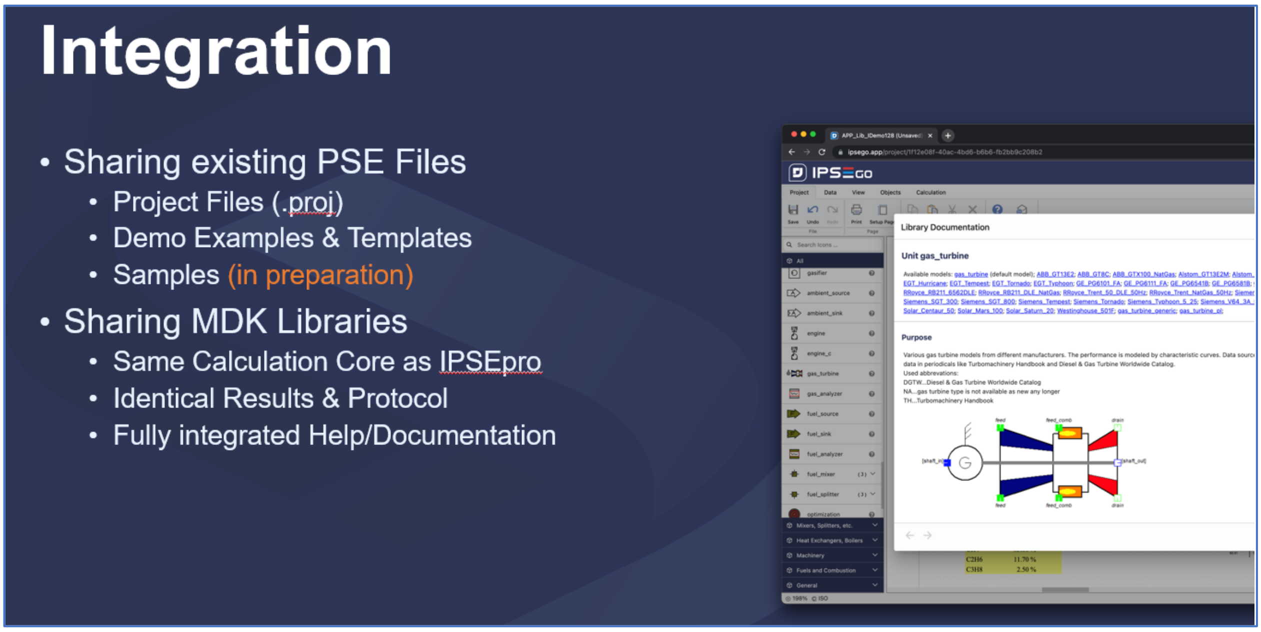


Figure 6: IPSE GO Integration Feature.

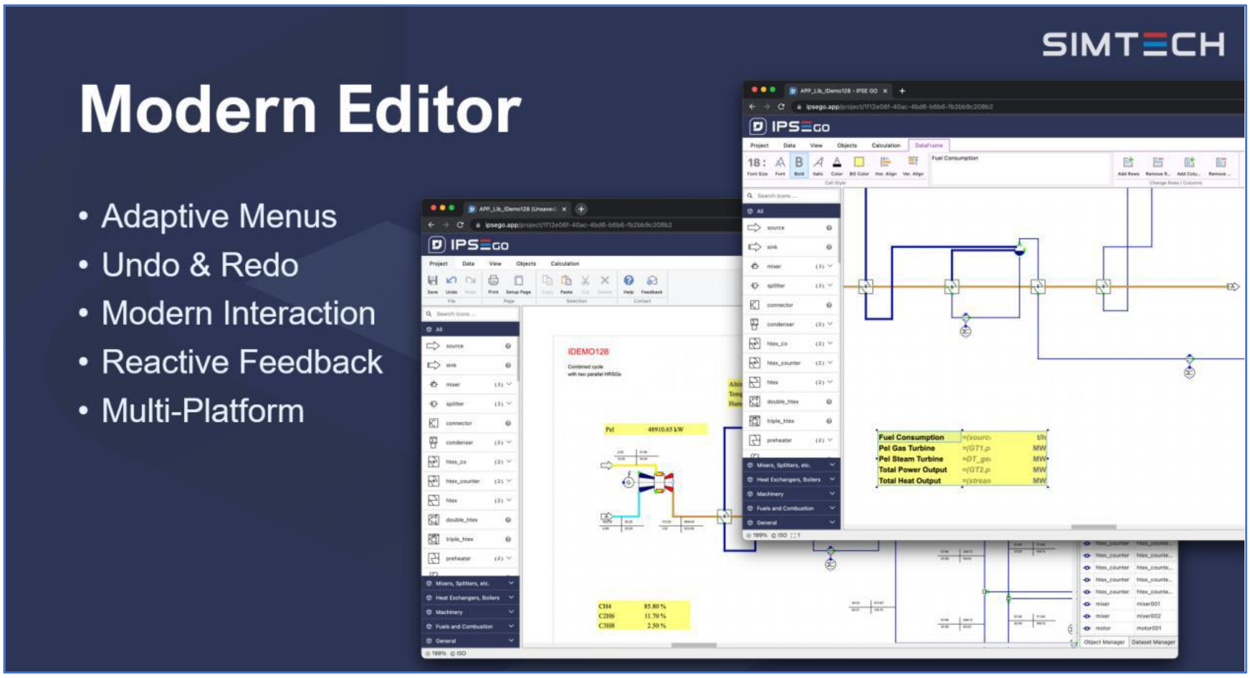


Figure 7: IPSE GO Modern Editor Feature.

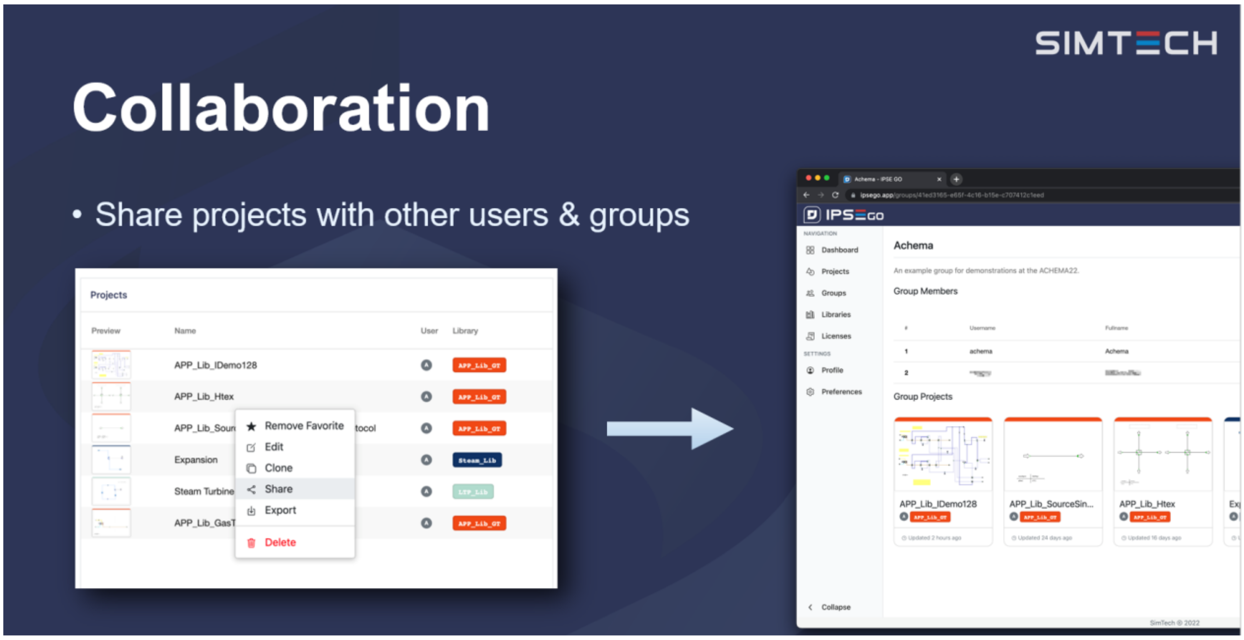


Figure 8: IPSE GO Collaboration Feature.

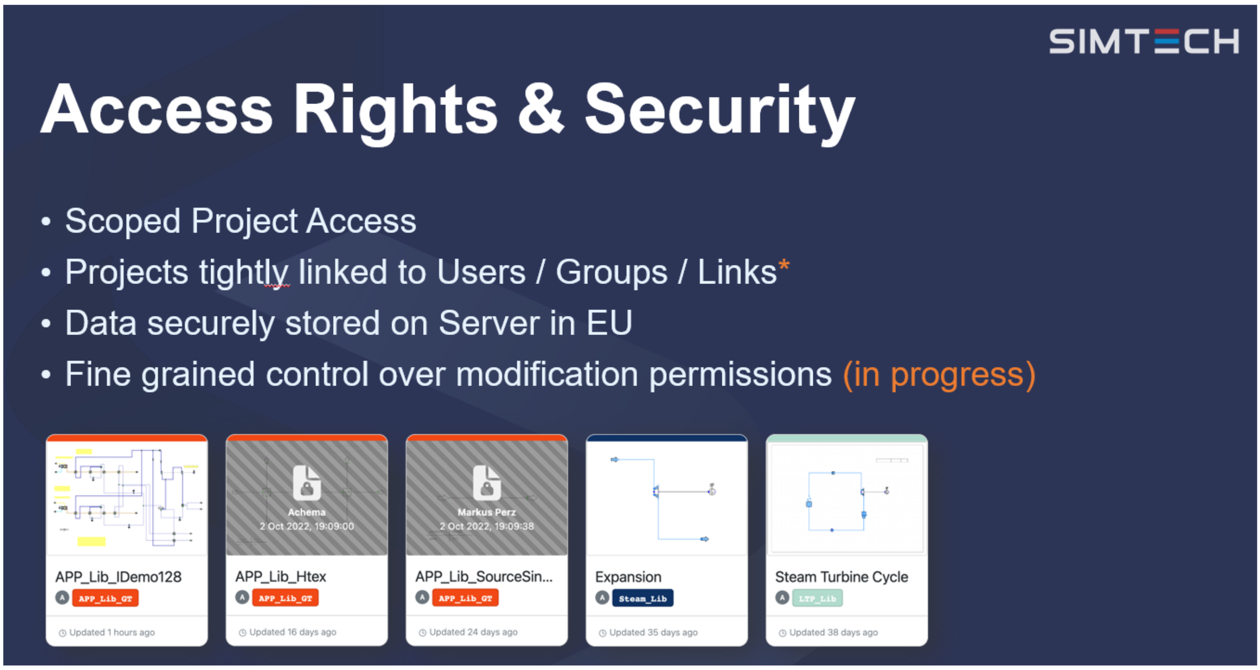


Figure 9: Access Rights & Security Feature.

2.1. Goals of the Simulation

The overall goal of the simulation within ALGAESOL system development, includes the precise behavioural and numerical representation of the involved components and process models of the fuel production paths, at a high accuracy level in relation to the real data provided, so that their evaluation and implementation within real-data virtual use-case scenarios can be validated. This entails that feasible further piloting stages of the system can take place with low implementation risks.

It is worth noting that in ALGAESOL, SIMTECH's Web-based Process Simulation Platform will be available for both project partners and end-users (during the project lifetime) to assist all project phases (design, development and testing), as well as to demonstrate the project's Use-Cases interacting with the ALGAESOL Stakeholder ecosystem for exploitation purposes.

Once ALGAESOL process models are made available online for stakeholders, the use cases can be simulated interactively by anyone interested in the technology. Additionally, stakeholders will be able to create their own testing cases, such that the number of different application examples will grow continuously.

The ALGAESOL_Lib library of components will be made available for the project Consortium Members in IPSEpro and also on the IPSE GO web platform. Modelling online training sessions guided by SIMTECH will be given to participants from the technical WPs of the project (all partners involved with WP5). Then, IPSE GO will also be made available to be tested and used by Consortium Members, with evolving ALGAESOL process models. Extensions and updates of both ALGAESOL_Lib and process models will continue to follow throughout the project.

2.2. Identification of Process Flows to Represent the ALGAESOL Renewable Fuel Production Paths

Considerations for Simulation in IPSEpro / IPSE GO: The simulation of the renewable fuel paths described here will be performed on the basis of the process flows used in each of the paths for the fuels production. The process flows have been identified from the process overview compiled in task T1.2 and are shown in Table 3. Figure 10 reproduces the illustration in Figure 3, with the various Process Flows (PF#) of the simulation indicated for each of the ALGAESOL Renewable Fuel Paths (1), (2), (3) and (4).

Table 3: Process flows for the process models simulation.

Process Flow PF#	PF Description	Main Constituent	Further Constituents	Process Connection PC#
PF1	Solar Irradiation	DII (direct incident irradiation)		- (local)
PF2	Organic Waste	see organic waste spec.	H2O	PC1
PF3	Carbon Dioxide	CO2	O2, N2, H2, H2O, CO, traces of other gas species	PC2
PF4	Methane	CH4	other gases	PC2
PF5	Methanol	CH3OH	H2O, CO, H2, CH4, HCOOH	PC3
PF6	Lipids	microalgae lipid extract	NADES, water, liposoluble substances, residual solid fraction	PC4
PF7	SAF	Sustainable Aviation Fuel	C8-C16 range hydrocarbons	PC3
PF8	Microalgae	aquaeous biological material		PC4
PF9	Water	H2O		PC1
PF10	Oxygen	O2		PC2
PF11	Acetate	acetate + biomass		PC1
PF12	Intermediate Gas Mix			PC2
PF13	Electrolyte	KHCO3		- (local)
PF14	Anolyte	alkaline solution (KOH)		- (local)
PF15	Catholyte	mineral medium		- (local)

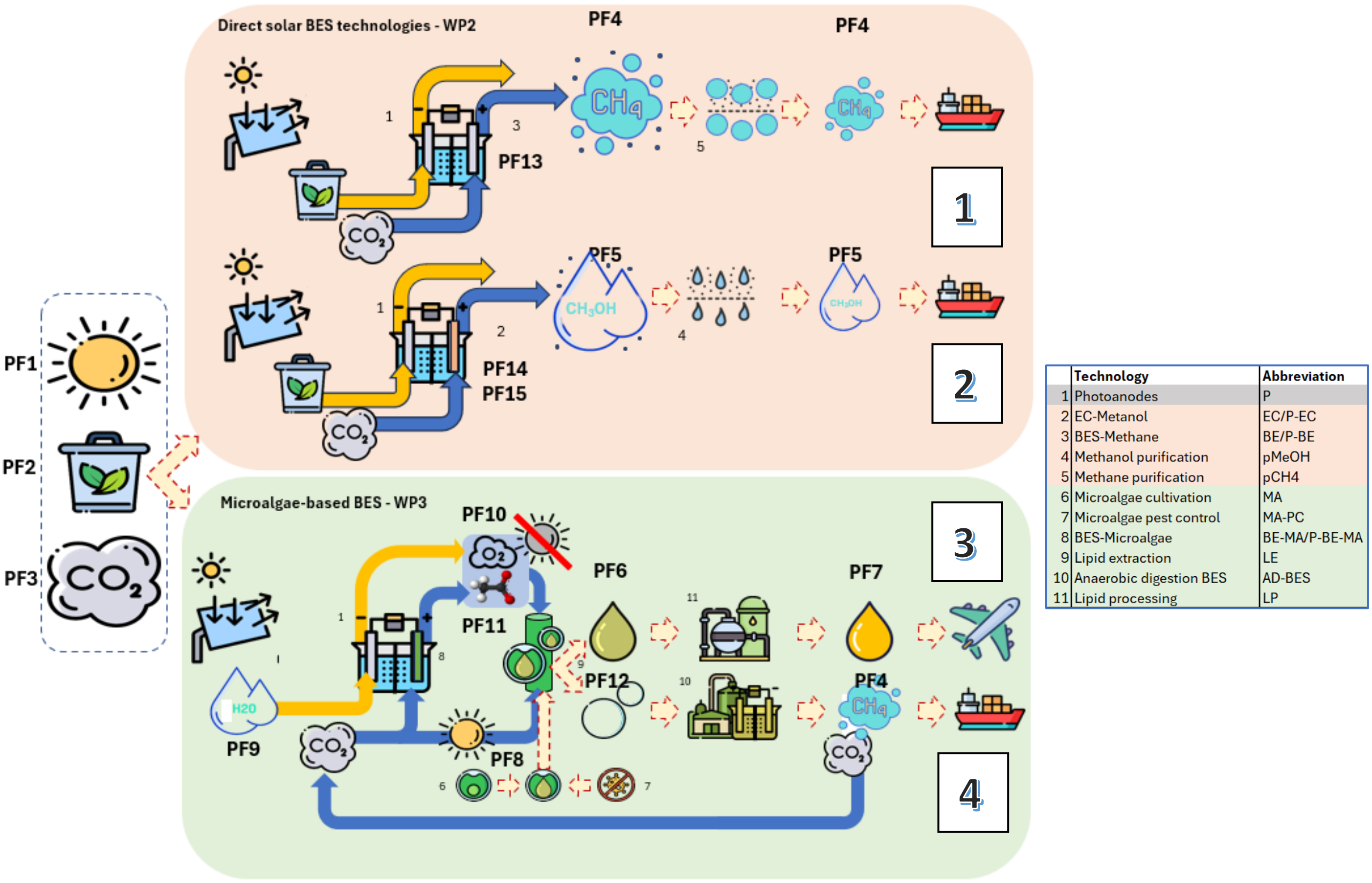


Figure 10:Process flows in renewable fuel production paths.

The process flows (PF) defined above will be grouped in several process connections (PC) which will have a more general specification. Thereby the number of models to be created will be reduced. In a process model, these connections will transfer information between the individual component models.

Specific parameters and variables have already been identified, with their typical values still to be completed, when creating the connections for process flows, the component models and subsequently the process models for the simulation and optimization of the ALGAESOL evaluated fuel paths.

Table 4: Process Connections to represent the Process Flows.

Process Connection (PC#)	Description	Connection Name
PC1	Aqueous organic waste	OW_Stream
PC2	Gas mixtures	G_Stream
PC3	Liquid fuels	LF_Stream
PC4	Microalgae and lipids	MAL_Stream

Table 5: Specification of the variables for aqueous organic waste.

Organic waste specification variables		Units
pressure	p	bar
temperature	t	°C
enthalpy	h	kJ/kg
specific volume	v	m^3/kg
mass flow	mass	kg/s
mass fraction of the organic substrate	w	kg/kg
volumetric flowrate	Q	L/s
chemical oxygen demand	COD	mg/L
chemical oxygen demand (vfa)	COD_vfa	mg/L
volatile fatty acids	VFA	mg/L
acetate	Acetate	mg/L
total suspended solids	TSS	mg/L
volatile suspended solids	VSS	mg/L

Table 6: Specification of the variables for gas mixtures.

Gas mixture specification variables		Units
pressure	p	bar
temperature	t	°C
enthalpy	h	kJ/kg
entropy	s	kJ/kgK
specific volume	v	m^3/kg
mass flow	mass	kg/s
mass fraction of Argon	AR	kg/kg
mass fraction of C2H6	C2H6	kg/kg
mass fraction of C3H8	C3H8	kg/kg
mass fraction of CH4	CH4	kg/kg
mass fraction of CO	CO	kg/kg
mass fraction of CO2	CO2	kg/kg
mass fraction of H2	H2	kg/kg
mass fraction of H2O	H2O	kg/kg
mass fraction of H2S	H2S	kg/kg
mass fraction of N2	N2	kg/kg
mass fraction of O2	O2	kg/kg
mass fraction of SO2	SO2	kg/kg

Table 7: Specification of the variables for liquid fuel mixtures.

MeOH and other liquid mixtures		Units
mass fraction of carbon	w_C	kg/kg
mass fraction of hydrogen	w_H	kg/kg
mass fraction of nitrogen	w_N	kg/kg
mass fraction of oxygen	w_O	kg/kg
mass fraction of sulphur	w_S	kg/kg
mass fraction of water	w_Water	kg/kg
mass fraction of ashes	w_Ash	kg/kg
specific heat capacity of the fuel	cp	kJ/kgK
lower heating value	LHV	kJ/kg
mass flow	mass	kg/s

Table 8: Specification of the variables for microalgae and lipids.

Microalgae and lipids specification variables		Units
pressure	p	bar
temperature	t	°C
specific heat capacity	cp	kJ/kgK
specific volume	v	m^3/kg
mass flow	mass	kg/s

All variables' identifications and definitions presented in the Tables 4-8 will be updated and augmented through the development of the component and process models for ALGAESOL in WP5, tasks T5.1 and T5.2. This also applies for Table 9.

2.3. Component Models in the Model Library ALGAESOL_Lib

This section describes how the component models to be created in IPSEpro-MDK will produce a customized library for ALGAESOL.

The technologies listed in Figure 10 and the Table 9 below will most likely form individual units, also called component models, which represent the process steps taken in fuel production. Unique names are required for the component models, so the core components obtain the prefix "AS_". Those more general component models which will be available for the different process connections, here a prefix "X_" has been used. In the actual implementation, instead of "X_" the prefix of the individual process connection will be used. X_Source stands for OW_Source (organic waste source), G_Source (gas source) etc.

All the process connections and component models together make up the model library ALGAESOL_Lib. Thereby, this library will be used for the modelling and simulation of the fuel production paths.

Table 9: Technologies and related component models.

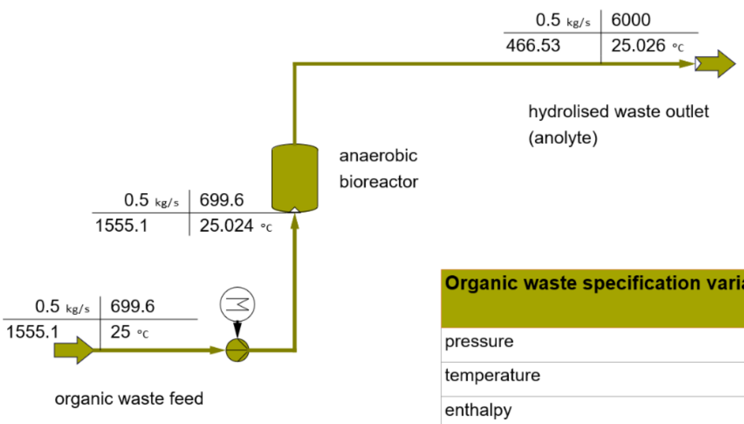
Technology	Abbreviations	Component Models
Photoanodes	P	Part of AS_P_EC, AS_P_BE and AS_P_BE_MA
EC-Methanol	EC/P-EC	AS_EC AS_P_EC
BES-Methane	BE/P-BE	AS_BE AS_P_BE
Methanol purification	pMeOH	AS_pMeOH
Methane purification	pCH4	AS_pCH4
Microalgae cultivation	MA	AS_MA
Microalgae pest control	MA-PC	AS_MA_PC
BES-Microalgae	BE-MA/P-BE-MA	AS_BE_MA AS_P_BE_MA
Lipid extraction	LE	AS_LE
Anaerobic digestion BES	AD-BES	AS_AD_BES
Lipid processing	LP	AS_LP
Sources, sinks	-	X_Source X_Sink
Pressure increase	-	X_Pump X_Compressor
Pressure decrease	-	X_Valve
Mixing and splitting of process connections	-	X_Mixer X_Splitter
Mechanical drive	-	motor

Example of a simple process model configured in IPSE GO

The illustration that follows (Figure 11) shows a simple process model flowsheet of an anaerobic digester developed in IPSE GO. The process flow specifications are listed in the displayed table. The organic waste feed specification is generic to allow various effluents to be represented via the same type of process connection.

Anaerobic digestion of aqeuous organic waste

Anaerobic digester for organic waste to increase availability of certain



Organic waste specification variables		OW_Stream001 org waste feed	OW_Stream003 org waste outlet	
pressure	p	1	1	bar
temperature	t	25	25.03	°C
enthalpy	h	104.9	104.9	kJ/kg
specific volume	v	0.001003	0.001003	m³/kg
mass flow	mass	0.5	0.5	kg/s
mass fraction of the organic substrate in the wa	w	0.000006018	0.000006018	kg/kg
volumetric flowrate	Q	0.5015	0.5015	L/s
chemical oxygen demand	COD	1555	466.5	mg/L
chemical oxygen demand (vfa)	COD_vfa	62.2	1555	mg/L
volatile fatty acids	VFA	1166	314.8	mg/L
acetate	Acetate	699.6	6000	mg/L
total suspended solids	TSS	110.9	66.54	mg/L
volatile suspended solids	VSS	1.109	77.63	mg/L

Figure 11: Example of a Process Model in IPSE GO.

3. ALGAESOL Use-Cases for Sustainable Fuel Production

In this section the use-cases for sustainable fuel production are described, with some details about the Sustainable Aviation Fuel (SAF) production, followed by some considerations about the production of shipping fuel for maritime transportation. The information in Section 3 was provided by ALGAESOL Partner SOCAR.

The criterion for selecting the virtual use cases for the project is based on choosing a real production line for fuels for aviation and shipping to allow realistic boundary conditions for an industrial case for ALGAESOL. The selected use case is connected to the production process of a refinery of the project partner SOCAR, the STAR Refinery which is located in Aliaga, Turkey[1] (see Figure 12). In 2021 the refinery was selected for the World Economic Forum (WEF) 'Global Lighthouse Network', which includes the facilities that best use Industry 4.0 technologies in production. It is a site at the forefront of technology and therefore well suited to serve as a use-case within the ALGAESOL. It will be the source for providing state of the art boundary conditions, being an example (scale, capacity etc.) for developing scale up strategies and as a case for benchmarking production costs and efficiency [1]. The site currently has a capacity of an annual gross production capacity up to 11 million tons for conventional fuel production but strives for an increasing share of biofuels in its output. Specific focus is put on producing biofuel via the conversion of algal lipids using catalysts, an expertise with which SOCAR contributes to the success of the project ALGAESOL in WP4, towards increasing the production efficiency of biofuels and specifically to reduce the costs for economic competitiveness with fossil fuels. Besides the optimisation of elements of the production process as developed in ALGAESOL, the evaluation of the entire value chain / production process is of importance. This includes the balancing of components in terms of their expected different operational characteristics as well as consideration of health, safety and environmental aspects as important aspects for industrialisation of the processes.

Challenges - Three of the challenges for the use-cases of sustainable fuels production are: (1) Implementing the ALGAESOL technology as a valuable and effective solution to exploit biofuels for aviation and shipping applications; (2) Developing a business case for the valorisation of the ALGAESOL solution for delivering its fuel to needs of the aviation and shipping industry; and (3) Simulating the application of the ALGAESOL for both sectors. Table 10 that follows describes in detail the use-case for Sustainable Aviation Fuel (SAF) production.

Table 10: Sustainable Aviation Fuel Production.

SUSTAINABLE AVIATION FUEL PRODUCTION
Use-Case Area of Application: AVIATION / Green SAF Production **Use-Case provider:** SOCAR – **Location:** SOCAR STAR Refinery (https://www.socar.com.tr/activity-fields/star-refinery)
Overview & Motivation: Crude oil-based fossil fuels and their derivatives have been used for decades in transportation, which ultimately have led to the emission of greenhouse gases (GHG) over the years. Notably, the transportation is the major contributor to air pollution. A noteworthy article by Zachariadis and Kouvaritakis (2003) underscores that CO2 emissions from the transport sector would be 70 % higher in 2030 as compared to those in 2000. Hence, the transition into carbon-neutral fuels becomes urgent to decrease environmental impacts in the near future. Nonetheless, a significant drawback in the production of biofuels is their high operating cost. For example, operating cost in biodiesel production from oil crops accounts for ~80 % of total expenses. On the other hand, it is not desirable to use oil crops in biodiesel production due to the increasing demand on these crops for human consumption. Thus, the key challenge is to investigate economically applicable biomass sources, like microalgae. The high lipid contents of aqua biomasses make them one of the strongest viable alternatives for proceeding sustainable evolution. The lipids, extracted from microalgal biomass, could be converted into transportation fuel, especially to Sustainable Aviation Fuel (SAF).

[1] https://www.socar.com.tr/activity-fields/star-refinery.

Therefore, the development of ALGAESOL is important to develop novel solutions to produce biofuels from algal lipids for SAF to decrease CAPEX and OPEX from conventional biofuel technologies. To this end, the current ALGAESOL use-case paves the pathway leading to set a background for the adaptation of the developed technologies into conventional production processes in the future.

Goals: To optimize the formulation of heterogeneous catalyst using the experimental design methodology for an active catalyst in the production of SAF from algal lipids; To produce biofuel using green technology via the conversion of algal lipids on the catalysts; To deploy a complete renewable solution to SAF production in the case of green hydrogen integration.

Use-Case Description: Use-Case I will pursue the need of sustainable aviation fuel production, as a viable solution to reach the zero-carbon emission target within the aviation value-chain. For the use-case implementation, a highly active novel catalyst will be improved to produce SAF from algal lipids at one-stage production route, which involves the development of a bifunctional catalyst for breaking down algal lipids into desired carbon range, followed by deoxygenation and isomerization in the presence of hydrogen. Acidic properties of the catalyst will play significant role to achieve this target. Both the acidity and the acidic strength of the catalyst will be critical in converting microalgal lipids into SAF. The experimental design will be performed to relate the acidity and acidic strength of the catalyst to the conversion of algal lipid into SAF to optimize the catalyst formulation. After the lab-scale production of sustainable aviation fuel over developed catalyst, produced SAF will be compared to conventional jet fuel which is produced in SOCAR STAR Refinery (an oil refinery located in Aliaga, Turkey). This performance test will lead to the evaluation whether the produced SAF via ALGAESOL solution could replace and/or be blended into conventional jet fuel after further exploitation up-scaling developments like pilot scale demonstrations.

Figure 12: SOCAR STAR Refinery (Turkey).

Methodology / Work to be done: To synthesize novel solid catalysts to produce sustainable aviation fuel (SAF) from algal lipids, the production route will follow the methodology illustrated in Figure 13. Modified single step sol-gel method will be used to synthesize a supported nickel catalyst. The acidity and acidic strength of the catalyst will play a key role in the production of SAF from algal lipids. To manipulate these crucial properties, different acids will be used in the sol-gel synthesis method. Specifically, the sulfuric acid, hydrochloric acid, and nitric acid will be used in sol-gel synthesize. In addition to acid types used in the synthesis, several other parameters, such as calcination temperature, metal & support content of the catalyst, will be optimized to aims to attain the desired acidity and acidic strength characteristics for the catalyst.

To investigate the effect of textural and crystallographic properties of the catalyst, the prepared catalysts will separately be calcined within the temperature range of 700^{o}C to 950^{o}C. In addition, the nickel amount will be changed from 2% to 10% in order to better address the hydrocracking and isomerization performance of the catalyst during the reaction. Subsequently, the reaction parameters, such as the ratio of catalyst amount to algal lipid, and residence time, will be fine-tunned in the presence of hydrogen gas in order to increase the yield of SAF. The initial identification of the SAF will be done by using gas chromatography equipped with a MS or FID detector. Then, the final product will be analysed with respect to standard methods, like ASTM, ISO, to compare the specifications to conventional jet fuel.

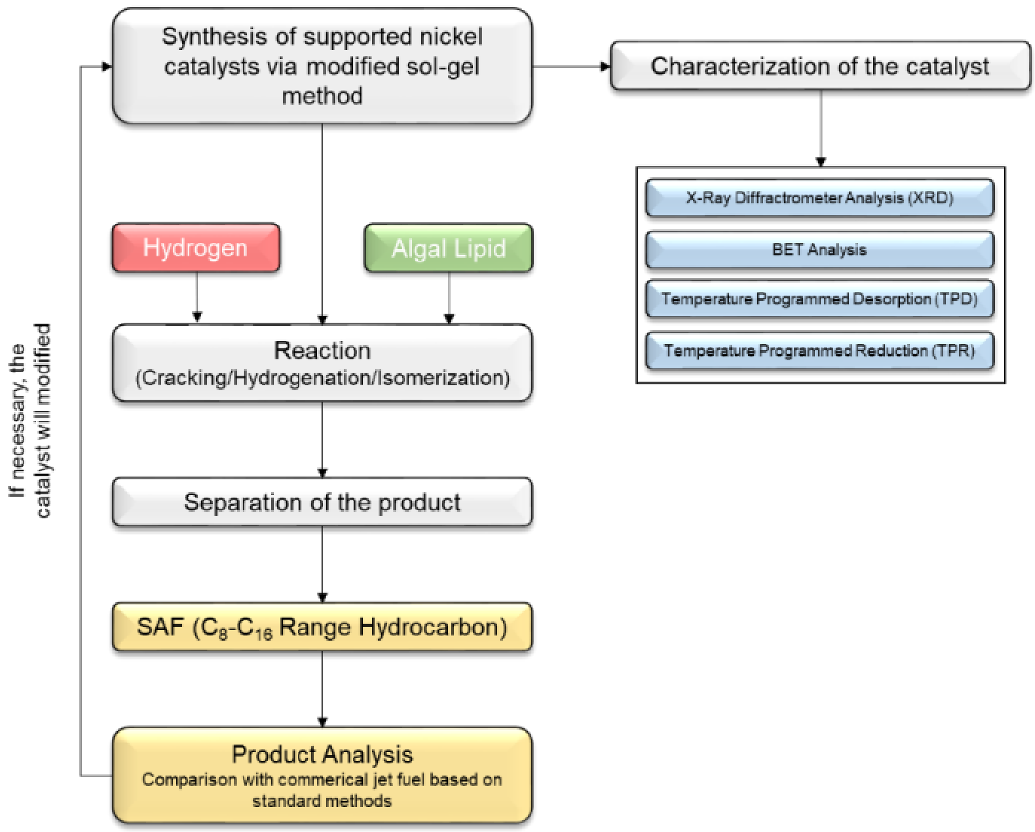


Figure 13: Methodology for the production of SAF from algal lipid.

ALGAESOL proposed solution: The feasibility of the ALGAESOL solution will be assessed in the Use-Case I, with the proof of concept for catalysis to utilize algal lipids into sustainable aviation fuel, through virtual process simulation and optimization, implemented in WP5. The Use-Case processes will be modelled within IPSE GO simulation web-platform, using the ALGAESOL customized library of component models and the data resulting from the use-case catalyst development and experiments. The Use-Case Model will be made available in IPSE GO via the web, for stakeholders' consultation and showcase for further exploitation routes of the ALGAESOL solution.

Expected Outcomes: Environmental Benefits: The production of biofuel using green technology via the conversion of algal lipids on the catalysts which are abundant, cost-effective, and non-toxic, will allow the mitigation of related adverse environmental impacts; Reduction of GHG emissions (aligned with the aviation industry strategy to decrease 1.5% emission per year, reducing the emission values in 2050, to be 50% less than the emission values in 2005). **Economic Benefits:** Decrease of CAPEX & OPEX compared to conventional biofuel technologies. Economically viable SAF for replacing fossil fuels in the aviation transportation sector.

Innovation potential: ALGAESOL innovative solution will allow SAF production and assessment compared to jet fuel and showcasing of use-case simulation, aligning with the sustainability strategy to reach zero carbon emission goal in 2050. with potential up-scaling for further real application in the aviation transportation sector. The implementation of Use-Case I will lead to increase the proposed solution TRL of the project, as it paves the way for further pilot demonstrations, as well as market up-scaling exploitation and deployment, enabling also new solutions to current HEFA technologies.

4. Simulation Overview for the Renewable Fuel Production Paths

This section presents details about the ALGAESOL Renewable Fuel Production Paths and their main parameters that will serve as inputs for their process modelling in the simulation tools.

4.1. ALGAESOL Renewable Fuel Production Paths (1, 2, 3 & 4)

This section presents in detail the four Renewable Fuel Production Paths evaluated in the ALGAESOL project.

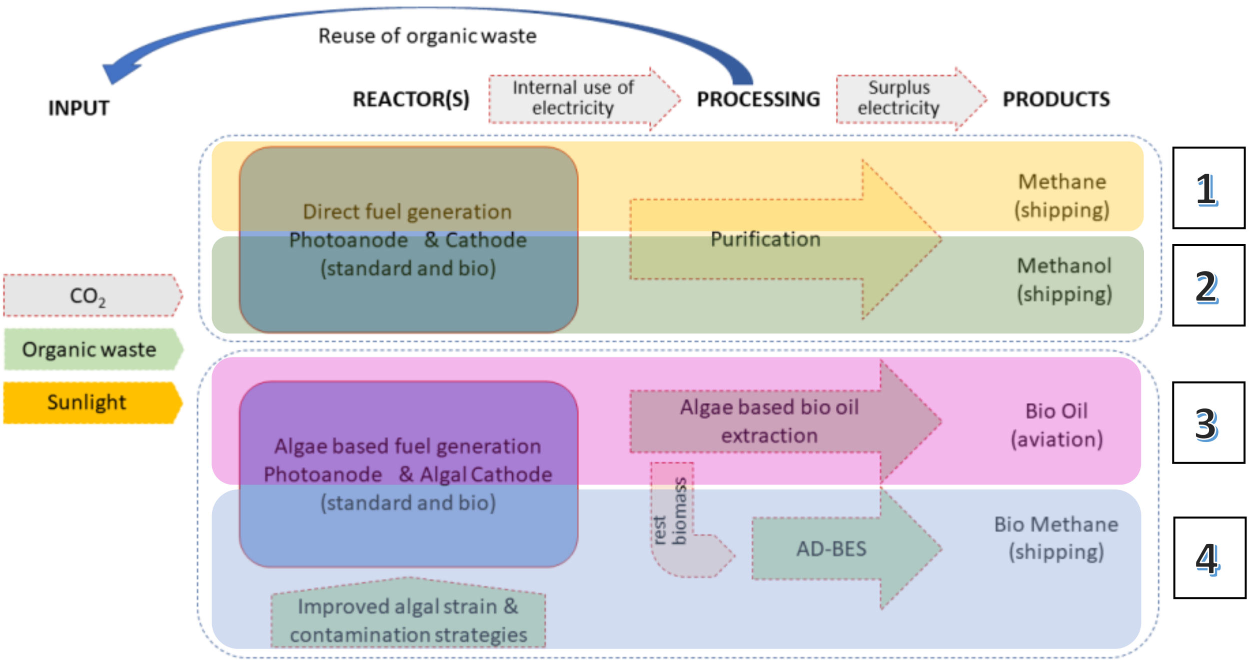


Figure 14: ALGAESOL Fuel Production Paths (1, 2, 3 & 4) for the Use-Cases.

The Renewable Fuel Path 1 deals with the Direct Solar conversion, using photo(bio)electrochemical technologies, for renewable fuel production (highlighted in yellow in Figure 14), enabling the production of the renewable fuel Methane, suitable for being used in shipping. Figure 15 illustrates the ALGAESOL Renewable Fuel Path 1, with the purification process for the production of Methane.

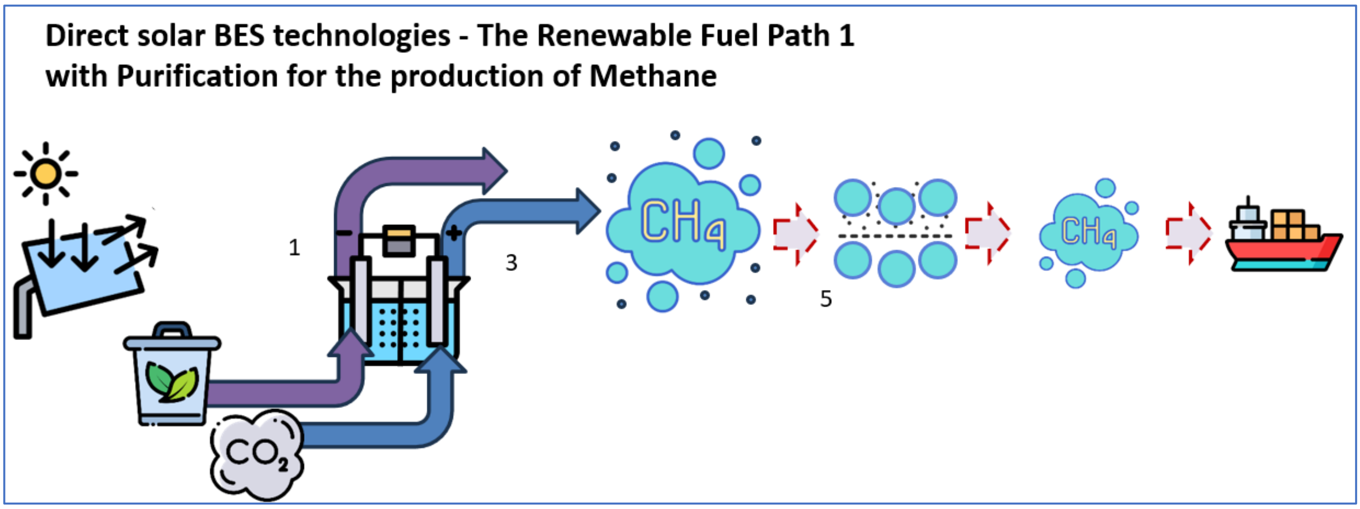


Figure 15: ALGAESOL Renewable Fuel Path 1, with Purification for the Production of Methane.

The Renewable Fuel Path 2 deals with the Direct Solar conversion, using photoelectrochemical technologies, for renewable fuel production (highlighted in green in Figure 14). This path enables the production of the renewable fuel Methanol, which is suitable for being used in shipping. Figure 16 illustrates the ALGAESOL Renewable Fuel Path 2, with purification process for the production of Methanol.

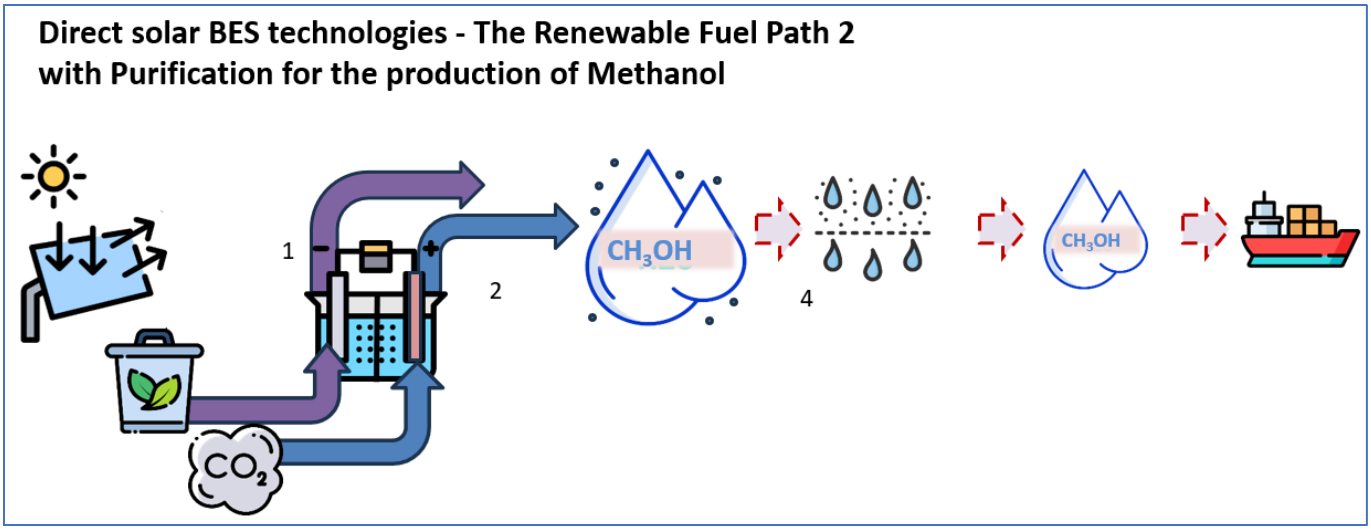


Figure 16: ALGAESOL Renewable Fuel Path 2, with Purification for the Production of Methanol.

The Renewable Fuel Path 3 deals with the Algae-based fuel generation, using photoanode and algal cathode technologies, for generating Bio-Oil from the process of Algae-based bio-oil extraction. This path is highlighted in pink in Figure 14. Path 3 enables the production of Bio-Oil, suitable for being used in aviation. Figure 17 illustrates the ALGAESOL Renewable Fuel Paths 3, for the production of Bio-Oil for aviation.

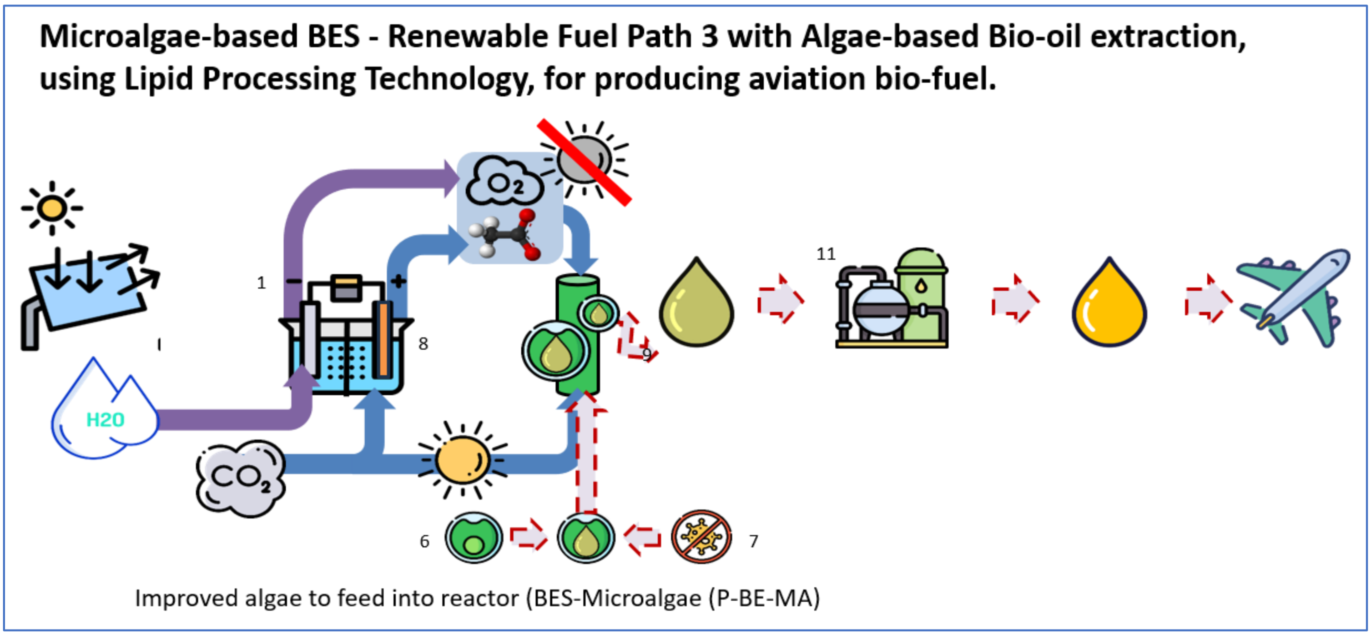


Figure 17: ALGAESOL Renewable Fuel Path 3, with the Production of Bio-Oil for Aviation.

The Renewable Fuel Path 4 deals with the Algae-based fuel generation, using photoanode and algal cathode technologies, for generating Bio-Methane via the process of the AD-BES (Anaerobic Digestion Bio-Electrochemical System) technology fed by the rest of the biomass used in the algae-based bio-oil extraction process from Path 3. This path is highlighted in blue in Figure 14. Path 4 enables the production of Bio-Methane, suitable for being used in shipping. Figure 18 illustrates the ALGAESOL Renewable Fuel Path 4, for the production of Bio-Methane for shipping.

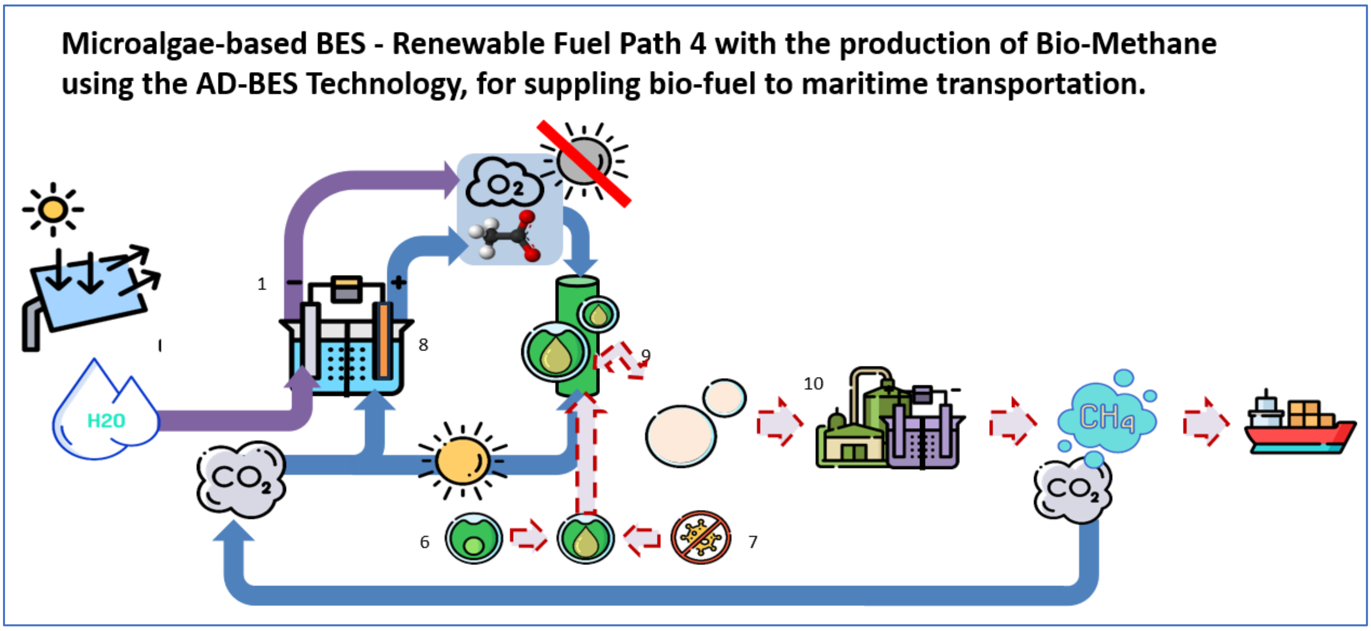


Figure 18: ALGAESOL Renewable Fuel Path 4, with the Production of Bio-Methane for Shipping.

4.2. Main Data Requirements for the Use-Cases and Renewable Fuel Production Paths

In order to model the Renewable Fuel Production Paths 1, 2, 3 and 4, as presented in Section 4.1, various interactions between SIMTECH's team and the team involved in WP1 Task T1.2 were necessary for the identification of the main parameters needed as input for the modelling of the component models needed for ALGAESOL_Lib, as well as for the process models related to the fuel production paths, which will be the output from WP5 enabling the Use-Cases to be specified within the work to be performed by SOCAR.

Examples of the main inputs per paths for the IPSEpro/IPSE GO simulations:

- For the Renewable Fuel Production Path 1, dealing with the Direct Solar conversion and using photo(bio)electrochemical technologies to enable the production of the renewable fuel Methane, the preliminary identified main inputs are: CO2; Aqueous Organic Waste; Solar Energy / Electricity; and Heat.
- For the Renewable Fuel Production Path 2, dealing with the Direct Solar conversion and using photoelectrochemical technologies to enable the production of the renewable fuel Methanol, the preliminary identified main inputs are: CO2; Aqueous Alkaline Electrolyte (optionally with Organic Wastes); Water; Electricity; and Heat.
- For the Renewable Fuel Production Path 3, dealing with Algae-based fuel generation and using photoanode and algal cathode technologies to enable the production of Bio-Oil suitable for SAF, the preliminary identified main inputs are: CO2; Water; Electrical Current; and Hours of Electrical Provision.
- For the Renewable Fuel Production Path 4, dealing with the Algae-based fuel generation and using photoanode and algal cathode technologies to enable the production of Bio-Methane, the preliminary identified main inputs are: Organic Residual from Micro-Algae; Water; Electricity; and Heat.

Figure 19 illustrates the main inputs identified in WP1, task T1.2, for modelling the renewable fuel production paths.

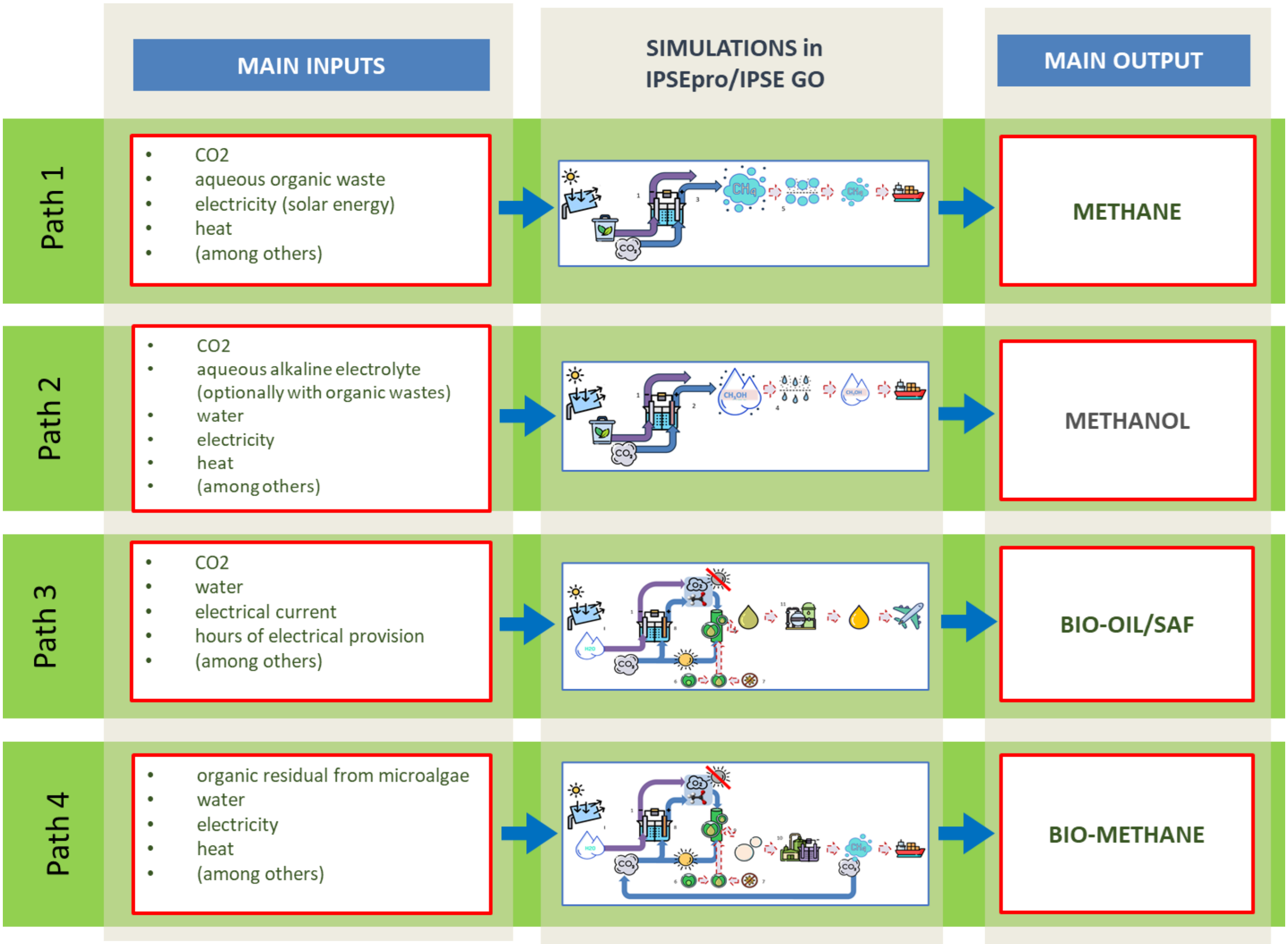


Figure 19: Main Inputs for Modelling the Renewable Fuel Production Paths.

5. Conclusions

Deliverable D1.3 reported the specifications of the process flows and requirements for implementing the component models; the process models of the Renewable Fuel Production Paths; and the further ALGAESOL Use-Cases. D1.3 was produced, based on the general guideline of the ALGAESOL overall concept, and focused on its modelling, emphasizing the simulation concept of the project and the adaption of the simulation tools for the design of the project process flows and use-cases process models, considering the boundary conditions imposed by each specific application. In this context, the document set out the general guidelines to be considered during the project process modelling and use-cases implementation.

In D1.3, a brief description of how the simulation is considered in the concept of ALGAESOL was given. An overview about the IPSEpro simulation environment and the IPSE GO web-platform was presented. The relevant aspects of the specifications and requirements for the implementation of the process models were described, within the overall goals of the simulation procedure, were presented. This led to the basic specification and requirements, such as: feasible computational effort, compatibility between models, adaptability to the web-platform, modularity and flexibility of the simulation tool and the process models, among others. The Process Flows for the representation of the ALGAESOL Renewable Fuel Production Paths were identified. The development of a customized library of component models, ALGAESOL_Lib, for the project was justified. An overview of the ALGAESOL Use-Cases, with information provided by SOCAR, was presented. A summary of the data required for the use-cases process modelling using IPSE GO, with the description of the four Renewable Fuel Production Paths was given in detail, including the preliminary identified main input data to implement their process models.

The outcomes of task T1.3 reported in this document will be relevant for all tasks related to the numerical models that represent ALGAESOL, for modelling its main system solution, as well as the simulation work in WP5 (T5.1 and T5.2), for the creation of customized component models in IPSEpro, and for simulating the overall processes representing the project's Renewable Fuel Production Paths, with the main aim to assess the developed ALGAESOL technology with real data of different use-case scenarios of the aviation and shipping applications.

With the preliminary specifications of D1.3, SIMTECH will build upon the experience brought from other research projects (see [6] and [29]) to accurately implement in WP5 the customized components and process models for ALGAESOL, considering its online simulation platform IPSE GO as a showcase tool for the modelled Renewable Fuel Production Paths and Use-Cases.

Degree of Progress

The degree of fulfilment of the activities within WP1-Task T1.3, with respect of what reported in the DoA, is estimated to be 100% completed, with the production of deliverable D1.3.

However, as Deliverable D1.3 was produced in M6, it includes some general specifications that were not possible to be yet further specified. Those will be defined in more detail during the development of the project within the work done in WP5, with inputs from the other technical WPs (WP2, WP3, WP4). This way, the defined requirements and specifications in D1.3 will be revisited and updated, when necessary, along with the development of the project.

Dissemination Level

As part of the Horizon Europe Programme, ALGAESOL project complies with the Open Science principle (see DMP [4]). Hence, deliverable D1.3, as a public dissemination-level document, will be made available in the Zenodo[2] open-science research data repository (https://zenodo.org/), within the Zenodo ALGAESOL Open-access Community for further reference and dissemination.

[2] https://about.zenodo.org/

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