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Deliverable D6.2

Generic LCA modelling

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1. Introduction

Genetic engineered phototrophic microalgae and cyanobacteria have great potential to significantly improve biofuel production. The modifications which are pursued in the PHOTOFUEL project are aiming to change the microbial cells in the way that they can excrete fuel precursors and compounds into the culture broth. By this, separation of the fuel precursors without culture harvesting and destroying of the cells and thus fuel production under steady state conditions is possible. The hypothesis regarding the Life Cycle Assessment (LCA) is that thereby energy balance can be improved and the nutrient demand and environmental impacts reduced. Whether this assumption is correct will be investigated by conducting LCA of the most promising PHOTOFUEL processes.

LCA on new technologies and processes such as the bio-catalytic production of fuel precursors is always tricky, because the technology is in its infancy and valid information and data are hardly available, especially from large-scale outdoor cultivation and harvesting systems. However, sustainability challenges related to new technologies and systems can be better addressed the earlier the assessment is carried out in the technology development phase. Therefore, it is necessary to carry out LCA if possible already in the technology design phase and to consider technical progress as well as possible changes in framework conditions to provide a deeper understanding of technical needs and environmental impacts of future technologies and systems for next generation biofuel production.

Generic LCA modelling is an important and highly valuable instrument to support and improve scoping and framing of new technologies and the preliminary assessment of the environmental impacts. It provides a platform to discuss and improve the units and processes of the bio-catalytic fuel production system. Besides, it facilitates the iterative adaptation and optimisation of the system by a continuous exchange of data, research results and insights from other work packages of the PHOTOFUEL Consortium, respectively with the project partners in WP2 and WP3, because in WP3 the modified strains with the best performance and bio-catalytic system developed in WP2 are scaled-up and cultivated in photobioreactors.

The generic modelling of the LCA is based on an inventory of the energy and materials flow within the defined boundaries of the investigated system. Thus, the design of the PHOTOFUEL processes is the first and crucial step in carrying out a generic LCA modelling. In the Deliverable D6.1 the system boundaries of three different PHOTOFUEL processes have been outlined:

- Cyanobacteria Synechocystis sp. PCC 6803 for the production of n-butanol and isobutanol;
- Cyanobacteria Synechocystis for the production of medium-chain alcohols and alkanes (iso fatty alkane) and sesquiterpenes;
- Chlamydomonas reinhardtii for the production of the bisabolene synthase.

In the meantime research in WP2 came up with new findings. Microbial production of free fatty acids (FFAs) with genetically modified Cyanobacteria Synechococcus sp. PCC 7002 has found to have great potential for biofuel production, because this strain has achieved high

volumetric productivity of FFAs under lab conditions. The FFAs producing strain has been cultivated and tested in the cultivation reactor of A4F in Portugal.

Due to these new insights in WP2 and WP3 we modified the design of the PHOTOFUEL processes considered for the generic LCA modelling set up in the Deliverable D6.1 and included the process of bio-catalytic FFA production. In this report the generic LCA modelling for the three improved strains producing different types of fuels precursors that have already been tested in WP3 are presented:

- Butanol from the Cyanobacteria Synechocystis sp. PCC 6803;
- Free fatty acids from the Cyanobacteria Synechococcus sp. PCC 7002;
- Bisabolene from Chlamydomonas reinhardtii.

The generic LCA modelling is built on three units:

- Production of the inoculum;
- Cultivation phase and the production of the fuel precursor;
- Harvest and separation of the precursor.

A schematic overview of the generic LCA model is given in Figure 1.

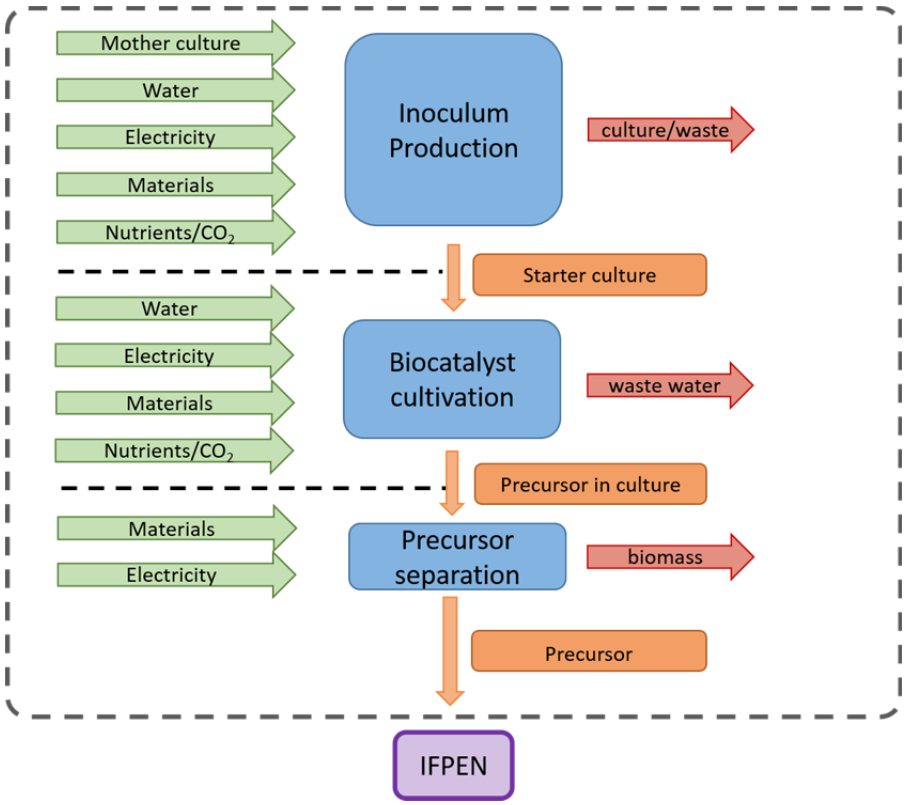

Figure 1: Schematic overview of the generic LCA model

It is assumed that for the production of the three PHOTOFUELS described above (butanol, free fatty acids and bisabolene) the production of the inoculum and the cultivation of the cyanobacteria and microalgae are similar while the harvesting processes are differing.

As the available knowledge of harvesting butanol is much more advanced than for harvesting FFAs or bisabolene the generic model for the butanol process is already much more developed than for the other two products. For this reason we have focused in this report on presenting the generic LCA modelling of butanol production. The generic model is built up on present information from WP2 and WP3, but can be easily adapted and modified if new findings are achieved during the project duration.

We assume that the technology will be continuously developed parallel to running trials. Adaptations will be made and the processes will be optimized. For the LCA this is connected with some challenging aspects. As we are dealing with a biological system that needs to be balanced, some process engineering parameters have to be adjusted and regulated. After the proof of concept, the operational times have to be extended to deliver a suitable baseline for the LCA data. Technical equipment related to material consumption can be optimally scaled according to its workload. To solve this complex proposition in the LCA model, some parameters have to be defined and assumptions taken. The following paragraphs describe the defined procedures according to the different phases of production.

2. Methodology

For the generic LCA modelling we used the open LCA software and preliminary project data and the database ecoinvent 3.2 [1], which provides very complex datasets to derive a proper LCI. Figure 5 gives an overview of the LCA model in the openLCA software. The impact assessment is carried out by calculating recommended impact categories according to the ILCD handbook [2].

The database for the processes comprises raw material extraction as well as the assembly to pre-products e.g. borosilicate tubes. However, transport, storage and end of life options are excluded because they are outside the system boundaries of the investigated processes. In addition to that, the delivery of inputs and raw materials to the production site as well as machine abrasion and disposal are defined to be outside the system boundaries of this study.

3. General assumptions

Improved engineering will make a significant impact on the productivity of PHOTOFUEL production. These improvements comprise efficient strategies for nutrient circulation and light exposure and the development and application of species that grow efficiently at certain climatic conditions, respectively light conditions and temperature. With the site-specific selection of the strains the yield potential can be fully exploited and the requirement for supplemental cooling or heating can be reduced or even avoided at the same time. As conditions differ considerably in winter and summer the conclusion is to cultivate different strains in summer and winter time if the light conditions and temperatures during winter time

are suitable for the cultivation of microalgae or cyanobacteria, such as it is the case at the location of A4F in Portugal.

In the generic LCA model a continuous cultivation and production period of 360 days is assumed. Here, we hypothesize two different strains for butanol production during summer and winter time: Different varieties of *Synechocystis* sp. PCC 6803 tolerating high temperatures with a productivity of 100 mg/l/d butanol in the summer period (May – Septemper → 5 months à 30 days) and a productivity of 15 mg/l/d butanol in the winter period (October –April → 7 months à 30 days, respectively, were assumed. Consequently in the LCA model we assume a weighted yearly average productivity of 50 mg/l/d butanol. The values for the summer productivity are forecasted according to UU whereas the winter productivity was measured in a first 14 days test run.

4. Inoculum production

The production of the inoculum for the cultivation of the three different PHOTOFUEL processes is assumed to be a small-scale production usually performed by laboratories. Thus, the design of the inoculum production comprises a stepwise up-scaling of inoculum production starting from a test tube and completing the process with inoculum production in a fiberglass cylinder as main reactor, which can hold 80 l of working volume (see Figure 2). It is assumed that this procedure will take twice per year to inoculate the cultivation reactor. In order to have a reliable and operational production of inoculum, three replicates are assumed to run in parallel. After one trail of these high density cultures has been successfully implanted in the cultivation reactor, the other two are discharged.

Nutrients are added to maintain optimal growth conditions. The uptake efficiency of nutrients is considered to be 100%. For the generic LCA model 12.4 g/l N of sodium nitrate and 3.4 g/l P_2O_5 provided by triple superphosphate, are applied. The amount of nutrients needed is based on the final target concentration of 1 g biomass/l and calculated on stoichiometric relations. Materials for glassware and plastics e.g. for shake flasks are recalled from the ecoinvent 3.2 database and typical lifetimes for lab equipment are considered.

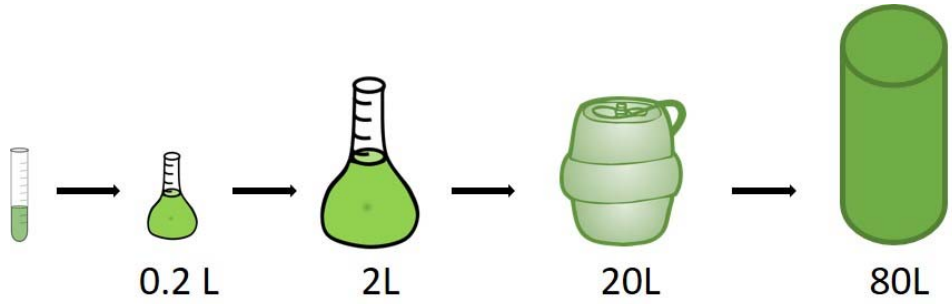

Figure 2: Production scheme for batch culture of algae (modified according to [3])

In a batch regime the culture is consecutively transferred to the next, bigger volume (see Figure 2). After about 30 days the culture is conveyed to the final cultivation reactor. This transfer takes place manually with no additional devices needed. Data for the inoculation equipment are based on literature and adapted according to practical experience from the EU project EnAlgae. The electricity consumption during inoculation is derived from experimental data. A compressor serves for gas exchange and for sufficient mixture to deliver the cells regularly to the light source represented by fluorescent light bulbs. The reactor is inoculated with 10% of the final cultivation medium. The inoculation of a 5 m^3 reactor requires five inoculation procedures per inoculation.

5. Cultivation

For the cultivation of the microalgae and cyanobacteria the LCA model is designed in a modular way assuming that a reactor with a volume of 5 m^3 serves as smallest production unit. Multiple of these production units are set up in series to increase the production capacities and to match with the technical layout of the harvesting equipment For the operation of the reactor modules different equipment, such as pumps, blowers, filters, sensors or heat exchangers, is designed in the LCA model (see Figure 3). The CO_2/air mixture (10%) will be provided by an upstream compressor. Regulation and automation of the flows to the modules will be supervised and guaranteed by sensors (pH, pressure, nutrients etc.). Pipelines for culture circulation, medium preparation, and cooling are considered in the model too. Given the uncertainties about the layout of the large-scale cultivation in the LCA modelling only the material and energy consumption of the circulation pump is included so far. For the electricity demand of the cultivation step we assume a value of 24 kWh/m^3/d based on data given by our project partner A4F in WP3.

The nutrient demand is calculated on the same baseline as for the inoculation procedure. On demand, the stock solution is pumped from the stock solution tank with high concentrated nutrients to the growth medium tank and if necessary diluted with fresh water prior to the transfer to the cultivation reactor (see Figure 3). The growth medium tank will serve as medium storage and should be continuously stirred and equipped with sampling units to measure the nutrient concentrations. Before fresh culture medium is pumped to the reactor units, it is filtered. After each separation it as assumed that most of the culture medium (90%) is recycled. Therefore, a recycling vessel linked to the culture medium tank is also considered.

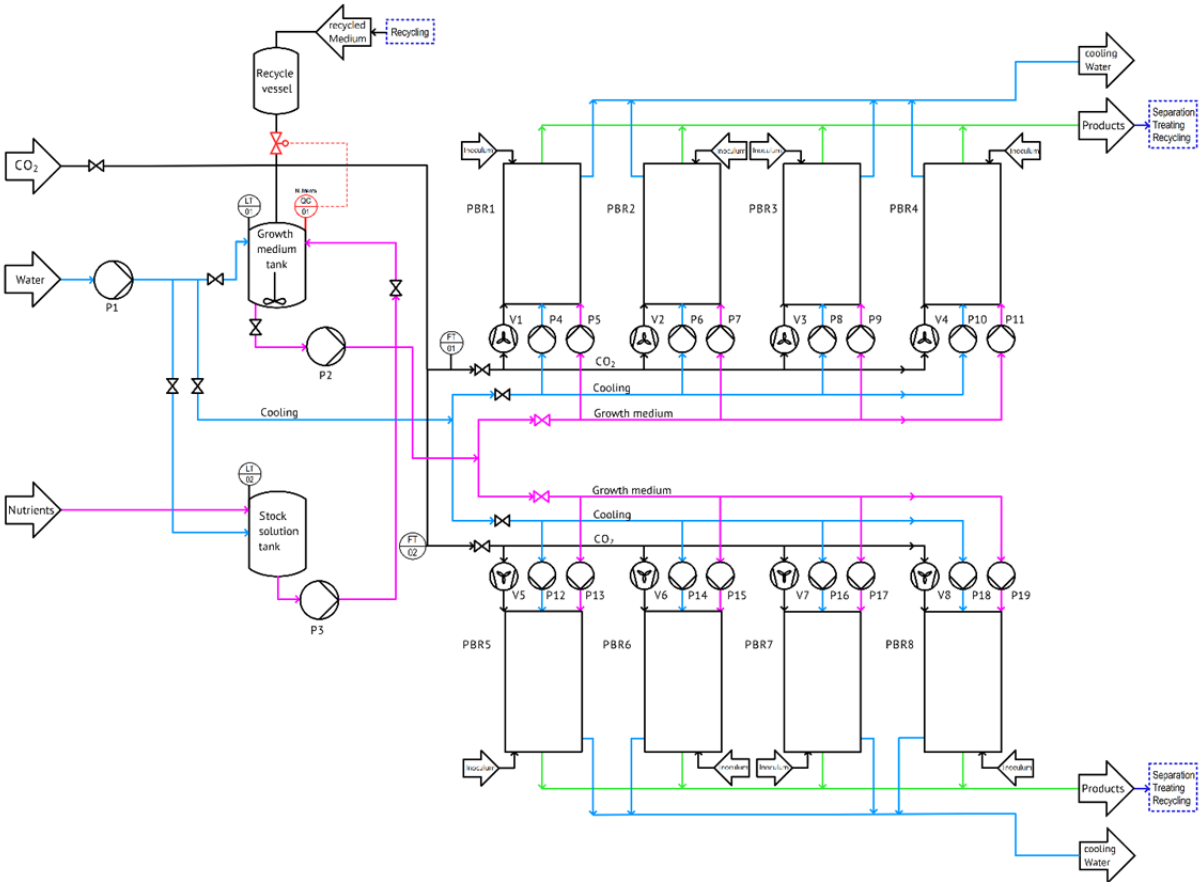

Figure 3: Process flow scheme of the cultivation module

6. Harvest and separation of the precursor

The culture regime is assumed to be continuous. The frequency of the harvests, however, still needs to be defined. In the generic model we assume that the butanol concentration is fixed to 1g/l. We assume that the reactor has reached this concentration 20 days after inoculation, and the continuous partial harvest of 30% of volume will occur every 6 days. Parallel to the harvests, medium including fresh fertilizer is added to maintain stable conditions. In Figure 4 the generic model of the harvesting and separation modules is displayed based mainly on the existing butanol production process.

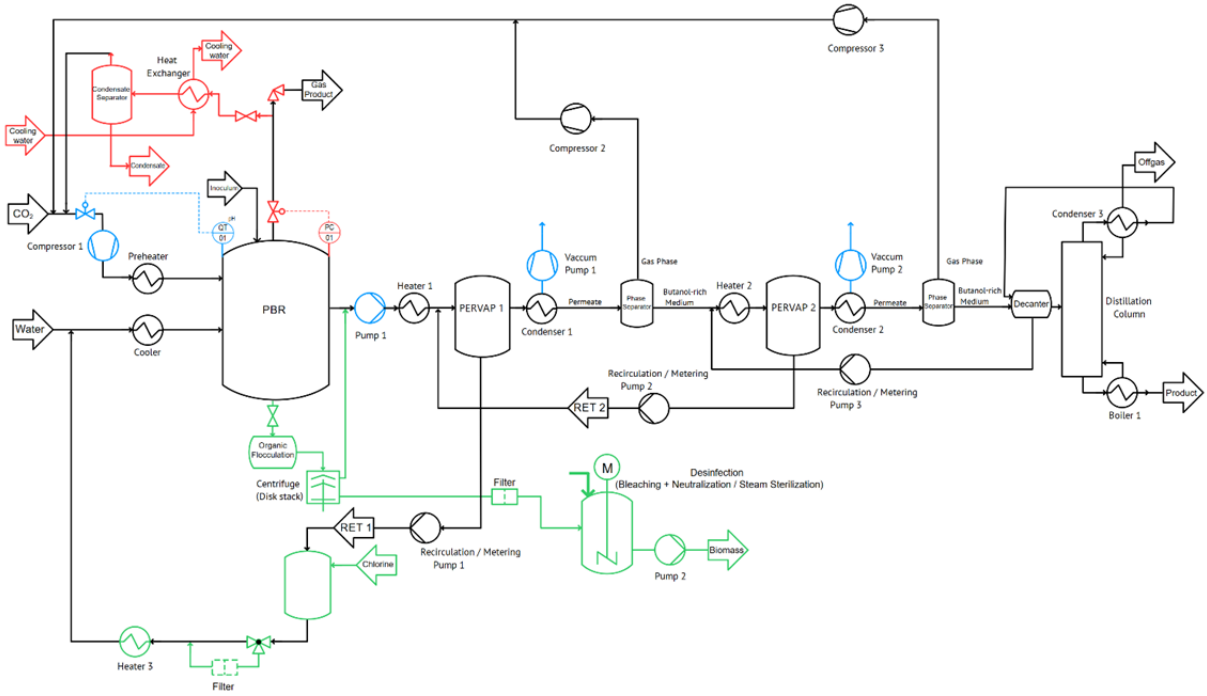

Figure 4: Flow diagram of the butanol production process (possible changes in future assessments in colours)

The butanol production rate is fixed against biomass production with a mass ratio of one. An optimal biomass concentration in the reactor is achieved by adding minimal levels of nutrients to keep a healthy culture and allow biomass growth in order to compensate for cell death. However, a viable constant biomass concentration within the reactor must be defined in order to avoid high biomass concentrations.

The maximum butanol concentration in the reactor is limited by the tolerance of the culture to elevated butanol concentrations. Current strains have shown good butanol tolerance up to concentrations of 4 g/l. However, this still must be reliably determined for chemostat operation. Two scenarios with different butanol level before harvesting have already been modelled in the PHOTOFUEL project. A rather low butanol scenario (1 g/l), which seems to be a realistic target, and a rather high butanol scenario (10 g/l), which is comparable to the butanol concentrations achieved in fermentative processes. However, only the 1 g/l scenario is analysed in the generic LCA model at this point.

The existing model does not consider any separation method of the butanol-rich medium and the produced biomass. At this stage, the biomass valorisation is not yet translated in the LCA calculation due to lack of data. The biomass pathway, however, will be included in the progress of this work to improve the overall efficiency of the system. Future assessments will also consider the use of different harvesting and separation methodologies since some relevant specific criteria about the harvesting module are not yet determined. For instance, a combination of two separation techniques would be interesting for the general energy balance to enhance the recovery efficiency and improve the economics. The first step would be an organic flocculation, as an initial dewatering step, coupled with disk stack centrifugation as a secondary treatment. As a result, less volume of biomass suspension would undergo the secondary energy-intensive treatment. After separation, the biomass would then be filtered, disinfected (depending on the future uses) and pumped.

On the other hand, the butanol-rich flow in the system undergoes a combination of two pervaporation steps and requires a final distillation column in order to purify the product. The pervaporation process is used to increase the butanol levels above the spontaneous butanol-water phase separation point. After this, it is possible to separate and recycle the aqueous phase back to the separation system and to recover the butanol from the organic phase through distillation. Each pervaporation unit requires a heater, a condenser, and a vacuum pump to reduce the outlet pressure. However, the vacuum pumps are not integrated in the generic LCA model.

All aqueous streams are being recycled in the generic LCA model to minimize the amount of required fresh water and to recover all residual butanol. In the future work we will also consider to treat this recycled stream with chlorine and to filter it, depending if there is a lot of material in suspension or not, and to use a recirculation pump. Then, it would be necessary to use a heater before reuse in order to avoid an accumulation of chlorine in the reactor.

The possibility of recycling all the gas streams and their energy use associated with compression will be analyzed in the future work too. In the particular case of the gas product from the reactor it might be necessary to dehumidify it before sending it back to the reactor by using a compressor. Also, in order to keep the appropriate pressure in the reactor, it would be necessary to control automatically the gas outlet and inlet.

7. Results of the generic LCA modelling

Materials and system inputs are translated to a one-year-baseline to account for different life times and input frequencies. For the reactor system and the technical equipment, the main embedded materials were considered. Market values were chosen for the supply of intermediate products (e.g. electricity) on a European scale. Furthermore, the cut-off system was applied, meaning that the production of materials and all respective impacts is allocated to the primary user and recycled materials bear only the impacts of the recycling processes.

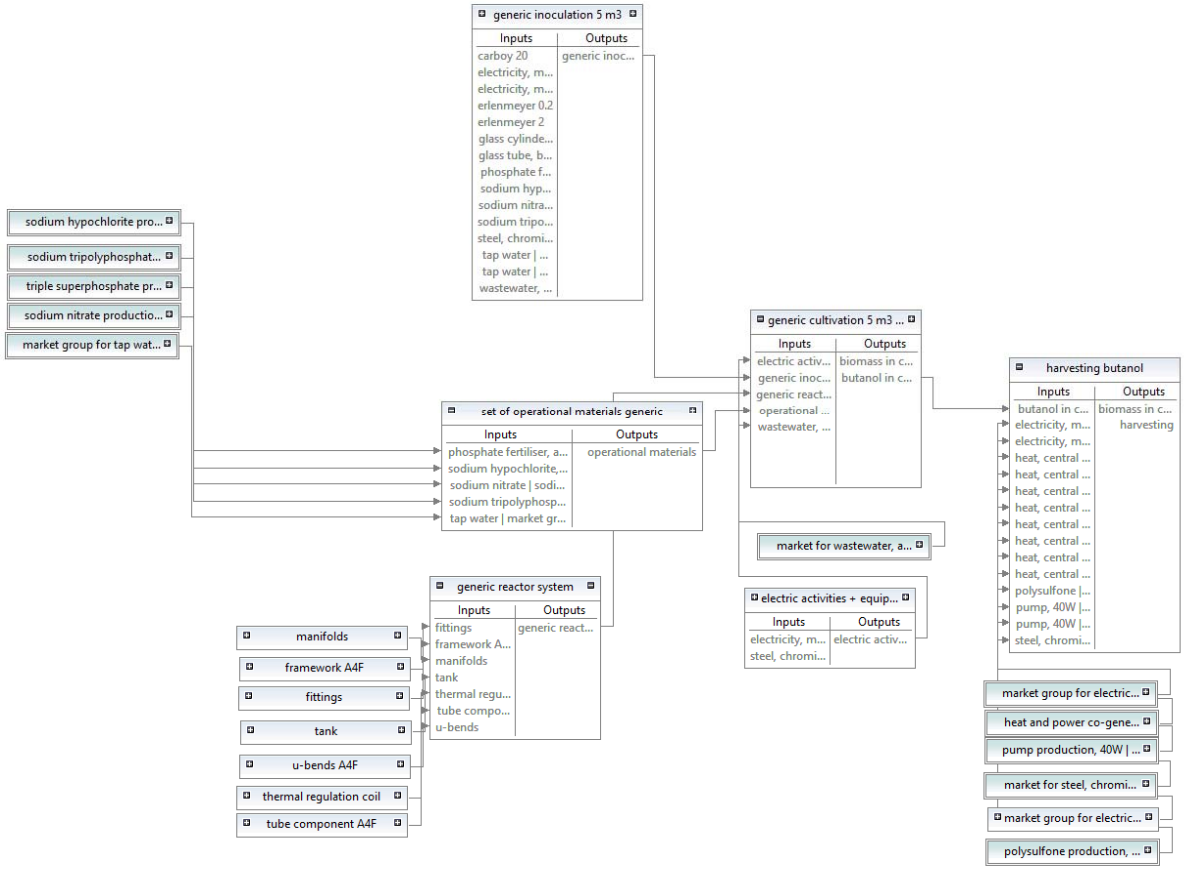

Figure 5: Illustration of the openLCA model

The results of the generic LCA modelling on the production of butanol are depicted and described in the following. The lifetime of the production system was assumed to be 20 years. During the cultivation period no maintenance and breakdowns were considered.

Figure 6 shows results of the recommended ILCD impact categories of the production of 1 kg of butanol. Main processes were considered as described above. Especially electricity, operational materials e.g. fertilizers and the embedded burdens of the materials used contribute to the impact assessment results. Processes contributing to less than 2% to each impact category were summarized to "others".

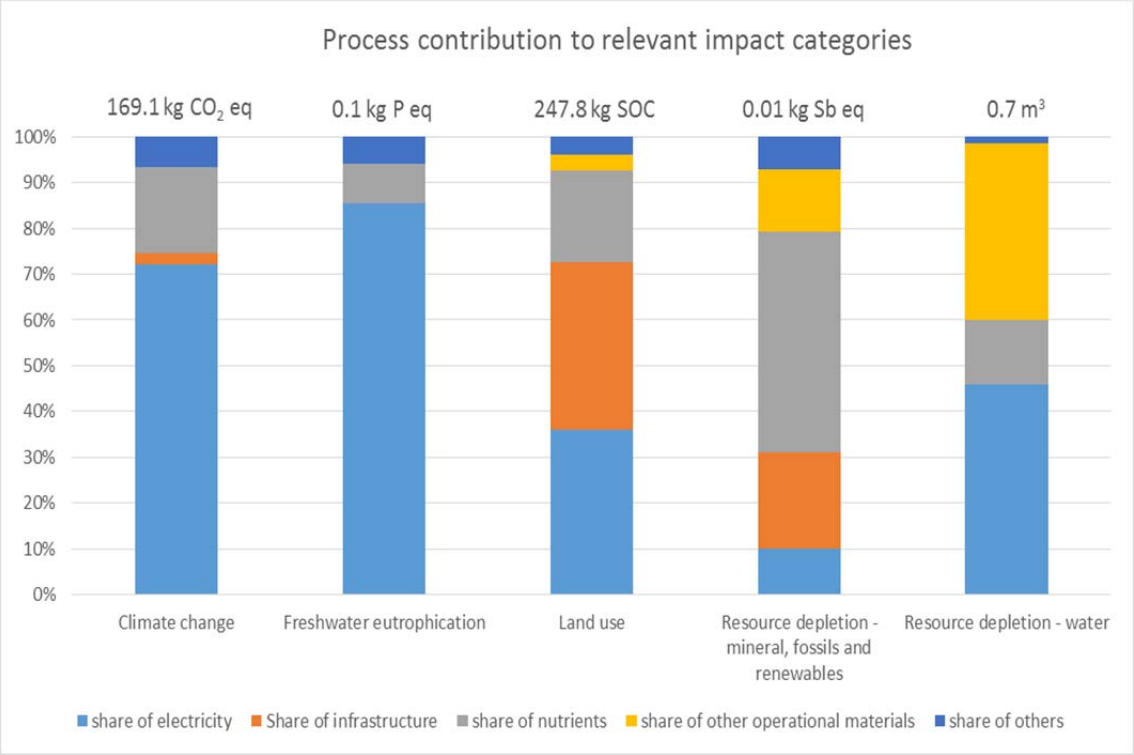

Figure 6: Contribution of clustered impacts to relevant impact categories recommended by the ILCD handbook

Highlighting the most prominent impact category of climate change, it can be stated that the production of 1 kg of Butanol results in the emissions of about 170 kg of CO_2 eq. Compared to conventional diesel production (0.56 kg CO_2 eq/kg diesel) this value is about 300 times higher. Nonetheless, these values cannot be directly compared, as butanol will serve as a blend component, not representing a full-value fuel itself. Therefore, looking at the production of ethyl tert-butyl ether, which is used as a bio-additive for bioethanol production the CO_2 eq emissions sum up to 0.13 kg. This means that the butanol production is about 1310 times more CO_2 intense than the production of the common bio-based fuel component. In general we can conclude that the butanol production is quite energy intense in the way we have modelled it so far. The share of electricity to the overall contribution to climate change is high with a share of about 72%. Besides, the other impact categories are also characterized by the electricity inputs in varying portions. The high electricity consumption is thus the major

obstacle that has to be overcome to achieve a competitive PHOTOFUEL process especially when looking at the global warming potential. It should be noted, however, that the process is still a young, small-scale technology that can be significantly improved by progress in biotechnology and process engineering. Besides, changes in the composition of the electricity mix will thus have a significant impact on the results of the LCA.

Considering the lifecycle phases, three major production steps, inoculum production, cultivation and harvesting/separation, are displayed inFigure 7. The results show that the main contributions are allocated to the cultivation phase. Here, we found the highest electricity inputs with about 43,200 kWh/a. In total about 300 kWh of electricity are used to produce 1 kg of butanol.

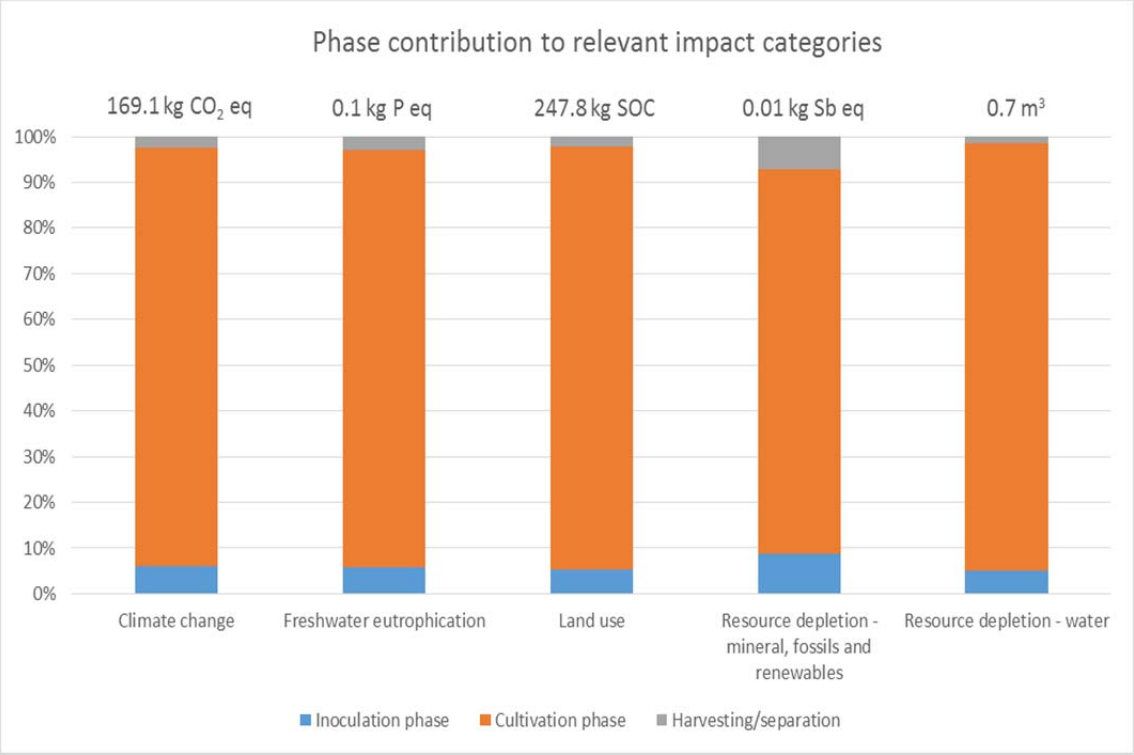

Figure 7: Contribution of production phases to relevant impact categories recommended by the ILCD handbook

8. Literature

[1] Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., and Weidema, B., 2016. (2016) The ecoinvent database version 3.

[2] JRC European commission. (2011) ILCD Handbook: Recommendations for Life Cycle Impact Assessment in the European context [Internet]. Vasa. http://dx.doi.org/10.278/33030

[3] Tamaru, C.S., FitzGerald, W.J.J. and Sato, V. (1993) Hatchery Manual for the artificial propagation of striped mullet.