

DanuP2Gas Optimization Tool

**User Manual**

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## DOCUMENT CONTROL SHEET

Short Description
User manual of DanuP2Gas Optimization Tool. It contains explanation of the tool's functionality and instructions on how to use it.

Version	Date	Description
V1.0	30.03.2022	User manual for the 1 <sup>st</sup> version of the tool available for the consortium of the project.
V2.0 (build 101)	31.07.2022	User manual for the 2 <sup>nd</sup> version of the tool available for the consortium of the project.
V2.0 (build 105)	17.08.2022	User manual for the 2 <sup>nd</sup> updated version of the tool available for the public.
V2.0 (build 111)	12.09.2022	Added part on using the tool, and the part about the underlying theory of the tool is set as Annexes. Added determination of default coefficients and prices.
V2.0 (build 117)	16.01.2024	Added scaling of electrical energy production profile of REP in the tool with description here. Added literature.

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## 1. INTRODUCTION

The interface to P2G Optimizer is the Excel document “DanuP2Gas Optimization Tool”. This file includes several main sheets: Optimization Tool, Plants and sources, P2G segments, and Charts. In the Optimization Tool, Plants and sources, and P2G segments sheets the user is supposed to enter data. Default values are given, but the user can enter new values in each field which is displayed in white colour. In the Results and, Charts sheets, results of the optimization are shown. Optimization result is not only the specification of the obtained P2G plant (given in sheet Results) but also includes time diagrams of consumed and produced energy and material (given in sheet Charts).

## 2. OPTIMIZATION TOOL SHEET

Several chapters of information are given in this sheet. In the **Investment parameters** are *Maximal Investment payoff period* as the maximal number of years needed to pay off the investment (default: 20 years), *Administration and building period* as the number of years it takes to build a P2G hub (default: 5 years), *Maximal investment* is the maximum of the investment that is given in Euros (default: 1 billion euros). Optimal results will often include investments in smaller amount than the maximal investment and shorter period than the maximal payoff period. Regarding investment, there is a possibility to add subsidy on the investment costs. Parameter *Use same subsidy for all parts of the P2G hub?*: in the case *yes* is selected, *Investment subsidy* is filled as a percentage and that value is applied to all processes. In the case *No* is selected, in the sheet P2G segments it is possible to apply different value of *Investment subsidy* for each particular segment of the P2G hub.

In the **Optimization parameters**, *Starting date of simulation* and *Last date of simulation* indicate the period in the simulation. No matter how short this period is, OT will scale Investment specifications presented in the Results sheet on the period of one year. Maximum time period between *Starting date of simulation* and *Last date of simulation* is 1 year. *Sampling time for electrical part* determines the OT's discrete-time step for electrical power calculation. With lower *Sampling time for electrical part* the results are more accurate, but the amount of required memory is higher. Sampling time for other processes is fixed to 24 hours (1 day). According to the entered values, *Amount of memory required (cca)* appears which tells the amount of RAM that the OT needs to run the simulation. With higher amount of the memory required, the longer will the OT require for finding the optimal solution. Full year simulation with 24-hour sampling time can last from few minutes up to 30 minutes to find the solution.

In the **Additional sales parameters**, *Price* as well as *Daily limits* for selling of hydrogen, oxygen, methane and biochar are given, with the corresponding units indicated. Additional sales refer to products that are sold directly at the P2G site, without using any grids. Here is also *Tax on CO<sub>2</sub> emissions*. All the default values are set to 0.

In the **Monthly precipitation** section, the precipitation values for each month can be entered. Default values are set to 0 as the precipitation data is not obtainable through the Atlas tool, but it can be easily found online for the desired location. If it is left as 0, the OT will consider the water grid as the only water source.

**Start Optimization** also appears on this page. By clicking on this field, optimization is started, and *Messages* in the **Optimization output** appear. The first message is about tool initialization and the last one is about the optimization end-results. End-results show if the tool has found the optimal solution. It also shows all the limits that are reached as the optimal solution. Reading the limits can be useful to explore the possibilities of the OT by changing the parameters that cause reaching those limits. For each message, *Date and time* of its appearance is also shown. If some of the data is not entered in the tool or if it is not entered correctly, error messages will appear in the Optimization output which will point to the exact cells and sheets where the error occurred. Warning messages can also appear which will tell if some value is not entered correctly but the tool will proceed with the calculation replacing that parameter with the one that can be used.

### 3. PLANTS AND SOURCES SHEET

In this sheet, data on **Renewable energy plant (REP), Industrial Plant (IP), Heat prices, Grid investment prices, Electricity prices, Gas prices, Water prices, Biomass (BM) prices, Biochar (BC) prices** is provided. It is possible to obtain all of these data from the Renewable Energy Atlas upon clicking in the **Import data from Atlas** field and selection of “json file” generated by the Atlas or to enter data manually in the fields given within this sheet. Even with the import from the Atlas tool, some data required for the OT might be missing due to missing values in the Atlas tool database, so this sheet should be checked before starting the optimization.

Data of the existing REP and IP that can be collocated and connected to the P2G hub is given through the **Renewable energy plant (REP)** and **Industrial plant (IP)** sections. If the data is entered manually, there are various possible selections under *Type of Plant* that can be chosen. *Photovoltaic, Wind, Hydro, Biogas, Biomass* types as well as *Custom* type are enabled in the case of REP. Upon the Type selection, typical production profiles are generated. Only when the *Custom* type is selected, it is up to the user to select appropriate production profile that will be used by the OT. In the case of IP, the following types are possible: *Weekdays, 24/7, Continuous* type and *Custom* type. *Weekdays* and *24/7* are profiles with generic oscillations of the consumption/production. In the profile *24/7* each day has the same profile, while profile *Weekdays* makes distinction between working days and weekends. *Continuous* type does not include any oscillation within a day nor difference between days. Apart from selecting the type of the REP and the profile type selection, annual production (or consumption) of electrical energy, gas and heat is needed. For electrical energy and gas connections of the REP and/or IP: type of the connection needs to be selected, and capacity of that connection needs to be given. The OT checks if the provided connection size is large enough for the combination of the

selected profile and given energy amount. If it is not large enough, the OT will automatically enlarge it and display a warning.

Similar to REP, upon *Custom* type selection for the IP, the user is required to supply the appropriate consumption profile. Supported file type is comma-separated values (.csv). The provided CSV file must have 1 column and either 365, 8760, or 35040 rows which correspond to 24-h, 1-h and 15-min sampling times.

When using REP, *Electrical energy production profile* is scaled according to [29] for *PV*, *Wind*, and *Hydro*. Other profiles are scaled only to match the entered *Annual electrical energy production*.

It is also possible to choose option *None* that manually excludes REP and IP which is indicated with grey colouring of all REP and IP data. If the User has selected collocation with both REP and IP, connection types of REP and IP must be the same as they are then considered a unique existing plant. This is needed for both (electricity and gas) connections. If they are not equal, OT cannot start with optimization and error message pops-up.

In this sheet, there are also seven chapters about prices: **Heat prices**, **Grid investment prices**, **Electricity prices**, **Gas prices**, **Water prices**, **Biomass (BM) prices** and **Biochar (BC) prices**.

In the **Heat prices**, *Price for produced heat* and *Price for consumed heat* are given. *Price for produced heat* is set by default to 0. The tool can run only if the *Price for produced heat* is less than or equal to the *Price for consumed heat*.

In the **Grid investment prices** electrical, gas and water grids are considered. In the general case, distances, and unit costs for each of them are to be provided, but in the case when REP or IP or both are collocated with the P2G, some inputs are set automatically. For example, when REP is collocated with the P2G, as REP already contains electrical grid connection, *Distance to the nearest electrical grid connection point* will be set to zero and its manual editing will be disabled, which is indicated with grey colouring. The fields *Capacity cost for electrical transmission grid connection* and *Capacity cost for electrical distribution grid connection* (due to possible increase of each connection capacity) always exists. The field *Calculated unit cost of electrical grid connection* will always be a positive non-zero value. In the case IP is collocated with the P2G hub, similar considerations are valid, not only for electricity, but for all three (Electrical, Gas, Water) grid connection investment calculations. This is the case since it is considered that IP already contains electrical, gas and water grid connections.

In **Electricity prices**, three possible tariffing periods (day, night, weekend) with all necessary data are to be given. Also, *Monthly peak power price* as well as *VAT percentage applicable to electricity business* are to be provided. Accordingly, *Prices for buying and selling electricity* for each tariffing period are calculated within this document and shown in grey colour to indicate that these fields are not for entry.

In **Gas prices**, as it is common to have different gas prices for colder and warmer part of the year, information on *Start* and *End of winter period* are to be given to the OT. Then, for each one of the periods (Winter and Summer) gas price components are to be supplied. In the case there is no difference between summer and winter, the same prices are to be filled. Finally, prices for buying and selling gas for winter and summer periods are calculated and shown in grey colour to indicate that these fields are not for entry as they are calculated based on other supplied data.

In **Water prices**, price for water supply is to be given.

In **Biomass (BM) prices** and **Biochar (BC) prices**, available biomass and biochar sources are shown. Upon filling of necessary data, *Calculated unit cost* for each source is automatically generated within this document. This value is shown in grey colour to indicate that field is not for entry. Using *Consider this source* it is possible to exclude each source from the optimization. Although biomass and biochar data are supposed to be taken from the Renewable Energy Atlas, it is also possible to manually include any other source or to correct the values obtained from the Atlas.

## 4. P2G SEGMENTS SHEET

Under this sheet, coefficients for technical description and valorisation for each P2G segment or subunit are given. These segments can be either different conversion processes or storages. They are as follows: Dry anaerobic digester (AD), Wet AD, Dry biomass to biochar plant (BM2BC), Wet biomass to biochar plant (BM2BC), Combined heat and power (CHP) or Fuel cell (FC), Carbon capture plant (CC), Gasification + water gas shift plant (GWGS), Methanation reactor, Gas compressor station, Electrolyser, Demineraliser, Precipitation collector, Heat exchanger, Dry biomass storage, Wet biomass storage, Biochar storage, Biogas storage, Hydrogen storage, Oxygen storage, Methane storage, Syngas storage, Carbon dioxide storage and Water storage.

Initial meaningful values of the parameters for all P2G hub segments are already provided as default values, but the expert/informed user can change them all and, in this way, adapt to the targeted equipment considered. Among all other, each process and storage contain the following parameters: investment subsidy, lifetime, and maximal size. *Lifetime* of each process/storage denotes the period after which the component should be replaced – financially it is reflected in yearly maintenance costs in the OT. Maximal size of a particular process is its maximum allowed nominal size / rating. With setting it to 0 the user prohibits to include certain segment in the optimized P2G hub.

In **Dry anaerobic digester (AD)** conversion coefficients of biomass to biochar, biomass to biogas, and biomass to residue are used as parameters. Coefficients for required heat as well as electricity for the dry AD segment of the P2G plant are also provided. *Unit price for Dry AD* as well as *Price of residue disposal* are also given as changeable parameters.

**Wet AD** is parametrized analogously to the dry AD subunit.

In **Dry biomass to biochar plant (BM2BC)**, the specific parameters are *coefficient of biomass to biochar conversion*, coefficients for required heat as well as electricity for Dry BM2BC and also *unit price for Dry BM2BC*.

**Wet biomass to biochar plant (BM2BC)** is parametrized analogously to the dry biomass to biochar plant.

In **Combined heat and power (CHP) or Fuel cell (FC)** it is enabled for the user to select between CHP or FC. Upon CHP selection, the user can modify the parameters maximal percentage of  $H_2$  in fuel of the CHP, electrical and heating efficiencies as well as CHP unit price which is based on CHP electrical power. Upon FC selection, the user can modify water retrieval efficiency of the FC, electrical and heating efficiencies as well as FC unit price which is based on FC electrical power.

**Carbon capture plant (CC)** contains parameters required heat and electricity per amount of captured  $CO_2$ , and unit price per amount of input  $CO_2$ .

**Gasification + water gas shift plant (GWGS)** contains *Mass efficiency of biochar to syngas conversion*, stoichiometric numbers in gasification, molar fractions in syngas and *Unit price per mass flow of input biochar* as well as *Price of tar disposal*.

In **Methanation reactor**, *Produced heat per amount of output  $CH_4$*  as well as *Required electricity per amount of output  $CH_4$*  can be changed by the user. *Unit price per molar flow of output  $CH_4$*  is also changeable.

In **Gas compressor station**, except from *Investment subsidy* and *Lifetime of the compressor station*, there is also changeable *Unit price per electrical power*.

In **Electrolyser**, depending on the used type of the electrolyser, the user can select *Consuming heat* and insert the value for *Heat required per amount of output  $H_2$* . In case of selecting *Producing heat*, the analogous parameter is *Heat produced per amount of output  $H_2$* . Except from that, electrical efficiency and unit price per nominal power are changeable.

In **Demineralizer**, *Required electricity for demineralization* and *Unit price per molar flow of input water* are changeable.

In **Precipitation collector**, *Unit price per collection area* is a changeable parameter while in **Heat exchanger** *Unit price per nominal power* is also changeable.

In each one of the **storages**, Unit price is left to be changeable.

## 5. RESULTS SHEET

After the optimization is successfully finished, its results appear in the Results sheet. It is organized in two parts. The first one on the left side of the page contains all **Investment specifications** and the second one on the right side of the page contains **Operational costs for selected period**.

In the **Investment specifications** resulting capacities (*Size*) and *Cost* for each *Process* and *Storage* are given. For each connection type (electricity, gas and water), *Size* and *Cost of Connection enlargement* is also given. When all total costs (*Total for processes*, *Total for storages* and *Total for connections*) are summed, *Total investment cost* is obtained.

In the **Operational costs for selected period**, Electrical, Heat, Gas and Water energy net calculations for the resulting P2G hub operation profile are provided. For all of them, collocation of P2G with REP and IP has to be considered. That is why electricity *Produced by REP* and *Electricity Consumed by IP* as well as their difference *Electrical energy > Net consumption without investment*, are set in the first rows. *Electrical energy > Mean peak power without investment* again refers only to the collocated REP and IP. Then, for the P2G investment *Electrical energy > Consumed by P2G* is shown. It is possible that the resulting P2G hub is composed of CHP or FC unit and without an electrolyser or any larger electrical consumer. In that case P2G is electricity producer which will be shown with the negative value of *Electrical energy > Consumed by P2G*. Final values of *Electrical energy > Net consumption with investment* and *Electrical energy > Mean peak power with investment* are obtained when the whole plant (REP, IP and P2G hub) is considered. In the *Heat* part, calculation is done in a similar way, with some differences. One of them is labelling of both of collocated plants REP, IP as heat production units: *Heat > Produced by REP*, *Heat > Produced by IP*. The second is that net heat is based on production: *Heat > Net production with investment*. In a similar way, *Gas > Net consumption with investment* is calculated. It could be noted that *Gas > Produced by P2G* can be both positive when P2G produces methane or negative when P2G takes methane from the gas grid or from the REP if it is a methane producer. For water, *Water > Water from the grid consumed by P2G* and *Water > Collected precipitation consumed by P2G* items exist.

While electricity, heat and gas are considered to be energy carriers, all other used and produced material are considered to be inputs and outputs. That is why **Operational costs for selected period** includes rows for *Input materials* and rows for *Additional sales* and for *Residues*. Input materials are *Dry biomass bought*, *Wet biomass bought*, and *Biochar bought*. In *Additional sales*, the following items are contained: *Hydrogen sold (in bottles)*, *Oxygen sold (in bottles)*, *Methane sold (in bottles)*, *Biochar sold*. *Residues* contains *Residue from dry anaerobic digester*, *Residue from wet anaerobic digester*, *Tar from gasification + water gas shift plant* and *CO<sub>2</sub> emitted*.

Then, using all above mentioned calculated operational costs, *Total operational cost without investment*, *Total operational cost with investment* as well as their difference *Savings with introduction of P2G* can be calculated. The last item (*Savings with introduction of P2G*) is used to calculate the *Payoff period* which is also dependent on: *Total investment*, *Maximal investment payoff period* and *Administration and building period* (last two are given in the Optimization tool sheet). If the simulation period (given in **Optimization parameters** in the Optimization Tool Sheet) is shorter than one year, OT will scale all operational costs up to the level of one year. Resulting *Payoff period* is shown

under *Total Investment* on the left side of the page. This data is obtained not only from the P2G operation savings, but it also takes into account *Administration and building period* and cost of equipment degradation.

## 6. CHARTS

Using Charts sheet, it is possible to see operation of the P2G hub throughout the complete period of simulation. This sheet includes all power profiles as well as input and output profiles: **Electricity profiles, Heat profiles, Gas (methane) profiles to/from the grid, Water profile, Input materials profiles, Additional sales profiles, Processes-mass flow profiles, Processes-molar flow profiles** and **Storages-mass profiles**. **Electricity profiles** include the following electrical attributes: *Electricity production of REP, Electricity consumption of IP, Electricity consumption of P2G, Electricity from the grid, Electricity used by electrolyser* and *Electricity produced by CHP/FC*. **Heat profiles** include the following heating attributes: *Heat production of REP, Heat production of IP, Heat consumption of P2G* and *Excess heat production*. **Gas (methane) profile to/from the grid** include the following attributes: *Biomethane production of REP, Methane consumption of IP, Biomethane production of P2G* and *Methane from the grid*. Units for each one of the attributes given within electricity, heat and gas profiles are in [kW]. **Water profile** contains only *Water from the grid* which is given in [m<sup>3</sup>/h]. **Input materials profiles** consists of *Dry biomass bought, Wet biomass bought, and Biochar bought*. All values are given in [kg/day]. **Additional sales profiles** includes: *Hydrogen sold (in bottles), Oxygen sold (in bottles), Methane sold (in bottles), Biochar sold (in bottles)*. All values are given in [kg/day]. In **Processes-mass flow profiles**, the following attributes are obtained: *Dry biomass into AD, Wet biomass into AD, Dry biomass into BM2BC, Wet biomass into BM2BC* and *Biochar into GWGS*. All values are given in [kg/s]. **Processes-molar flow profiles** gives: *CH<sub>4</sub> out of methanation* and *CO<sub>2</sub> captured by CC*. All values are given in [mol/s]. **Storages-mass profiles** encompasses all storages. It contains the following attributes: *Mass of dry biomass in storage, Mass of wet biomass in storage, Mass of biochar in storage, Mass of syngas in storage, Mass of biogas in storage, Mass of CO<sub>2</sub> in storage, Mass of O<sub>2</sub> in storage, Mass of CH<sub>4</sub> in storage, Mass of H<sub>2</sub> in storage* and *Volume of H<sub>2</sub>O in storage*. All attributes are given in [kg] except of the volume of H<sub>2</sub>O which is given in m<sup>3</sup>.

Image of each of the given profiles can be saved by clicking on *Save chart as image* and *Save data* buttons.

## 7. HOW TO USE IT

On the web page of the DanuP2Gas project Atlas (web GIS-based tool) together with the DanuP2Gas Optimization Tool can be found. The optimization tool can be unzipped in some folder on the user's computer. In the unpacked folder the Excel file described here can be located. The user's first step is a simple mouse click to select the site of P2G hub. Then, biomass sources shown on the Atlas are to be selected. Due to the lack of Biochar

sources, all of them will be automatically selected. The Atlas will give feedback on possible REP and IP that could be collocated with P2G which means that P2G hub can use existing electrical and gas connection points. The User has the option to select the offered REP, IP or not. Afterwards the Atlas will automatically find the rest of needed connection points. The user's next step is to click in the *Import data from Atlas* located in the Excel interface file, sheet Plant and sources. User can then change any of changeable attributes of the Excel interface file, and finally must click on *Start optimization* located in the Optimization tool sheet. After that the user waits for OT computation followed by message release in **Optimization output**.

## 8. PARAMETER RECAPITULATION

According to the interface excel file, table with list of all parameters of the OT is given in this section (Table 1). This alphabetical listing also includes description of the certain parameter together with its unit.

Table 1. List of all parameters

<i>Parameter</i>	<i>Description</i>	<i>Unit</i>
Administration and building period		years
Amount of water needed in GWGS per mass of BC		mol/kg
Average pressure inside methane storage		bar
Biochar (BC) prices >Production capacity		t/year
Biochar (BC) prices >Purchase cost		€/t
Biochar (BC) prices>Consider this source?	Selection Yes or No is possible	N/A
Biochar source name		
Biochar storage> Investment subsidy		%
Biochar storage> Lifetime of the storage		years
Biochar storage> Maximal size of the storage		kg
Biochar storage> Unit price		€/kg
Biogas storage> Investment subsidy		%
Biogas storage> Lifetime of the storage		years
Biogas storage> Maximal size of the storage		kg

Biogas storage> Unit price		€/kg
Biomass (BM) prices>Consider this source?	Selection Yes or No is possible	N/A
Biomass (BM) prices>Production capacity		t/year
Biomass (BM) prices>Purchase cost		€/t
Biomass source name		N/A
Capacity cost for electrical distribution grid connection		€/kW
Capacity cost for electrical transmission grid connection		€/kW
Capacity cost for gas distribution grid connection		€/kW
Capacity cost for gas transmission grid connection		€/kW
Capacity cost for water grid connection		€/ (m <sup>3</sup> /h)
Carbon capture plant (CC)> Investment subsidy		%
Carbon capture plant (CC)> Lifetime of the plant		years
Carbon capture plant (CC)> Maximal size of the plant		mol/s
Carbon dioxide storage> Investment subsidy		%
Carbon dioxide storage> Lifetime of the storage		years
Carbon dioxide storage> Maximal size of the storage		kg
Carbon dioxide storage> Unit price		€/kg
Combined heat and power (CHP) or Fuel cell (FC)	Selection between CHP and FC is possible	N/A
Combined heat and power (CHP) or Fuel cell (FC) > Electrical efficiency		%
Combined heat and power (CHP) or Fuel cell (FC) > Heating efficiency		%
Combined heat and power (CHP) or Fuel cell (FC) > Investment subsidy		%
Day tariff> Electricity price without grid operator fees, including taxes		€/kWh

Day tariff> Grid operator fees of the distribution system, including taxes		€/kWh
Day tariff> Grid operator fees of the transmission system, including taxes		€/kWh
Demineraliser> Investment subsidy		%
Distance between transport hubs THT1 and THT2		km
Distance between transport hubs THW1 and THW2		km
Dry anaerobic digester (AD)> Coefficient of biomass to biochar conversion		N/A
Dry anaerobic digester (AD)> Coefficient of biomass to biogas conversion		N/A
Dry anaerobic digester (AD)> Coefficient of biomass to residue conversion		N/A
Dry anaerobic digester (AD)> Investment subsidy		%
Dry anaerobic digester (AD)> Lifetime of the digester		years
Dry anaerobic digester (AD)> Maximal size of the digester		kg/s
Dry anaerobic digester (AD)> Price of residue disposal		€/kg
Dry anaerobic digester (AD)> Required electricity per mass of input biomass		kJ/kg
Dry anaerobic digester (AD)> Required heat per mass of input biomass		kJ/kg
Dry anaerobic digester (AD)> Unit price per mass flow of input biomass		€/(kg/s)
Dry biomass storage> Investment subsidy		%
Dry biomass storage> Lifetime of the storage		years
Dry biomass storage> Maximal size of the storage		kg
Dry biomass storage> Unit price		€/kg

Dry biomass to biochar plant (BM2BC)> Coefficient of biomass to biochar conversion		N/A
Dry biomass to biochar plant (BM2BC)> Investment subsidy		%
Dry biomass to biochar plant (BM2BC)> Lifetime of the plant		years
Dry biomass to biochar plant (BM2BC)> Maximal size of the plant		kg/s
Dry biomass to biochar plant (BM2BC)> Required electricity per mass of input biomass		kJ/kg
Dry biomass to biochar plant (BM2BC)> Required heat per mass of input biomass		kJ/kg
Dry biomass to biochar plant (BM2BC)> Unit price per mass flow of input biomass		€/ (kg/s)
Electricity prices> Use custom yearly profile of prices instead?	Selection Yes or No is possible	N/A
Electricity prices>File	File upload in the case Yes is previously selected	N/A
Electrolyser > Electrical efficiency		%
Electrolyser> Investment subsidy		%
Electrolyser> Unit price per nominal power		€/kW
End time of day tariff		h
End time of weekend tariff		h
End time of winter period		N/A
Gas compressor station> Investment subsidy		%
Gas compressor station> Unit price per electrical power		€/kW
Gas prices> Use custom yearly profile of prices instead?	Selection Yes or No is possible	N/A
Gas prices>File	File upload in the case Yes is previously selected	N/A
Gasification + water gas shift plant (GWGS)> Investment subsidy		%
Gasification + water gas shift plant (GWGS)> Lifetime of the plant		years
Gasification + water gas shift plant (GWGS)> Maximal size of the plant		kg/s
Heat exchanger> Investment subsidy		%

Heat exchanger> Unit price per nominal power		€/kW
Heat produced per amount of H <sub>2</sub>	Active upon <i>Producing heat</i> selection	kJ/mol
Heat required per amount of H <sub>2</sub>	Active upon <i>Consuming heat</i> selection	kJ/mol
Hydrogen storage> Investment subsidy		%
Hydrogen storage> Lifetime of the storage		years
Hydrogen storage> Maximal size of the storage		kg
Hydrogen storage> Unit price		€/kg
Investment subsidy		%
IP> Annual heat production	Enabled when REP>Type of plant Biogas, Biomass or Custom is selected; Average heat production	MWh
IP> Electrical energy consumption profile	Is enabled in the case Custom is previously selected; Selection between electrical energy consumption profiles or Custom is possible	N/A
IP> Electrical energy consumption profile> File	File upload in the case Custom is previously selected	N/A
IP> Heat production profile	Selection between various predefined profiles and Custom is possible	N/A
IP> Heat production profile>File	File upload in the case Custom is previously selected	N/A
IP>Annual biomethane (gas) consumption	Average biomethane (gas) consumption	MWh
IP>Annual electrical energy consumption		MWh
IP>Biomethane consumption profile	Enabled when IP>Type of plant Custom is selected; Selection between various predefined profiles and Custom is possible	N/A
IP>Biomethane consumption profile >File	File upload in the case Custom is previously selected	N/A
IP>Existing electrical connection capacity		MW
IP>Existing gas connection capacity		MW
IP>Internal gas network pressure		bar

IP>Pressure of the gas network	Data is taken directly from the Atlas	bar
IP>Type of existing electrical connection	Selection between Distribution and Transmission	N/A
IP>Type of existing gas connection	Selection between Distribution, Transmission and Custom	N/A
IP>Type of plant	IP type selection or Custom	N/A
Last date of simulation		N/A
Lifetime of CHP/FC		years
Lifetime of the compressor station		years
Lifetime of the demineraliser		years
Lifetime of the electrolyser		years
Lifetime of the heat exchanger		years
Lifetime of the precipitation collector		years
Limit of daily biochar sale		kg/day
Limit of daily hydrogen sale		kg/day
Limit of daily methane sale		kg/day
Limit of daily oxygen sale		kg/day
Mass efficiency of biochar to syngas conversion		%
Maximal area of rainfall collection		m <sup>2</sup>
Maximal investment		€
Maximal investment payoff period		years
Maximal percentage of H <sub>2</sub> in fuel of the CHP	Active upon CHP selection	%
Maximal size of CHP/FC		kW <sub>e</sub>
Maximal size of demineraliser		mol/s
Maximal size of the electrolyzer		kW
Methanation reactor> Investment subsidy		%
Methanation reactor> Lifetime of the plant		years
Methanation reactor> Maximal size of the plant		mol/s
Methane storage> Investment subsidy		%
Methane storage> Lifetime of the storage		years
Methane storage> Maximal size of the storage		kg
Methane storage> Unit price		€/kg

Molar fraction of CH <sub>4</sub> in biogas		N/A
Molar fraction of CO <sub>2</sub> in biogas		N/A
Molar fraction of CO <sub>2</sub> in syngas		N/A
Molar fraction of H <sub>2</sub> in syngas		N/A
Monthly peak power price		€/kW
Monthly precipitation >April	Average precipitation on P2G site	mm
Monthly precipitation >August	Average precipitation on P2G site	mm
Monthly precipitation >December	Average precipitation on P2G site	mm
Monthly precipitation >February	Average precipitation on P2G site	mm
Monthly precipitation >January	Average precipitation on P2G site	mm
Monthly precipitation >July	Average precipitation on P2G site	mm
Monthly precipitation >June	Average precipitation on P2G site	mm
Monthly precipitation >March	Average precipitation on P2G site	mm
Monthly precipitation >May	Average precipitation on P2G site	mm
Monthly precipitation >November	Average precipitation on P2G site	mm
Monthly precipitation >October	Average precipitation on P2G site	mm
Monthly precipitation >September	Average precipitation on P2G site	mm
Night tariff> Electricity price without grid operator fees, including taxes		€/kWh
Night tariff> Grid operator fees of the distribution system, including taxes		€/kWh
Night tariff> Grid operator fees of the transmission system, including taxes		€/kWh
Oxygen storage> Investment subsidy		%
Oxygen storage> Lifetime of the storage		years
Oxygen storage> Maximal size of the storage		kg
Oxygen storage> Unit price		€/kg
Precipitation collector> Investment subsidy		%
Price for consumed heat		€/MWh
Price for produced heat		€/MWh
Price for selling biochar		€/kg
Price for selling hydrogen		€/kg
Price for selling methane		€/kg
Price for selling oxygen		€/kg
Price for water supply, excluding sewerage and wastewater		€/m <sup>3</sup>

cleaning cost, including operators/grid fees and taxes		
Price of tar disposal		€/kg
Produced heat per amount of output CH <sub>4</sub>		kJ/mol
REP> Annual heat production	Enabled when REP>Type of plant Biogas, Biomass or Custom is selected; Average heat production	MWh
REP> Electrical energy production profile	Selection between electrical energy production profiles or Custom is possible	N/A
REP> Electrical energy production profile> File	File upload in the case Custom is previously selected	N/A
REP> Heat production profile	Enabled when REP>Type of plant Biogas, Biomass or Custom is selected; Selection between Continuous and Custom is possible	N/A
REP> Heat production profile>File	File upload in the case Biogas, Biomass or Custom is previously selected	N/A
REP> Price for produced heat		€/MWh
REP>Annual biomethane (gas) production	Enabled when REP>Type of plant Biogas or Custom is selected; Average biomethane production	MWh
REP>Annual electrical energy production		MWh
REP>Biomethane production profile	Enabled when REP>Type of plant Biogas or Custom is selected; Selection between Continuous and Custom is possible	N/A
REP>Biomethane production profile>File	File upload in the case Custom is previously selected	N/A
REP>Existing electrical connection capacity		MW
REP>Existing gas connection capacity		MW
REP>Internal gas network pressure	Enabled when REP>Type of plant Biogas or Custom is selected	bar
REP>Pressure of the gas network	Data is taken directly from the Atlas	bar
REP>Type of existing electrical connection	Selection between Distribution and Transmission	N/A
REP>Type of existing gas connection	Enabled when REP>Type of plant Biogas or Custom is selected;	N/A

	Selection between Distribution, Transmission or Custom	
REP>Type of plant	REP type selection or Custom	N/A
Required electricity for demineralization		kJ/mol
Required electricity per amount of captured CO <sub>2</sub>		kJ/mol
Required electricity per amount of output CH <sub>4</sub>		kJ/mol
Required electricity per mass of input biochar		kJ/kg
Required heat per amount of captured CO <sub>2</sub>		kJ/mol
Required heat per mass of input biochar		kJ/kg
Road distance from the BC source to the nearest railroad transport hub (THT1)		km
Road distance from the BC source to the nearest waterway transport hub (THW1)		km
Road distance from the BC source to the P2G hub		km
Road distance from the P2G hub and the nearest railroad transport hub (THT2)		km
Road distance from the P2G hub and the nearest waterway transport hub (THW2)		km
Road distance to P2G hub		km
Road transport cost		€/ (t km)
Road transport cost from the BC source to the P2G hub		€/ (t km)
Road transport cost from the P2G hub to the BC source		€/ (t km)
Sampling time for electrical part		h
Start time of day tariff		h
Start time of weekend tariff		h
Start time of winter period		h
Starting date of simulation		N/A
Stoichiometric number of H <sub>2</sub> O in gasification		N/A
Stoichiometric number of O <sub>2</sub> in gasification		N/A

Summer period> Distribution system fee for consumption, including taxes		€/kWh
Summer period> Distribution system fee for injection, including taxes		€/kWh
Summer period> Gas price without grid/operator fees, including taxes		€/kWh
Summer period> Gas supply fee, including taxes		€/kWh
Summer period> Transmission system fee for consumption, including taxes		€/(kWh /day)
Summer period> Transmission system fee for injection, including taxes		€/(kWh /day)
Syngas storage> Investment subsidy		%
Syngas storage> Lifetime of the storage		years
Syngas storage> Maximal size of the storage		kg
Syngas storage> Unit price		€/kg
Tax on CO2 emissions		€/kg
Total energy production from biogas	Active upon CHP selection	MJ/kg
Total energy production from hydrogen		MJ/kg
Total energy production from methane	Active upon CHP selection	MJ/kg
Type	Biomass type selection according to the percentage of wet content	N/A
Type of electrolyser	Selection between <i>Producing heat</i> and <i>Consuming heat</i> is possible	N/A
Unit cost for electrical distribution grid connection		€/(kW km)
Unit cost for electrical transmission grid connection		€/(kW km)
Unit cost for gas distribution grid connection		€/(kW km)
Unit cost for gas transmission grid connection		€/(kW km)
Unit cost for water grid connection		€/ ((m <sup>3</sup> /h) km)

Unit price per amount of input CO <sub>2</sub>		€/ (mol/s)
Unit price per collection area		€/m <sup>3</sup>
Unit price per electrical power		€/kW <sub>e</sub>
Unit price per mass flow input biochar		€/ (kg/s)
Unit price per molar flow of input water		€/ (mol/s)
Unit price per molar flow of output CH <sub>4</sub>		€/ (mol/s)
Unit transport cost of the THT1 (THT1 to THT2)		€/ (t km)
Unit transport cost of the THT2 (THT1 to THT2)		€/ (t km)
Unit transport cost of the THW1 (THW1 to THW2)		€/ (t km)
Unit transport cost of the THW2 (THW1 to THW2)		€/ (t km)
Use same subsidy for all parts of the P2G hub?		N/A
VAT percentage applicable to electricity business		%
VAT percentage applicable to gas business		%
Water retrieval efficiency of the FC	Active upon FC selection	N/A
Water storage> Investment subsidy		%
Water storage> Lifetime of the storage		years
Water storage> Maximal size of the storage		m <sup>3</sup>
Water storage> Unit price		€/m <sup>3</sup>
Wet anaerobic digester (AD)> Coefficient of biomass to biochar conversion		N/A
Wet anaerobic digester (AD)> Coefficient of biomass to biogas conversion		N/A
Wet anaerobic digester (AD)> Coefficient of biomass to residue conversion		N/A

Wet anaerobic digester (AD)> Investment subsidy		%
Wet anaerobic digester (AD)> Lifetime of the digester		years
Wet anaerobic digester (AD)> Maximal size of the digester		kg/s
Wet anaerobic digester (AD)> Price of residue disposal		€/kg
Wet anaerobic digester (AD)> Required electricity per mass of input biomass		kJ/kg
Wet anaerobic digester (AD)> Required heat per mass of input biomass		kJ/kg
Wet anaerobic digester (AD)> Unit price per mass flow of input biomass		€/(kg/s)
Wet biomass storage> Investment subsidy		%
Wet biomass storage> Lifetime of the storage		years
Wet biomass storage> Maximal size of the storage		kg
Wet biomass storage> Unit price		€/kg
Wet biomass to biochar plant (BM2BC)> Coefficient of biomass to biochar conversion		N/A
Wet biomass to biochar plant (BM2BC)> Investment subsidy		%
Wet biomass to biochar plant (BM2BC)> Lifetime of the plant		years
Wet biomass to biochar plant (BM2BC)> Maximal size of the plant		kg/s
Wet biomass to biochar plant (BM2BC)> Required electricity per mass of input biomass		kJ/kg
Wet biomass to biochar plant (BM2BC)> Required heat per mass of input biomass		kJ/kg
Wet biomass to biochar plant (BM2BC)> Unit price per mass flow of input biomass		€/(kg/s)
Winter period> Distribution system fee for consumption, including taxes		€/kWh

Winter period> Distribution system fee for injection, including taxes		€/kWh
Winter period> Gas price without grid/operator fees, including taxes		€/kWh
Winter period> Gas supply fee, including taxes		€/kWh
Winter period> Transmission system fee for consumption, including taxes		€/(kWh /day)
Winter period> Transmission system fee for injection, including taxes		€/(kWh /day)

N/A - Not applicable

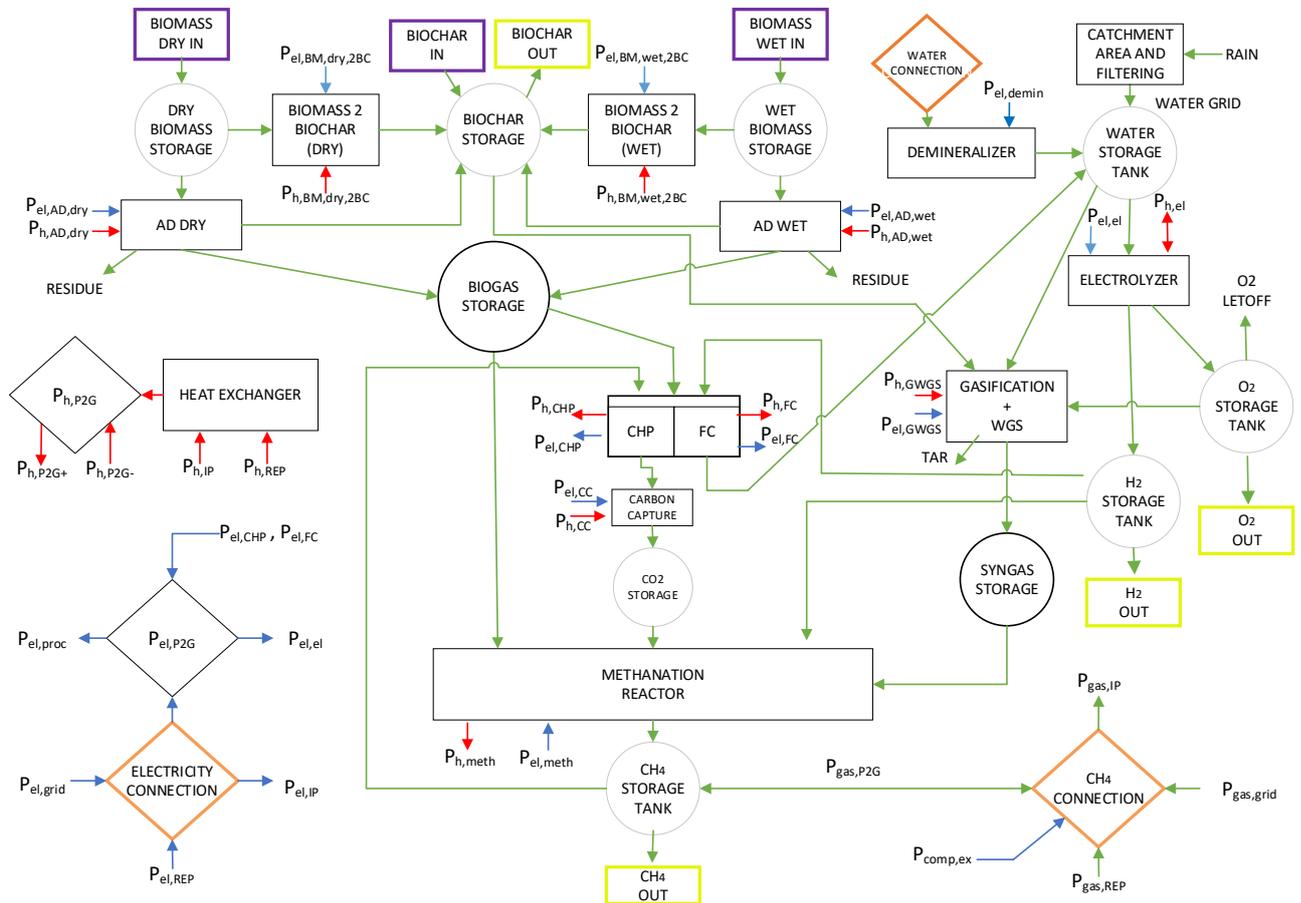
# ANNEXES

## 1. MATHEMATICAL BACKGROUND

### 1.1 POWER TO GAS OVERALL CONCEPT

To include versatile ways for P2G realization, the P2G concept will include not only “Biochar P2G” (Annex 2.) but also “Biogas P2G”. “Biogas P2G” is based on biogas power plant with addition of biogas upgrade to biomethane. Except from that, P2G concept contains biochar production by a Biomass2Biochar as well as production of hydrogen. The P2G system enables connection to industrial plants (IPs) as well as to the renewable power plants (REPs). Each industrial facility that has significant amount of methane consumption could be regarded as IP. Each wind, photovoltaic, hydro and biomass power plant of a certain level of electricity/gas production could be regarded as REP. The complete scheme of the P2G concept is given in Figure 1.

Figure 1: Overall concept of the Power to Gas Plant



Without biochar part (Gasification + WGS, O<sub>2</sub> storage) the concept is reduced to “Biogas P2G”. For its heat and electricity production (CHP/FC), not only biogas but also a mixture of biogas and hydrogen is possible to use as feedstock. Exhaust CO<sub>2</sub> from the CHP can be captured and stored in the CO<sub>2</sub> storage. Instead of CHP, to produce heat and electricity, it is possible to use fuel cells (FC). In that case the only feedstock is hydrogen

and as the water is coproduct in FC operation it can be saved and used for other processes.

Similarly, without biogas part (AD, CHP/ FC, Carbon Capture, CO<sub>2</sub> storage) the concept is reduced to “Biochar P2G”. If everything except from Biomass2Biochar is removed, the concept is reduced to Biomass to Biochar plant that will only do the production of the biochar. The concept could be also reduced only to the hydrogen production plant. If all components given in Figure 1 are incorporated, simultaneous operation of “Biogas P2G” and “Biochar P2G” as well as biochar and hydrogen production is also allowed by this concept. According to the given processes, their electrical and heat production and consumption are also depicted. Electricity is shown in blue, heat in red and mass and gas paths in green colour.

## 1.2 MODELLING OF POWER TO GAS PROCESSES

### 1.2.1 MODELLING OF BIOMASS STORAGES DYNAMICS

It is assumed that biomass can be stored at the site of the P2G plant. Two types of biomass feedstock, dry and wet biomass, are considered. Dynamics of the biomass is given as follows:

$$\dot{m}_{BM,dry,store} = \dot{m}_{BM,dry,in} - \dot{m}_{BM,dry,AD} - \dot{m}_{BM,dry,2BC} \quad (A1.1a)$$

$$\dot{m}_{BM,wet,store} = \dot{m}_{BM,wet,in} - \dot{m}_{BM,wet,AD} - \dot{m}_{BM,wet,2BC} \quad (A1.1b)$$

where the annotation is:

$m_{BM,dry,store}$  = mass of dry biomass stored at the site [kg]

$\dot{m}_{BM,dry,in}$  = dry biomass delivered to the site [kg/s]

$\dot{m}_{BM,dry,AD}$  = dry biomass consumed by AD [kg/s]

$\dot{m}_{BM,dry,2BC}$  = dry biomass consumed by BM2BC plant [kg/s]

$m_{BM,wet,store}$  = mass of wet biomass stored at the site [kg]

$\dot{m}_{BM,wet,in}$  = wet biomass delivered to the site [kg/s]

$\dot{m}_{BM,wet,AD}$  = wet biomass consumed by AD [kg/s]

$\dot{m}_{BM,wet,2BC}$  = wet biomass consumed by BM2BC plant [kg/s]

Optimization tool will manipulate with the following variables:  $\dot{m}_{BM,dry,in}$ ,  $\dot{m}_{BM,dry,AD}$ ,  $\dot{m}_{BM,dry,2BC}$ ,  $\dot{m}_{BM,wet,in}$ ,  $\dot{m}_{BM,wet,AD}$ ,  $\dot{m}_{BM,wet,2BC}$ , within the following conditions:

$$m_{BM,dry,store} \geq 0; \dot{m}_{BM,dry,in} \geq 0; \dot{m}_{BM,dry,AD} \geq 0; \dot{m}_{BM,dry,2BC} \geq 0$$

$$m_{BM,wet,store} \geq 0; \dot{m}_{BM,wet,in} \geq 0; \dot{m}_{BM,wet,AD} \geq 0; \dot{m}_{BM,wet,2BC} \geq 0$$

Maximal values of both dry and wet biomass storages are to be found throughout the complete time horizon. Therefore, two more conditions are to be added:

$$m_{BM,dry,store} \leq M_{BM,dry,store}$$

$$m_{BM,wet,store} \leq M_{BM,wet,store}$$

where  $M_{BM,dry,store}$  and  $M_{BM,wet,store}$  are the capacities in [kg] of dry and wet biomass storages.

Also, maximal values for AD and BM2BC process capacities are to be determined:

$$\dot{m}_{BM,dry,AD} \leq \dot{M}_{BM,dry,AD}$$

$$\dot{m}_{BM,wet,AD} \leq \dot{M}_{BM,wet,AD}$$

$$\dot{m}_{BM,dry2BC} \leq \dot{M}_{BM,dry2BC}$$

$$\dot{m}_{BM,wet2BC} \leq \dot{M}_{BM,wet,2BC}$$

where  $\dot{M}_{BM,dry,AD}$  and  $\dot{M}_{BM,wet,AD}$  are nominal mass flows in [kg/s] at the input of dry and wet ADs, while  $\dot{M}_{BM,dry2BC}$  and  $\dot{M}_{BM,wet,2BC}$  are nominal mass flows in [kg/s] at the input of dry and wet BM2BC plants.

## 1.2.2 MODELLING OF BIOCHAR STORAGE AND SYNGAS PRODUCTION AND STORAGE DYNAMICS

It is assumed that biochar can be stored at the site of the P2G plant. According to Figure 1, dynamic of the biochar is:

$$\begin{aligned} \dot{m}_{BC,store} = \dot{m}_{BC,in} - \dot{m}_{BC,out} + \alpha_{dry} \dot{m}_{BM,dry,AD} + \alpha_{wet} \dot{m}_{BM,wet,AD} + \beta_{dry} \dot{m}_{BM,dry,2BC} + \\ + \beta_{wet} \dot{m}_{BM,wet,2BC} - \dot{m}_{BC,GWGS} \end{aligned} \quad (A1.2)$$

where:

$m_{BC,store}$  = mass of biochar stored at the site [kg]

$\dot{m}_{BC,in}$  = biochar delivered to the site [kg/s]

$\dot{m}_{BC,out}$  = biochar taken from the site [kg/s]

$\alpha_{dry}$  = coefficient of biomass to biochar conversion during dry AD [-]

$\alpha_{wet}$  = coefficient of biomass to biochar conversion during wet [-]

$\beta_{dry}$  = coefficient of biomass to biochar conversion during dry BM2BC [-]

$\beta_{wet}$  = coefficient of biomass to biochar conversion during wet BM2BC [-]

$\dot{m}_{BC,GWGS}$  = biochar mass consumption rate during the gasification process [kg/s]

Optimization tool will manipulate with the following variables:  $\dot{m}_{BC,in}$ ,  $\dot{m}_{BC,out}$ ,  $\dot{m}_{BC,GWGS}$

Manipulation will be limited to the following conditions:

$$m_{BC,store} \geq 0; \dot{m}_{BC,in} \geq 0; \dot{m}_{BC,out} \geq 0; \dot{m}_{BC,GWGS} \geq 0$$

Also, throughout the complete time horizon maximal biochar storage value is to be found as well as maximal capacity of Gasification + WGS (GWGS) process:

$$m_{BC,store} \leq M_{BC,store}$$

$$\dot{m}_{BC,GWGS} \leq \dot{M}_{BC,GWGS}$$

where  $M_{BC,store}$  is the capacity in [kg] of the biochar storage, and  $\dot{M}_{BC,GWGS}$  is the nominal mass flow in [kg/s] at the input of the GWGS process.

Result of the Gasification + WGS process is syngas:

$$\dot{m}_{SG,GWGS} = \eta_{BC \rightarrow SG} \dot{m}_{BC,GWGS} \quad (A1.3a)$$

which is given in molar notation as:

$$\dot{n}_{SG,GWGS} = \eta'_{BC \rightarrow SG} \dot{m}_{BC,GWGS} \quad (A1.3b)$$

Mass efficiency  $\eta_{BC \rightarrow SG}$  of biochar to syngas conversion used to calculate molar efficiency is calculated as:

$$\eta'_{BC \rightarrow SG} = \frac{\eta_{BC \rightarrow SG}}{M_{SG}[\text{kg/mol}]} \quad (A1.4)$$

where molar mass of syngas  $M_{SG}$  as well as syngas mole fraction of  $H_2$  ( $g_1'$ ) and  $CO_2$  ( $g_2'$ ) after WGS are obtained according to elaboration given in 3.1.3.

In the gasification process, a certain amount of tar is produced:

$$\dot{m}_{TAR,GWGS} = k_{TAR} \dot{m}_{BC,GWGS} \quad (A1.5)$$

Parameter  $k_{TAR}$  that determines amount of tar should be limited with the following constraint:

$$k_{TAR} + \eta_{BC \rightarrow SG} = 1$$

Tar is considered to be waste that needs to be managed.

After syngas is produced in GWGS it is stored in the syngas storage before it is used in the methanation reactor. Syngas storage dynamics is:

$$\dot{n}_{SG,store} = \dot{n}_{SG,GWGS} - \dot{n}_{SG,meth} \quad (A1.6)$$

where:

$$n_{SG,store} = \text{syngas in its storage [mol]}$$

$$\dot{n}_{SG,GWGS} = \text{syngas produced in GWGS [mol/s]}$$

$\dot{n}_{SG, meth} = \text{syngas released to the methanation reactor [mol/s]}$

Its composition is the same as the composition of syngas produced in GWGS:

$$\dot{n}_{H_2, SG} = g'_1 \dot{n}_{SG, meth} \quad (A1.7a)$$

$$\dot{n}_{CO_2, SG} = g'_2 \dot{n}_{SG, meth} \quad (A1.7b)$$

where:

$\dot{n}_{H_2, SG} = H_2 \text{ from syngas to methanation [mol/s]}$

$\dot{n}_{CO_2, SG} = CO_2 \text{ from syngas to methanation [mol/s]}$

The optimization tool manipulates with  $\dot{n}_{SG, meth}$ . The manipulation is constrained with the following conditions:

$$n_{SG, store} \geq 0 ; \dot{n}_{SG, meth} \geq 0$$

Also, throughout the complete time horizon maximal syngas storage value is to be found:

$$n_{SG, store} \leq N_{SG, store}$$

where  $N_{SG, store}$  is the capacity in [mol] of the syngas storage.

### 1.2.3 MODELLING OF BIOGAS STORAGE DYNAMICS AND CHP/FC UNIT

Biogas storage is used to possibly offset biogas production and consumption. Biogas is produced in AD processes while its consumption occurs in CHP/FC and Methanation processes:

$$\dot{m}_{BG, store} = \gamma_{dry} \dot{m}_{BM, dry, AD} + \gamma_{wet} \dot{m}_{BM, wet, AD} - \dot{m}_{BG, CHP/FC} - \dot{m}_{BG, meth} \quad (A1.8)$$

where:

$m_{BG, store} = \text{mass of biogas in storage [kg]}$

$\dot{m}_{BG, CHP/FC} = \text{mass of biogas consumed by CHP/FC [kg/s]}$

$\dot{m}_{BG, meth} = \text{mass of biogas for the methanation reactor [kg/s]}$

$\gamma_{dry} = \text{conversion coefficient of dry biomass mass to biogas amount during AD}$

$\gamma_{wet} = \text{conversion coefficient of wet biomass mass to biogas amount during AD}$

Similar to the analysis given for syngas, dynamics of the biogas going into methanation reactor could be noted:

$$\dot{n}_{CH_4, BG} = S'_M \frac{\dot{m}_{BG, meth}}{M_{BG}} \quad [\text{mol/s}] \quad (A1.9a)$$

$$\dot{n}_{CO_2,BG} = s'_C \frac{\dot{m}_{BG, meth}}{M_{BG}} \quad [\text{mol/s}] \quad (\text{A1.9b})$$

where:

$s'_M$  = molar fraction of  $CH_4$  in biogas

$s'_C$  = molar fraction of  $CO_2$  in biogas

$M_{BG}$  = molar mass of biogas (60%  $CH_4$ , 40%  $CO_2$ ) = 0.027[kg/mol]

To make a switch in equations from molar to mass equalities, and vice versa, molar fractions, as well as mass fractions, of  $CH_4$  and  $CO_2$  in biogas are needed. Molar fractions are defined, and mass fractions are:

$$s_M = s'_M \frac{M_{CH_4}}{M_{BG}} = \text{mass fraction of } CH_4 \text{ in biogas}$$

$$s_C = s'_C \frac{M_{CO_2}}{M_{BG}} = \text{mass fraction of } CO_2 \text{ in biogas}$$

According to Fig. 1, CHP/FC can be supplied from three sources: methane, biogas and hydrogen. Total gas power of the CHP/FC is:

$$P_{total,CHP/FC} = k_{CH_4} \dot{m}_{CH_4,CHP/FC} + k_{BG} \dot{m}_{BG,CHP/FC} + k_{H_2} \dot{m}_{H_2,CHP/FC} \quad (\text{A1.10})$$

where:

$\dot{m}_{CH_4,CHP/FC}$  = methane delivered to CHP/FC from the methane storage [kg/s]

$\dot{m}_{BG,CHP/FC}$  = biogas delivered to CHP/FC [kg/s]

$\dot{m}_{H_2,CHP/FC}$  = hydrogen delivered to CHP/FC [kg/s]

and  $k_{CH_4} = 50000$  [kWs/kg],  $k_{H_2} = 120000$  [kWs/kg] are heating values of gases. Heating value of biogas is expressed as a function of methane heating value:

$$k_{BG} = s_M k_{CH_4} = s'_M \frac{M_{CH_4}}{M_{BG}} k_{CH_4} \quad (\text{A1.11})$$

OT will give the User possibility to choose between CHP and FC (Fuel Cells stack) options. Accordingly, an auxiliary logical variable “x” will be created. In the case CHP is selected it will take the value “0” and when the User has selected FC, it will take the value “1”. Production of electricity and heat from the CHP unit is then obtained:

$$P_{el,CHP} = \eta_{el,CHP} (1 - x) P_{total,CHP/FC} \quad (\text{A1.12a})$$

$$P_{h,CHP} = \eta_{h,CHP} (1 - x) P_{total,CHP/FC} \quad (\text{A1.12b})$$

where  $\eta_{el,CHP}$  and  $\eta_{h,CHP}$  are electrical and heating efficiencies of the CHP process whose values are restricted with the following condition:

$$\eta_{el,CHP} + \eta_{h,CHP} \leq 1.$$

Since there is an option for the User to choose between the CHP and FC, operation of FC is also defined. Its electricity and heat production are:

$$P_{el,FC} = \eta_{el,FC} \times P_{total,CHP/FC} \quad (A1.13a)$$

$$P_{h,FC} = \eta_{h,FC} \times P_{total,CHP/FC} \quad (A1.13b)$$

where  $\eta_{el,FC}$  and  $\eta_{h,FC}$  are electrical and heating efficiencies of the FC which are restricted with the following condition:

$$\eta_{el,FC} + \eta_{h,FC} \leq 1.$$

According to the stoichiometry of the CHP process, the amount of the produced CO<sub>2</sub> is:

$$\dot{m}_{CO_2,CHP/FC} = \frac{M_{CO_2}}{M_{BG}} \dot{m}_{BG,CHP/FC} + \frac{M_{CO_2}}{M_{CH_4}} \dot{m}_{CH_4,CHP/FC} \quad (A1.14)$$

During the FC chemical reaction, liquid water production can be noted as:

$$\dot{m}_{H_2O,CHP/FC} = \eta_{FC,H_2O} \frac{M_{H_2O}}{M_{H_2}} \dot{m}_{H_2,CHP/FC} \quad (A1.15)$$

where:

$\eta_{FC,H_2O}$  =  
share of water (produced during FC operation), gained in liquid phase for return into  
the water storage tank

Regarding biogas, the optimization tool will manipulate with  $\dot{m}_{BG, meth}$  and with  $\dot{m}_{BG, CHP/FC}$ .

Manipulation will be limited to the following conditions:

$$\dot{m}_{BG, store} \geq 0 ; \dot{m}_{BG, meth} \geq 0 ; \dot{m}_{BG, CHP/FC} \geq 0$$

The optimization tool will also manipulate with  $\dot{m}_{H_2, CHP/FC}$ . The first manipulation limit will be the following condition:  $\dot{m}_{H_2, CHP/FC} \geq 0$ .

With the following set of equations, that use the auxiliary variable "x", usage of  $\dot{m}_{H_2, CHP/FC}$  in CHP option is limited and usage of  $\dot{m}_{CH_4, CHP/FC}$  and  $\dot{m}_{BG, CHP/FC}$  in FC option is disabled:

$$0 \leq \dot{m}_{H_2, CHP/FC} \leq (x + \alpha_{H_2}) (\dot{m}_{CH_4, CHP/FC} + \dot{m}_{BG, CHP/FC} + \dot{m}_{H_2, CHP/FC}) \quad (A1.16a)$$

$$0 \leq \dot{m}_{BG, CHP/FC} \leq (1 - x) \dot{m}_{BG, CHP/FC} \quad (A1.16b)$$

$$0 \leq \dot{m}_{CH_4, CHP/FC} \leq (1 - x) \dot{m}_{CH_4, CHP/FC} \quad (A1.16c)$$

Inequations (A1.16) are rearranged to obtain a form more suitable to OT:

$$[1 - (x + \alpha_{H_2})] \dot{m}_{H_2, CHP/FC} - (x + \alpha_{H_2}) \dot{m}_{BG, CHP/FC} - (x + \alpha_{H_2}) \dot{m}_{CH_4, CHP/FC} \leq 0 \quad (A1.17a)$$

$$x \dot{m}_{BG, CHP/FC} \leq 0 \quad (A1.17b)$$

$$x\dot{m}_{CH_4,CHP/FC} \leq 0 \quad (A1.17c)$$

$$\dot{m}_{H_2,CHP/FC} \geq 0 \quad (A1.17d)$$

$$\dot{m}_{BG,CHP/FC} \geq 0 \quad (A1.17e)$$

$$\dot{m}_{CH_4,CHP/FC} \geq 0 \quad (A1.17f)$$

where:

$\alpha_{H_2}$  = allowed weight ratio of hydrogen in the gas mixture

Residues of the AD processes are also considered. Accordingly, the following constraints must hold due to the mass conservation principle:

$$\alpha_{dry} + \gamma_{dry} + \gamma_{dry,res} \leq 1 \quad (A1.18a)$$

$$\alpha_{wet} + \gamma_{wet} + \gamma_{wet,res} \leq 1 \quad (A1.18b)$$

and these constraints are checked when parameters are entered by the user in the user interface of the optimisation tool.

where:

$\gamma_{dry,res}$  = coefficient of biomass mass residue in dry AD

$\gamma_{wet,res}$  = coefficient of biomass mass residue in wet AD

## 1.2.4 MODELLING OF CO<sub>2</sub> STORAGE DYNAMICS

According to Fig. 1, dynamic of CO<sub>2</sub> storage is analysed:

$$\dot{n}_{CO_2,store} = \dot{n}_{CO_2,store,in} - \dot{n}_{CO_2,store,out} \quad (A1.19)$$

where:

$n_{CO_2,store}$  = molar amount of CO<sub>2</sub> in storage [mol]

$\dot{n}_{CO_2,store,in}$  = molar rate of captured CO<sub>2</sub> [mol/s]

$\dot{n}_{CO_2,store,out}$  = molar rate of CO<sub>2</sub> for the methanation reactor [mol/s]

Carbon dioxide is produced during CHP operation, then it can be captured and stored, and thereafter released in the methanation reactor. Stoichiometry of the methane burning in the CHP tells that one mole of burned methane produces one mole of carbon dioxide. By following (A1.14), the molar rate of carbon dioxide generation via burning in the CHP/FC unit is:

$$\dot{n}_{CO_2,burned} = \frac{1}{M_{CO_2}} \dot{m}_{CO_2,CHP/FC} = \frac{1}{M_{BG}} \dot{m}_{BG,CHP/FC} + \frac{1}{M_{CH_4}} \dot{m}_{CH_4,CHP/FC} \quad (A1.20)$$

P2G will not be forced to collect the total amount of burned carbon dioxide. Therefore, a variable  $\dot{n}_{CO_2,store,in}$  is introduced. OT can manipulate this variable within the following limits:

$$0 \leq \dot{n}_{CO_2,store,in} \leq \dot{n}_{CO_2,burned}$$

Also, throughout the complete time horizon consisting of  $N$  discrete-time steps  $k$ , maximal value of  $\dot{n}_{CO_2,store,in}$  is to be found:  $\dot{N}_{CC} = \max(\dot{n}_{CO_2,store,in}(k))$ , where  $k \in \{0, 1, \dots, N - 1\}$  – it determines the sizing/capacity of the carbon capture unit.

Manipulation of  $\dot{n}_{CO_2,store,out}$  is possible indirectly, but due to simplicity  $\dot{n}_{CO_2,store,out}$  is made to be a function of other optimisation variables and is not used as an optimisation variable in the OT directly – it concerns attaining of the required supply ratio between  $CO_2$  and  $H_2$  in the methanation reactor. This variable must be kept positive:

$$\dot{n}_{CO_2,store,out} \geq 0$$

Manipulation with carbon dioxide in the storage is limited with:

$$n_{CO_2,store} \geq 0$$

Also, throughout the complete time horizon, maximal value of  $n_{CO_2,store}$  is to be found:

$$N_{CO_2} = \max(n_{CO_2,store}(k)), \forall k \in \{0, 1, \dots, N - 1\},$$

since it determines the needed capacity of the  $CO_2$  storage in the P2G hub.

## 1.2.5 THE METHANATION REACTOR AND BALANCE OF METHANATION GASES

To achieve ideal methane production, stoichiometric ratio of the delivered  $CO_2$  and  $H_2$  in the methanation reactor should be equal to 1:4. As it is shown in Figure 2, there are many ways of  $CO_2$  and  $H_2$  supply to the methanation reactor. The overall gas balance and methane production equation is:

$$\dot{n}_{CO_2,store,out} + \dot{n}_{CO_2,BG} + \dot{n}_{CO_2,SG} = k_{stoch} \dot{n}_{H_2, meth} = \dot{n}_{CH_4, meth} \quad (A1.21)$$

where:

$$k_{stoch} = \text{stoichiometric number of methanation reaction} = \frac{1}{4}$$

$\dot{n}_{CO_2,BG}$  = molar rate of carbon dioxide directly from the biogas injected  
in the methanation process, according to (A1.9b) [mol/s]

$\dot{n}_{H_2, meth}$  = molar rate of hydrogen injected in the methanation process [mol/s]

$\dot{n}_{CH_4, meth}$  = molar rate of methane produced in the methanation process [mol/s]

Further on,  $\dot{n}_{H_2, meth}$  is defined as sum of molar rate of hydrogen from the hydrogen storage to the methanation process and molar rate of hydrogen contained in syngas that is delivered with syngas from the syngas storage to the methanation process:

$$\dot{n}_{H_2, meth} = \dot{n}_{H_2, store, meth} + \dot{n}_{H_2, SG} \quad (A1.22)$$

Optimization variables for the OT regarding biogas and syngas dosage into the methanation process are already introduced before – they are  $\dot{m}_{BG, meth}$  and  $\dot{n}_{SG, meth}$  and according to them  $\dot{n}_{CO_2, BG}$ ,  $\dot{n}_{CO_2, SG}$  and  $\dot{n}_{H_2, SG}$  are determined. The additional optimization variable to fully determine the methanation process input is  $\dot{n}_{H_2, store, meth}$ .

Thus:

$$\begin{aligned} \dot{n}_{CO_2, store, out} &= k_{stoch}(\dot{n}_{H_2, store, meth} + \dot{n}_{H_2, SG}) - \dot{n}_{CO_2, BG} - \dot{n}_{CO_2, SG} = \\ &= k_{stoch}\dot{n}_{H_2, store, meth} + k_{stoch}g'_1\dot{n}_{SG, meth} - \frac{s'_c}{M_{BG}}\dot{m}_{BG, meth} - g'_2\dot{n}_{SG, meth} = k_{stoch}\dot{n}_{H_2, store, meth} + \\ &\quad (k_{stoch}g'_1 - g'_2)\dot{n}_{SG, meth} - \frac{s'_c}{M_{BG}}\dot{m}_{BG, meth} \end{aligned} \quad (A1.23)$$

As assessed in the previous section related to CO<sub>2</sub> storage dynamics, it must hold also that  $\dot{n}_{CO_2, store, out} \geq 0$  and also that  $n_{CO_2, store} \geq 0$  which indirectly requires to establish the carbon capture unit whenever it happens that  $\dot{n}_{CO_2, store, out} > 0$ .

The produced methane in the methanation reactor is also tied with the introduced optimization variables due to (A1.21):

$$\dot{n}_{CH_4, meth} = k_{stoch}\dot{n}_{H_2, meth} = k_{stoch}(\dot{n}_{H_2, store, meth} + \dot{n}_{H_2, SG}) = k_{stoch}\dot{n}_{H_2, store, meth} + k_{stoch}g'_1\dot{n}_{SG, meth} \quad (A1.24)$$

Methane input  $\dot{n}_{CH_4, BG}$  from biogas directly in the methanation reactor is already defined by (A1.9a) and it is assumed to be just forwarded through the methanation reactor, though it is considered that it also consumes a part of the methanation reactor capacity. The sizing/capacity of the methanation reactor is thus determined with:

$$\begin{aligned} \dot{N}_{meth, M} &= \max(\dot{n}_{CH_4, meth} + \dot{n}_{CH_4, BG}) \\ &= \max\left(k_{stoch}\dot{n}_{H_2, store, meth} + k_{stoch}g'_1\dot{n}_{SG, meth} + \frac{s'_M}{M_{BG}}\dot{m}_{BG, meth}\right) \end{aligned}$$

## 1.2.6 MODELLING OF H<sub>2</sub>O STORAGE DYNAMICS

Dynamics of the P2G hub water storage is:

$$\dot{n}_{H_2O, store} = \dot{n}_{H_2O, grid} + \frac{\dot{m}_{H_2O, CHP/FC}}{M_{H_2O}} + \dot{n}_{H_2O, rain} - \dot{n}_{H_2O, feed} \quad (A1.25)$$

where:

$\dot{m}_{H_2O,CHP/FC}$  = mass rate of FC water production according to (A1.15)[kg/s]

$n_{H_2O,store}$  = amount of water in the water storage (demineralized water)[mol]

$\dot{n}_{H_2O,grid}$  = molar rate of water supplied from the water distribution system which is additionally demineralized  $\left[\frac{\text{mol}}{\text{s}}\right] = \frac{Q_{H_2O,grid} \rho_{H_2O}}{3600 M_{H_2O}} = k_{H_2O} Q_{H_2O,grid}$

$Q_{H_2O,grid}$  = volume flow of the water coming from the grid  $\left[\frac{\text{m}^3}{\text{h}}\right]$

$k_{H_2O} = 15 \left[\frac{\text{mol h}}{\text{m}^3 \text{s}}\right]$

$\dot{n}_{H_2O,rain}$  – molar rate of rainwater that is fetched at the P2G hub site [mol/s]

$\dot{n}_{H_2O,feed}$

– molar rate of water needed for electrolysis and gasification (demineralized water) [mol/s]

The molar rate of water needed for electrolysis and gasification is:

$$\dot{n}_{H_2O,feed} = \dot{n}_{H_2O,store,in} + \dot{n}_{H_2O,GWGS} \quad (\text{A1.26})$$

where:

$\dot{n}_{H_2O,store,in}$  – molar rate of water needed for electrolysis  $\left[\frac{\text{mol}}{\text{s}}\right]$

$\dot{n}_{H_2O,GWGS}$  – molar rate of water needed for GWGS reaction  $\left[\frac{\text{mol}}{\text{s}}\right]$

Water needed for electrolysis  $\dot{n}_{H_2O,store,in}$  is used as optimization variable restricted with the following:

$$\dot{n}_{H_2O,store,in} \geq 0$$

Throughout the complete time horizon, maximal value of  $\dot{n}_{H_2O,store,in}$  is to be found for determination of sizing/capacity for the electrolyser:

$$\dot{N}_{H_2O,store,in} = \max\left(\dot{n}_{H_2O,store,in}(k)\right), \text{ where } k \in \{0, 1, \dots, N - 1\}$$

Needed water supply for gasification and afterwards for WGS can be calculated:

$$\dot{n}_{H_2O,GWGS} = k_{H_2O,GWGS} \dot{n}_{SG,GWGS} \quad (\text{A1.27a})$$

where:

$k_{H_2O,GWGS}$  – coefficient of water needed for GWGS [–]

Expression (A1.27a) can be bonded to the manipulation variable:

$$\dot{n}_{H_2O,GWGS} = k_{H_2O,GWGS} \eta'_{BC \rightarrow SG} \dot{m}_{BC,GWGS} \quad (A1.27b)$$

Now, using (A1.26) and (A1.27b), the final expression for the needed amount of demineralized water is obtained:

$$\dot{n}_{H_2O,feed} = \dot{n}_{H_2O,store,in} + k_{H_2O,GWGS} \eta'_{BC \rightarrow SG} \dot{m}_{BC,GWGS} \quad (A1.28a)$$

or:

$$\dot{n}_{H_2O,feed} = \dot{n}_{H_2O,store,in} + k_{supp,GWGS} \dot{m}_{BC,GWGS} \quad (A1.28b)$$

where  $k_{supp,GWGS}$  is introduced:

$$k_{supp,GWGS} = k_{H_2O,GWGS} \eta'_{BC \rightarrow SG}$$

Quantity of precipitation used at the P2G site is:

$$\dot{n}_{H_2O,rain} = A_{drain} k_{rain} \quad (A1.29)$$

$A_{drain}$  = drainage area [m<sup>2</sup>] is manipulated variable ;

$$k_{rain} = \text{average precipitation quantity per unit area and time [mol/(m}^2 \text{ s)]} = \frac{\rho_{H_2O}}{M_{H_2O}} \dot{h}_{rain}$$

where  $\dot{h}_{rain}$  is the profile of the rainfall at the site extracted from a single value of monthly rainfall in units [mm/month] converted to [m/s].

Catchment of rainwater is determined by manipulation with drainage area  $A_{drain}$ . It is also possible to manipulate with  $\dot{n}_{H_2O,grid}$ . Manipulations are restricted to the following conditions:

$$n_{H_2O,store} \geq 0; \dot{n}_{H_2O,grid} \geq 0$$

$$0 \leq A_{drain} \leq A_{drain,max}$$

where  $A_{drain,max}$  (maximal drainage area at the site of the P2G hub) is provided by the OT User.

Throughout the complete time horizon, maximal value of  $n_{H_2O,store}$  is found to assess the needed size of the water storage:

$$N_{H_2O,store} = \max(\dot{n}_{H_2O,store}(k)), \text{ where } k \in \{0, 1, \dots, N - 1\},$$

The needed size of the connection point to the water distribution grid is determined as

$$\dot{N}_{H_2O,grid} = \max(\dot{n}_{H_2O,grid}(k)), \text{ where } k \in \{0, 1, \dots, N - 1\}.$$

Before water from the public distribution grid  $\dot{n}_{H_2O,grid}$  enters the P2G (according to the Fig. 1), it is demineralized. For sizing of the demineralization unit, again  $\dot{N}_{H_2O,grid}$  is used.

## 1.2.7 MODELLING OF ELECTROLYZER AND H<sub>2</sub> STORAGE DYNAMICS

According to Figure 1, input to hydrogen storage is hydrogen produced by electrolyser:

$$\dot{n}_{H_2,store,in} = \frac{\eta_{el,electrolyzer} P_{el,electrolyzer}}{\varepsilon_s} \quad (A1.30)$$

where:

$P_{el,electrolyzer}$  = electrical power needed for  $\dot{n}_{H_2,store,in}$  production [kW]

$\varepsilon_s$  = specific energy needed for splitting of one mole of water into hydrogen and oxygen = 260 kW/mol

$\eta_{el,electrolyzer}$  = efficiency of electrolyzer

There are three hydrogen outputs: the first one is hydrogen for the CHP/FC, the second is hydrogen that goes to methanation reactor and the third is hydrogen that could possibly go to a hydrogen consumer such as hydrogen fuelling station. Accordingly, hydrogen storage dynamic is:

$$\dot{n}_{H_2,store} = \dot{n}_{H_2,store,in} - \dot{n}_{H_2,CHP/FC} - \dot{n}_{H_2,store,meth} - \dot{n}_{H_2,store,out} \quad (A1.31)$$

where:

$n_{H_2,store}$  = amount of hydrogen in hydrogen storage [mol]

$\dot{n}_{H_2,store,in}$  = hydrogen into hydrogen storage [mol/s]

$\dot{n}_{H_2,store,meth}$  = hydrogen from hydrogen storage to methanation reactor [mol/s]

$\dot{n}_{H_2,store,out}$  = hydrogen from hydrogen storage to another purpose [mol/s]

Manipulation with  $\dot{n}_{H_2,CHP/FC}$  is already described in 1.2.3. Besides that, OT manipulates with the following variables:  $\dot{n}_{H_2,store,in}$ ,  $\dot{n}_{H_2,store,meth}$  and  $\dot{n}_{H_2,store,out}$ .

The manipulation is limited with the following constraints:

$$n_{H_2,store} \geq 0 ; \dot{n}_{H_2,store,meth} \geq 0 ; \dot{n}_{H_2,store,out} \geq 0$$

Also, throughout the complete time horizon, maximal value of  $n_{H_2,store}$  is to be found for determination of sizing/capacity for the hydrogen storage:

$$N_{H_2,store} = \max(n_{H_2,store}(k)), \text{ where } k \in \{0, 1, \dots, N - 1\}$$

## 1.2.8 MODELLING OF O<sub>2</sub> STORAGE DYNAMICS

Dynamics of the oxygen storage is:

$$\dot{n}_{O_2,store} = \dot{n}_{O_2,store,in} - \dot{n}_{O_2,store,GWGS} - \dot{n}_{O_2,store,out} - \dot{n}_{O_2,store,letoff} \quad (A1.32)$$

where:

$n_{O_2,store}$  = amount of oxygen in the oxygen storage

$\dot{n}_{O_2,store,in}$  = oxygen injected to the oxygen storage from the electrolyzer [mol/s]

$\dot{n}_{O_2,store,GWGS}$  = oxygen from the oxygen storage to gasification [mol/s]

$\dot{n}_{O_2,store,out}$  = oxygen from the oxygen storage to external purpose (for selling) [mol/s]

$\dot{n}_{O_2,store,letoff}$  = oxygen from the oxygen storage released to the atmosphere [mol/s]

According to Chapter 2.4.2 where electrolyser is elaborated,  $\dot{n}_{O_2,store,in}$  is:

$$\dot{n}_{O_2,store,in} = v_1 \dot{n}_{H_2,store,in} \quad (A1.33)$$

where:

$v_1$  = stoichiometric number of oxygen in electrolysis  $\left\{ H_2O \rightarrow H_2 + \frac{1}{2} O_2 \right\}$  reaction:  $= \frac{1}{2}$

The amount of oxygen needed for gasification is determined by the gasification dynamics given with:

$$\dot{n}_{O_2,store,GWGS} = v_2 \eta'_{BC \rightarrow SG} \dot{m}_{BC,GWGS} \quad (A1.34)$$

where:

$v_2$  = stoichiometric number of oxygen in gasification, and

$\eta'_{BC \rightarrow SG}$  is provided in (A1.4).

The oxygen from the storage can be also released to the atmosphere ( $\dot{n}_{O_2,store,letoff}$ ) or can be used for selling in healthcare, industry etc. ( $\dot{n}_{O_2,store,out}$ ).

Due to the fact that variables given in (A1.33) and (A1.34) are already used, the optimization tool can here additionally manipulate with  $\dot{n}_{O_2,store,out}$  and  $\dot{n}_{O_2,store,letoff}$ . The manipulation is constrained by the following conditions:

$$n_{O_2,store} \geq 0; \dot{n}_{O_2,store,out} \geq 0; \dot{n}_{O_2,store,letoff} \geq 0$$

Also, throughout the complete time horizon, maximal value of  $n_{O_2,store}$  is to be found which corresponds to the oxygen storage capacity:

$$N_{O_2,store} = \max(n_{O_2,store}(k)), \text{ where } k \in \{0, 1, \dots, N - 1\}.$$

## 1.2.9 MODELLING OF CH<sub>4</sub> STORAGE DYNAMICS

Dynamics of the methane storage comprises of the transfer to/from the gas connection point (positive sign means the export of gas, negative the import of gas), gas inputs obtained from the methanation reactor, and gas outputs: the first for transport selling

purpose, the second for transfer to the gas connection point and the third for gas (methane) line from the methane storage to the CHP/FC:

$$\dot{n}_{CH_4,store} = \dot{n}_{CH_4,meth} + \dot{n}_{CH_4,BG} - \dot{n}_{CH_4,out} - \dot{n}_{gas,P2G,conn} - \dot{n}_{CH_4,CHP/FC} \quad (A1.35)$$

where:

$$\dot{n}_{gas,P2G,conn} = P_{gas,P2G} k_{kw2mol} \quad (A1.36)$$

$\dot{n}_{gas,P2G,conn}$  = gas transfer between CH<sub>4</sub> storage and gas connection point [mol/s]

$P_{gas,P2G}$  = gas  $\dot{n}_{gas,P2G,conn}$  transfer given in [kW]

$k_{kw2mol}$  = conversion from kW to mol = 1/805 [(mol/s) / kW]

$n_{CH_4,store}$  = amount of methane in the methane storage tank [mol]

$\dot{n}_{CH_4,meth}$  = gas produced in the methanation reactor (A1.24) [mol/s]

$\dot{n}_{CH_4,BG}$  = gas already contained within biogas (A1.9a) [mol/s]

$\dot{n}_{CH_4,out}$  = gas that is sold in a transportable container [mol/s]

$\dot{n}_{CH_4,CHP/FC}$  = gas released from CH<sub>4</sub> storage to the CHP/FC [mol/s]

In the OT, in addition to the already introduced optimization variables, it is possible to do manipulation with additionally with variables:  $\dot{n}_{CH_4,out}$  and  $P_{gas,P2G}$ . Variable  $P_{gas,P2G}$  is also used in assessment of compression in 1.3.5.

Gas bidirectional flow from the storage to the gas connection point and vice versa is also enabled. Accordingly, OT will have the following limitations:

$$n_{CH_4,store} \geq 0; \dot{n}_{CH_4,out} \geq 0; \dot{n}_{CH_4,CHP/FC} \geq 0$$

Also, throughout the complete time horizon, maximal value of  $n_{CH_4,store}$  is determined, as the needed capacity of the CH<sub>4</sub> storage tank:

$$N_{CH_4,store} = \max(n_{CH_4,store}(k)), \forall k.$$

## 1.2.10 BALANCE OF THERMAL ENERGY (HEAT)

Heat system of the complete P2G system (REP and IP included) comprises of heat consumed and produced by the P2G hub, as well as by the REP and the IP connected to the hub. The complete P2G system net consumption (REP and IP included) is:

$$P_{h,net,cons} = P_{h,P2G} - P_{h,REP} - P_{h,IP} \quad (A1.37)$$

where

$P_{h,P2G}$  = heat power consumed(+)/produced(-) by the P2G hub [kW]

$P_{h,REP}$  = heat power produced(+)/consumed(-) by the REP connected to the P2G hub [kW]

$P_{h,IP}$  = heat power produced(+)/consumed(-) by the IP connected to the P2G hub [kW]

Heat produced by the P2G hub can be noted as:

$$P_{h,P2G} = P_{h,P2G+} - P_{h,P2G-} \quad (A1.38)$$

where

$P_{h,P2G-}$  = cumulative sum of produced heat (with + sign) of processes of the P2G hub that produce heat [kW],

$P_{h,P2G+}$  = cumulative sum of consumed heat (with + sign) of processes of the P2G hub that consume heat [kW].

Namely, a P2G hub, depending on its configuration and operation at a certain moment, can be either a net producer or a net consumer of heat. Operation of CHP/FC and methanation produce heat, while for the electrolyser it is possible for it to be either a heat producer or a heat consumer. For distinguishing between the two cases, in the pre-processing part of the OT an auxiliary variable  $y$  is used that can be selected by the user:

$$\begin{aligned} y &= 1 \text{ if the electrolyser is a heat producer;} \\ y &= -1 \text{ if the electrolyser is a heat consumer.} \end{aligned}$$

Accordingly, heat production of the P2G hub can be noted as:

$$P_{h,P2G-} = \frac{1+y}{2} P_{h,el} + P_{h,CHP} + P_{h,FC} + P_{h,meth} \quad (A1.39)$$

On the other hand, several internal processes of a P2G are heat consumers: carbon capture (CC), AD, Biomass2Biochar and GWGS processes. Using the auxiliary variable  $y$ , possibility of heat consumption of the electrolyser is also included:

$$P_{h,P2G+} = \frac{1-y}{2} P_{h,el} + P_{h,cc} + P_{h,AD,dry} + P_{h,AD,wet} + P_{h,BM,dry,2BC} + P_{h,BM,wet,2BC} + P_{h,GWGS} \quad (A1.40)$$

where:

$P_{h,el}$  = heat power produced( $y = 1$ )/consumed ( $y = -1$ ) by the electrolyzer [kW],

$P_{h,CHP}$  = heat power produced by the CHP unit ( $P_{h,CHP}$  – A1.12b) [kW],

$P_{h,FC}$  = heat power produced by the FC unit ( $P_{h,FC}$  – A1.13b) [kW],

$P_{h,meth}$  = heat power produced by methanation [kW],

$P_{h,cc}$  = heat power consumed by the carbon capture [kW],

$P_{h,AD,dry}$  = heat power consumed by the dry AD [kW],

$P_{h,AD,wet}$  = heat power consumed by the wet AD [kW],

$P_{h,BM,dry,2BC}$  = heat power consumed by the dry BM2BC [kW],

$P_{h,BM,wet,2BC}$  = heat power consumed by the wet BM2BC [kW],

$P_{h,GWGS}$  = heat power consumed by the GWGS [kW].

With the common heat exchanger circuit, produced heat can be used to supply heat consuming processes. Power of the heat exchanger is defined by the maximal heat transfer to the P2G hub. Both directions (production/consumption) are taken into consideration:

$$P_{h,HE,max} \geq P_{h,P2G+,max} = \frac{1-y}{2} P_{h,el,max} + P_{h,cc,max} + P_{h,AD,dry,max} + P_{h,AD,wet,max} + P_{h,BM,dry,2BC} + P_{h,BM,wet,2BC} + P_{h,GWGS,max} \quad (A1.41a)$$

$$P_{h,HE,max} \geq P_{h,P2G-,max} = \frac{1+y}{2} P_{h,el,max} + P_{h,CHP,max} + P_{h,FC,max} + P_{h,meth,max} \quad (A1.41b)$$

where:

$P_{h,HE,max}$  is the rated power of the heat exchanger obtained by intersecting (A1.41a) and (A1.41b).

$\frac{1-y}{2} P_{h,el,max}$ ,  $P_{h,cc,max}$ ,  $P_{h,AD,dry,max}$ ,  $P_{h,AD,wet,max}$ ,  $P_{h,BM,dry,2BC}$ ,  $P_{h,BM,wet,2BC}$ ,  $P_{h,GWGS,max}$  are maxima of heat consumption by the corresponding processes throughout the complete time horizon.

$\frac{1+y}{2} P_{h,el,max}$ ,  $P_{h,CHP,max}$ ,  $P_{h,FC,max}$ ,  $P_{h,meth,max}$  are maxima of heat production by the corresponding processes throughout the complete time horizon.

Calculation for each heat component is given next. Heat power produced ( $y=1$ ) or consumed ( $y=-1$ ) by the electrolyser is:

$$\text{Consumed: } P_{h,el} = \frac{1+y}{2} k_{h,el} \dot{n}_{H2,store,in} \quad (A1.42a)$$

$$\text{Produced: } P_{h,el} = \frac{1-y}{2} k_{h,el} \dot{n}_{H2,store,in} \quad (A1.42b)$$

Heat power produced by the CHP unit is given in (A1.12b) and heat produced by the FC unit is given in (A1.13b), while heat power produced by the methanation reactor is:

$$P_{h,met} = k_{h,met} (\dot{n}_{CH4,met} + \dot{n}_{CH4,BG}) \quad (A1.43)$$

Heat power consumed by the carbon capture unit is determined by the carbon capture heat coefficient  $k_{h,CC}$  and rate of carbon capture:

$$P_{h,CC} = k_{h,CC} \dot{n}_{CO2,store,in} \quad (A1.44)$$

Heat power needed for ADs is:

$$P_{h,AD,dry} = k_{h,dry,AD} \dot{m}_{BM,dry,AD} \quad (A1.45a)$$

$$P_{h,AD,wet} = k_{h,wet,AD} \dot{m}_{BM,wet,AD} \quad (A1.45b)$$

Heat power needed for BM2BCs is:

$$P_{h,BM,dry,2BC} = k_{h,BM,dry,2BC} \dot{m}_{BM,dry,2BC} \quad (A1.46a)$$

$$P_{h,BM,wet,2BC} = k_{h,BM,wet,2BC} \dot{m}_{BM,wet,2BC} \quad (A1.46b)$$

Heat power needed for gasification and WGS is

$$P_{h,GWGS} = k_{h,GWGS} \dot{m}_{BC,GWGS} \quad (A1.47)$$

The coefficients used in the previous equations depend on the technology used, and here are suggested the values which are used as default in the OT, but the expert user can freely change them:

$$k_{h,el} = \text{heat coefficient of electrolysis} = 32 \left[ \frac{\text{kW}}{\text{mol/s}} \right],$$

$$k_{h,meth} = \text{heat coefficient of methanation} = 250 \left[ \frac{\text{kW}}{\text{mol/s}} \right],$$

$$k_{h,CC} = \text{carbon capture heat coefficient} = 170 \left[ \frac{\text{kW}}{\text{mol/s}} \right],$$

$$k_{h,dry,AD} = \text{heat coefficient of dry AD} = 250 \left[ \frac{\text{kW}}{\text{kg/s}} \right],$$

$$k_{h,wet,AD} = \text{heat coefficient of wet AD} = 270 \left[ \frac{\text{kW}}{\text{kg/s}} \right],$$

$$k_{h,BMdry2BC} = \text{heat coefficient of dry BM2BC} = 0 \left[ \frac{\text{kW}}{\text{kg/s}} \right],$$

$$k_{h,BMwet2BC} = \text{heat coefficient of wet BM2BC} = 0 \left[ \frac{\text{kW}}{\text{kg/s}} \right],$$

$$k_{h,GWGS} = \text{heat coefficient of GWGS} = 100 \left[ \frac{\text{kW}}{\text{kg/s}} \right].$$

Each of the given values is backed up with the literature as is given in 3. Determination of coefficients and prices.

### 1.2.11 BALANCE OF ELECTRICAL ENERGY

According to Figure 1, electrical balance of the P2G plant can be noted:

$$P_{el,grid} = P_{el,P2G} + P_{comp,ex} - P_{el,REP} + P_{el,IP} \quad (A1.48)$$

where:

$P_{el,grid}$  = electrical power of electrical grid system (+sign means consumption from the grid,

– sign means export to the grid) [kW] ,

$P_{el,P2G}$  = consumed electrical power of the P2G hub [kW]

$P_{comp,ex}$  = consumed electrical power required for gas compression in the pipeline of the P2G + REP + IP system and towards the gas grid [kW].

$P_{el,REP}$  = produced electrical power of the REP connected to the P2G hub [kW] ,

$P_{el,IP}$  = consumed electrical power of the IP connected to the P2G hub [kW].

Total electrical power of the P2G hub is:

$$P_{el,P2G} = P_{el,in} - P_{el,out} \quad (A1.49)$$

where:

$P_{el,in}$  = electrical power consumed by processes of the P2G plant [kW]

$P_{el,out} = P_{el,CHP} + P_{el,FC}$  = el. power produced by the CHP unit ( $P_{el,CHP}$  – A1.12a) or FC ( $P_{el,FC}$  – A1.13a) [kW]

Then,  $P_{el,in}$  can be noted as:

$$P_{el,in} = P_{el,electrolyser} + P_{el,proc} \quad (A1.50)$$

where:

$P_{el,electrolyser}$  the electrical consumption of the electrolyser,

and  $P_{el,proc}$  encompasses consumption of all other processes of the P2G plant.

When all components are included,  $P_{el,P2G}$  becomes:

$$P_{el,P2G} = P_{el,electrolyzer} + P_{el,cc} + P_{el,AD,dry} + P_{el,AD,wet} + P_{el,BM,dry,2BC} + P_{el,BM,wet,2BC} + P_{el,GWGS} + P_{el,meth} + P_{el,demin} - P_{el,CHP} - P_{el,FC} \quad (A1.51)$$

where:

$P_{el,cc}$  = electrical power consumption of carbon capture [kW]

$P_{el,AD,dry}$  = electrical power consumption of dry AD [kW]

$P_{el,AD,wet}$  = electrical power consumption of wet AD [kW]

$P_{el,BM,dry,2BC}$  = electrical power consumption of dry BM2BC [kW]

$P_{el,BM,wet,2BC}$  = electrical power consumption of wet BM2BC [kW]

$P_{el,GWGS}$  = electrical power consumption of GWGS [kW]

$P_{el,meth}$  = electrical power of methanation [kW]

$P_{el,demin}$  = electrical power consumption of water demineralization [kW]

Calculation for each of the given electrical power consumptions can be obtained:

$$P_{el,electrolyser} = \frac{\varepsilon_s}{\eta_{el,electrolyser}} \dot{n}_{H2,store,in} \quad (A1.52)$$

$$P_{el,CC} = k_{el,CC} \dot{n}_{CO2,store,in} \quad (A1.53)$$

$$P_{el,AD,dry} = k_{el,AD,dry} \dot{m}_{BM,dry,AD} \quad (A1.54)$$

$$P_{el,AD,wet} = k_{el,AD,wet} \dot{m}_{BM,wet,AD} \quad (A1.55)$$

$$P_{el,BM,dry,2BC} = k_{el,BM,dry,2BC} \dot{m}_{BM,dry,2BC} \quad (A1.56)$$

$$P_{el,BM,wet,2BC} = k_{el,BM,wet,2BC} \dot{m}_{BM,wet,2BC} \quad (A1.57)$$

$$P_{el,GWGS} = k_{el,GWGS} \dot{m}_{BC,GWGS} \quad (A1.58)$$

$$P_{el,meth} = k_{el,meth} (\dot{n}_{CH4,meth} + \dot{n}_{CH4,BG}) \quad (A1.59)$$

$$P_{el,demin} = k_{el,demin} \dot{n}_{H2O,grid} \quad (A1.60)$$

The coefficients used in the previous equations depend on the technology used, and here are suggested the values which are used as default in the OT, but the expert user can freely change them  $k_{el,CC} = \text{carbon capture electrical coefficient} = 20 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$

$$k_{el,dryAD} = \text{electrical coefficient of dry AD} = 150 \left[ \frac{\text{kW}}{\text{kg/s}} \right]$$

$$k_{el,wetAD} = \text{electrical coefficient of wet AD} = 170 \left[ \frac{\text{kW}}{\text{kg/s}} \right]$$

$$k_{el,BMdry2BC} = \text{electrical coefficient of dry BM2BC} = 8700 \left[ \frac{\text{kW}}{\text{kg/s}} \right]$$

$$k_{el,BMwet2BC} = \text{electrical coefficient of wet BM2BC} = 8700 \left[ \frac{\text{kW}}{\text{kg/s}} \right]$$

$$k_{el,GWGS} = \text{electrical coefficient of GWGS} = 100 \left[ \frac{\text{kW}}{\text{kg/s}} \right]$$

$$k_{el,meth} = \text{electrical coefficient of methanation} = 800 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$$

$$k_{el,demin} = \text{electrical coefficient of demineralization} = 7.5 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$$

Each of the given values is backed up with the literature as it is given in 3. Determination of coefficients and prices.

Due to possibility of bidirectional flow of  $\dot{n}_{gas,P2G,conn}$ , electrical power needed for compression to the gas grid  $P_{comp,ex}$  is determined in 1.3.2.3.

## 1.2.12 DISCRETIZATION OF P2G SYSTEM DYNAMICS

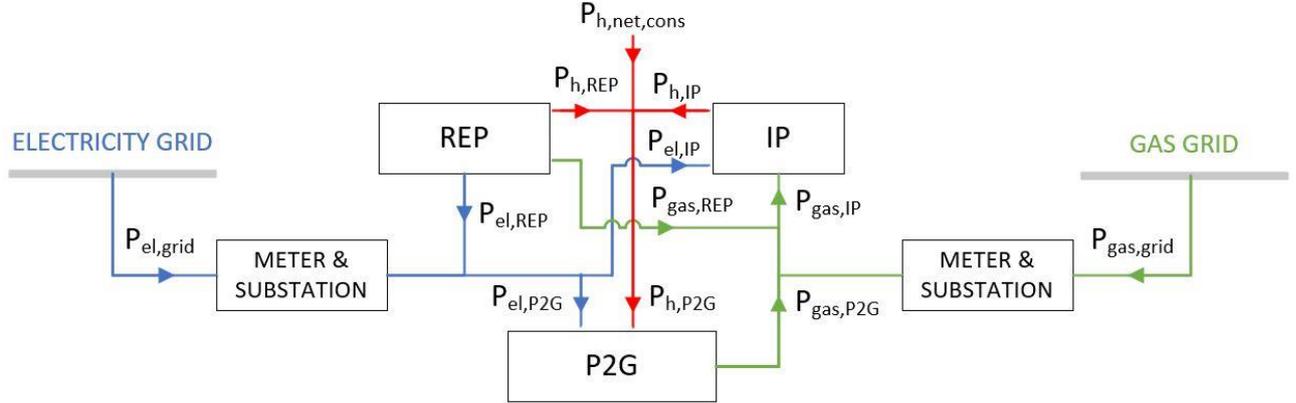
Model of the P2G system is to be discretized with two sampling times. Faster sampling time  $T_{el}$  will be used for P2G dynamics that are related to electricity and for other (gas, heat) slower sampling times:  $T_{gas}, T_{heat}$  are used. Sampling time of the slower sampling is  $T_{day} = T_{gas} = T_{heat} = 1$  day (24h) while faster sampling time  $T_{el}$  can be selected in the range: 1 hour-24 hours. Slower sampling will be indicated with (d), while for faster sampling designation (k) is used.

## 1.3 POWER TO GAS SYSTEM COST ASSESMENT

### 1.3.1 SYSTEM DESCRIPTION

According to Fig. 2, the complete P2G system is considered. Electricity, gas and heat are depicted in blue, red and green colour.

Figure 2: Complete P2G connection system



According to the electricity and gas grid connections as well as interconnections between P2G, REP and IP given in the scheme, the following equation system is obtained:

$$P_{el,grid}(k) = P_{el,IP}(k) - P_{el,REP}(k) + P_{el,P2G}(k) \quad (A1.61)$$

$$P_{gas,grid}(d) = P_{gas,IP}(d) - P_{gas,REP}(d) - P_{gas,P2G}(d) \quad (A1.62)$$

$$P_{h,net,cons}(d) = P_{h,P2G}(d) - P_{h,REP}(d) - P_{h,IP}(d) \quad (A1.63)$$

where:

$P_{el,grid}, P_{el,P2G}, P_{el,REP}, P_{el,IP}$  = electrical power of Electricity grid, P2G, REP, IP

$P_{gas,grid}, P_{gas,P2G}, P_{gas,REP}, P_{gas,IP}$  = gas power of Gas grid, P2G, REP, IP

$P_{h,P2G}, P_{h,REP}, P_{h,IP}, P_{h,net,cons}$  = heat power of P2G, REP, IP and net heat power

For the given system, operation, investment, and degradation cost calculation is given in this section.

### 1.3.2 OPERATION COST

#### 1.3.2.1 ASSESSMENT OF COSTS FOR BIOMASS AND BIOCHAR IMPORT IN THE P2G HUB

Unit cost of each biomass or biochar source, indexed with  $i$ , is calculated as the sum of the transport cost and the market cost:

$$p_{i,dry} = p_{i,dry,T} + p_{i,dry,M} \quad (A1.64a)$$

$$p_{i,wet} = p_{i,wet,T} + p_{i,wet,M} \quad (A1.64b)$$

$$p_{i,BC} = p_{i,BC,T} + p_{i,BC,M} \quad (A1.64c)$$

where:

$p_{i,dry,T}$  = unit transport cost for a dry biomass source  $i$  [€/t]

$p_{i,dry,M}$  = unit market cost of a dry biomass source  $i$  [€/t]

$p_{i,wet,T}$  = unit transport cost for a wet biomass source  $i$  [€/t]

$p_{i,wet,M}$  = unit market cost of a wet biomass source  $i$  [€/t]

$p_{i,BC,T}$  = unit transport cost for a certain biochar source [€/t]

$p_{i,BC,M}$  = unit market cost of a certain biochar source [€/t]

Biomass will be transported only by road which makes its transport cost calculation:

$$p_{i,dry,T} = k_{i,BM,T} d_{TL,i} \quad (A1.65a)$$

$$p_{i,wet,T} = k_{i,BM,T} d_{TL,i} \quad (A1.65b)$$

where:

$k_{BM,T}$  = transport cost for biomass [€/(km t)]

$d_{TL,i}$  = distance of a certain transport leg [km]

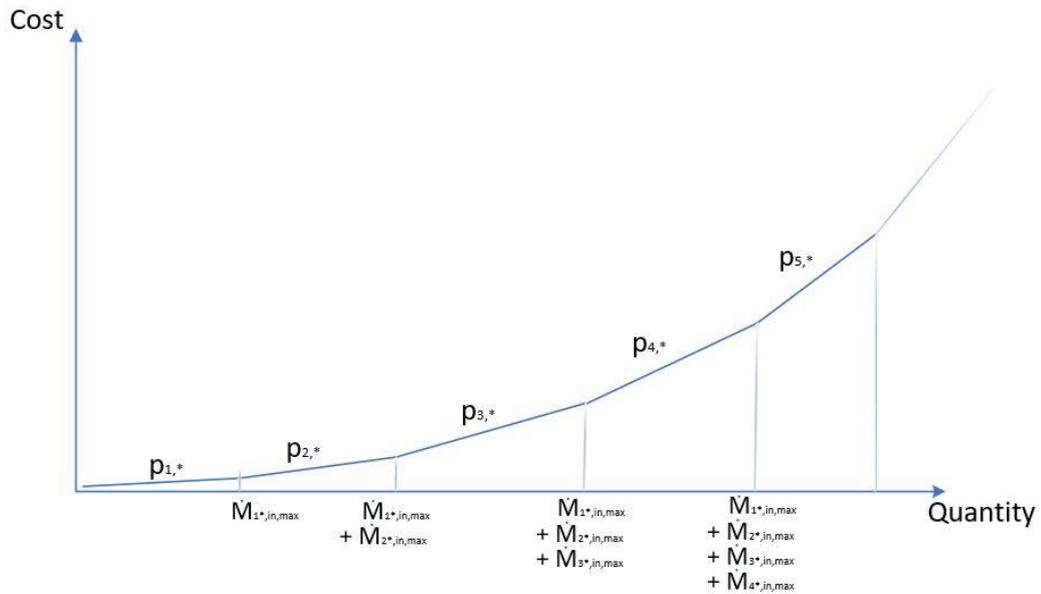
For biochar transport, cost of different transport options is calculated, and the minimal value is taken:

$$p_{i,BC,T} = \min(\text{transport cost over different transport options}) \quad (A1.65c)$$

To enable this calculation, data regarding transport hubs, their distances and cost for each transport type are needed. Such data are preferably automatically generated for the OT, e.g. with the help of Renewable Energy Atlas.

Once the costs for the different sources are determined, they are integrated in the OT optimisation problem. Operation of the OT includes manipulation with  $\dot{m}_{BM,dry,in}$ ,  $\dot{m}_{BM,wet,in}$  and  $\dot{m}_{BC,in}$ . Those variables can be obtained by stacking the contributions of multiple biomass and biochar sources, which means that different costs and available amounts of sources should be considered. Obviously, the best way is to use all available amount of the cheapest source at first, then the second cheapest and so on. This could be easily implemented by sorting the array of the sources from the lowest cost value  $p_{i,dry}, p_{i,wet}, p_{i,BC}$  to the higher values. In Figure 3, a favourable curve of source cost versus the amount of source taken by P2G, is drawn. Actually, three curves are to be obtained: two for biomass (dry and wet) and third one for biochar sources which is in the figure illustrated with asterisk.

Figure 3: Cost curve for multiple sources



Depending on the amount (quantity) of the source ( $\dot{m}_{BM,dry,in}$ ,  $\dot{m}_{BM,wet,in}$  and  $\dot{m}_{BC,in}$ ) considered in the OT, to obtain a favourable cost curve, the sources must be properly ordered. In the following considerations dry biomass source prices sorted in the ascending order are noted as  $p_{1,dry}, p_{2,dry}, p_{3,dry} \dots p_{Nsd,dry}$  while their maximal daily amounts as  $\dot{M}_{1,dry}, \dot{M}_{2,dry}, \dot{M}_{3,dry} \dots \dot{M}_{Nsd,dry}$  respectively. Wet biomass source attributes are analogously noted as  $p_{1,wet}, p_{2,wet}, p_{3,wet} \dots p_{Nsw,wet}$  and  $\dot{M}_{1,wet}, \dot{M}_{2,wet}, \dot{M}_{3,wet} \dots \dot{M}_{Nsw,wet}$ . Biochar sources attributes are analogously noted:  $p_{1,BC}, p_{2,BC}, p_{3,BC} \dots p_{Nsb,BC}$  and  $\dot{M}_{1,BC}, \dot{M}_{2,BC}, \dot{M}_{3,BC} \dots \dot{M}_{Nsb,BC}$ . Biomass input quantities ( $\dot{m}_{BM,dry,in}$ ,  $\dot{m}_{BM,wet,in}$ ) and biochar

input quantity ( $\dot{m}_{BC,in}$ ) are represented by  $u_{**}$  in general. Novel optimization variable  $\varepsilon_{**}$  corresponding to  $u_{**}$  are introduced as the supremum of the good (biomass or biochar) cost over all segments of the cost curve for the opted daily amount  $u_{**}$  of the good. Conditions for an arbitrary pair  $(\varepsilon_{**}, u_{**})$  with overall  $N_{s^*}$  sources are:

$$\varepsilon_{**} \geq u_{**} p_{1,*} \quad (\text{A1.66a})$$

$$\varepsilon_{**} \geq \dot{M}_{1,*} p_{1,*} + (u_{**} - \dot{M}_{1,*}) p_{2,*} \quad (\text{A1.66b})$$

$$\varepsilon_{**} \geq \dot{M}_{1,*} p_{1,*} + \dot{M}_{2,*} p_{2,*} + [u_{**} - (\dot{M}_{1,*} + \dot{M}_{2,*})] p_{3,*} \quad (\text{A1.66c})$$

⋮

$$\varepsilon_{**} \geq \sum_{i=1}^{N_{s^*}-1} \dot{M}_{i,*} p_{i,*} + [u_{**} - \sum_{i=1}^{N_{s^*}-1} \dot{M}_{i,*}] p_{N_{s^*},*} \quad (\text{A1.66d})$$

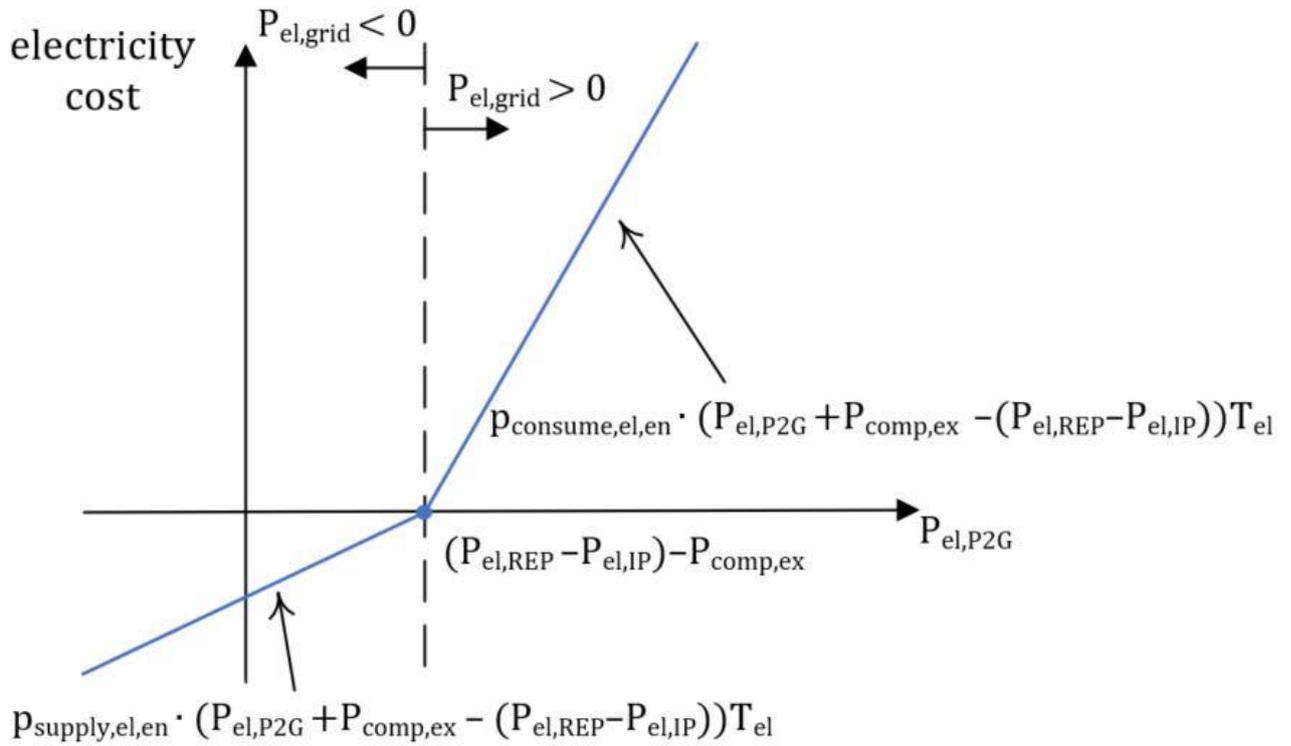
$$0 \leq u_{**} \leq \sum_{i=1}^{N_{s^*}} \dot{M}_{i,*} \quad (\text{A1.66e})$$

For any feasible value of  $u_{**}$  ( $0 \leq u_{**} \leq \sum_{i=1}^{N_{s^*}} \dot{M}_{i,*}$ ) the inequation system (A1.66a)-(A1.66e) when subject to minimisation of  $\varepsilon_{**}$  picks the cheapest sources available and disregards the non-needed overly expensive sources.

### 1.3.2.2 ASSESSMENT OF COSTS FOR ELECTRICITY, GAS, AND HEAT

In the complete P2G system configuration, REP and IP are included. REP and IP are producer and consumer of electrical power which enables the complete P2G system to be either a producer or a consumer of electricity at a certain time instant. According to the national electricity regulations, there are different prices for the produced and the consumed energy. Also, the tariff system may include the prices that vary for day and night production/consumption and also prices for the weekend period may be different. In Figure 4 a change of unit electricity cost due to the change from the electricity producer ( $p_{supply,el,en}$ ) to consumer ( $p_{consume,el,en}$ ) is given.

Figure 4: The electricity cost curve for the overall P2G system



where:

$p_{supply,el,en}$  – cost of supplied electricity [€/kWh]

$p_{consume,el,en}$  – cost of consumed electricity [€/kWh]

Mathematical representation of  $P_{el,grid}$  cost calculation is similar to the considerations from 1.2.11. In each time step, there are two conditions, that are denoted using Figure 4:

$$\varepsilon_{el} \geq p_{supply,el,en} [P_{el,P2G}(k) + P_{comp,ex}(k) - (P_{el,REP}(k) - P_{el,IP}(k))] T_{el} \quad (A1.67a)$$

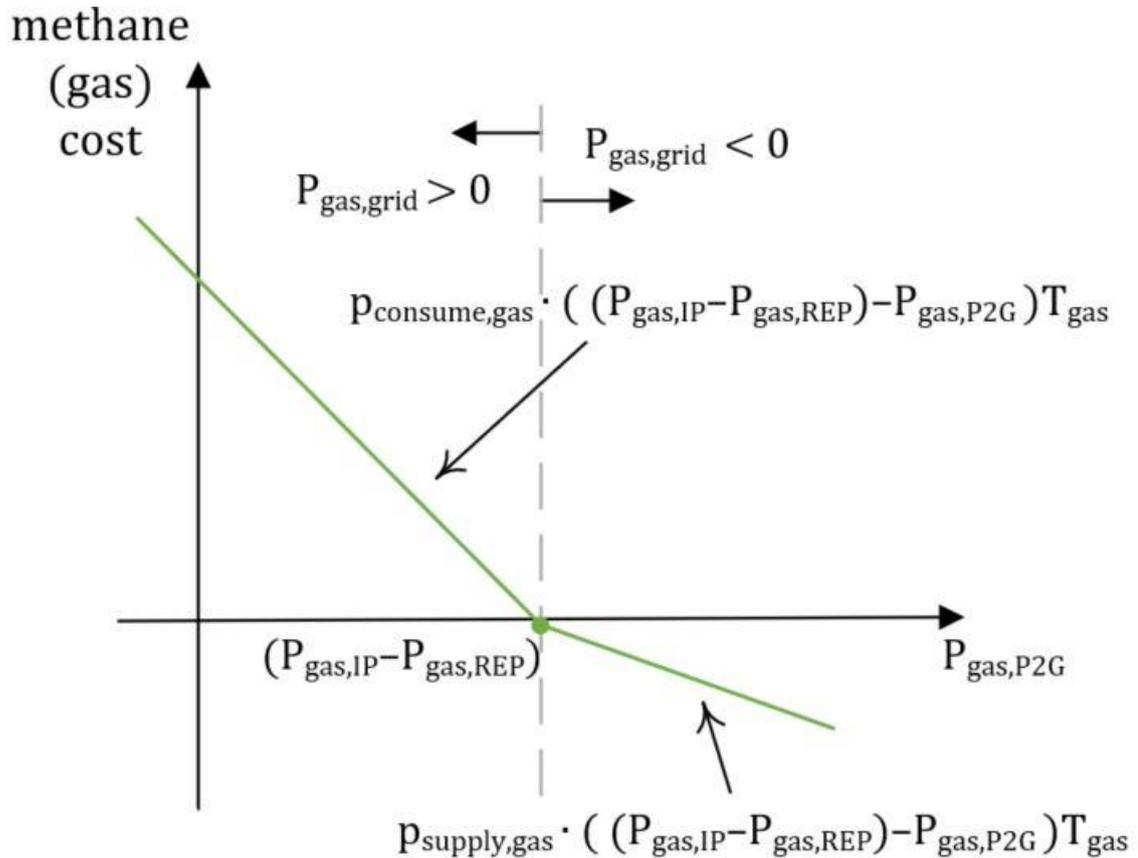
$$\varepsilon_{el} \geq p_{consume,el,en} [P_{el,P2G}(k) + P_{comp,ex}(k) - (P_{el,REP}(k) - P_{el,IP}(k))] T_{el} \quad (A1.67b)$$

where  $\varepsilon_{el}$ , supremum of the cost of electrical energy, is used for calculation of the cost by applying the minimisation function to  $\varepsilon_{el}$ . All powers mentioned are mean powers over a time period of duration  $T_{el}$ . Due to the tariff for costing the monthly peak power, the maximal mean consumed power on a tariffing interval  $T_{el}$  must be assessed as well.

Similar to electrical power, the complete P2G system configuration can be either a producer or a consumer of gas at a certain time instant. There are also different prices in place for the case of consumption and for the case of gas production. According to the national regulations, there are also different seasonal prices: ones for the winter and another ones for the summer period.

In Figure 5 a characteristic change of unit gas cost due to a change from consumer ( $p_{consume,gas}$ ), to producer ( $p_{supply,gas}$ ) is given.

Figure 5: Characteristic of the gas cost



where:

$p_{consume,gas}$  – cost of consumed methane [€/kWh]

$p_{supply,gas}$  – cost of supplied methane [€/kWh]

Mathematical representation of the gas cost calculation is similar to the electricity cost calculation. According to Figure 5, two conditions exist:

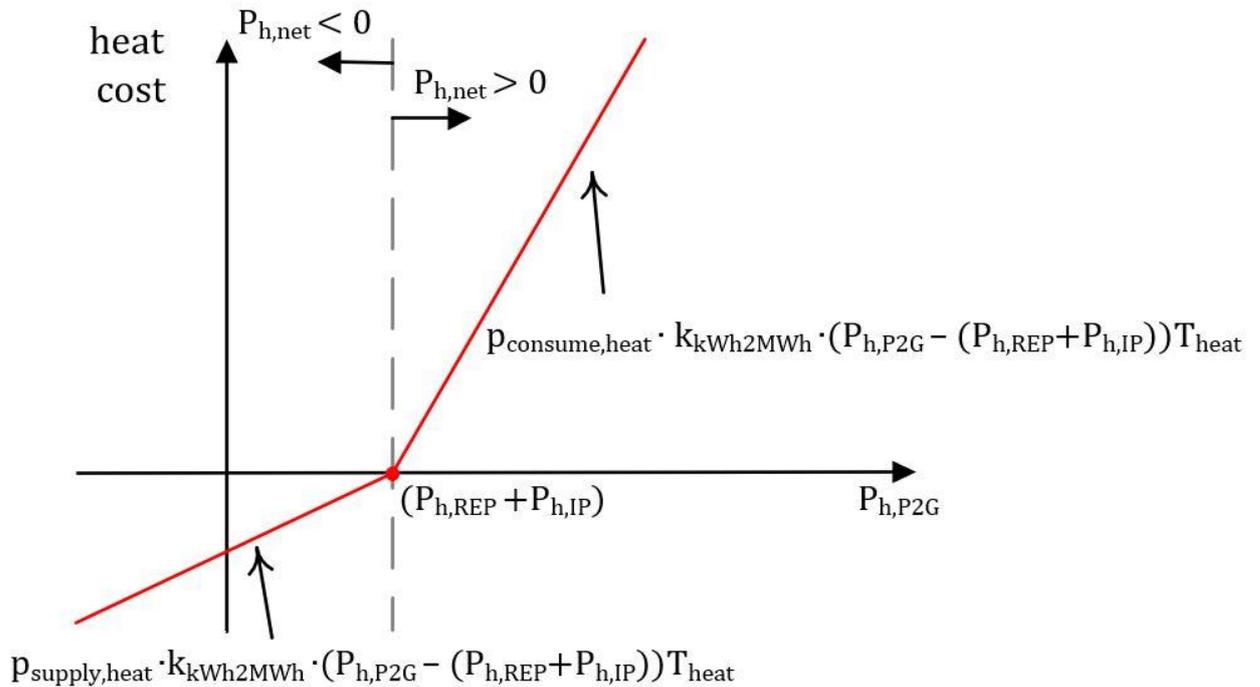
$$\varepsilon_{gas} \geq p_{consume,gas} [P_{gas,IP}(d) - P_{gas,REP}(d) - P_{gas,P2G}(d)] T_{gas} \quad (A1.68a)$$

$$\varepsilon_{gas} \geq p_{supply,gas} [P_{gas,IP}(d) - P_{gas,REP}(d) - P_{gas,P2G}(d)] T_{gas} \quad (A1.68b)$$

where  $\varepsilon_{gas}$  is a supremum of the cost of the supplied gas. It should be noted that charging of the gas production/consumption will be considered on a daily basis ( $T_{gas} = 24$  h).

As it is depicted in Figure 6, the complete P2G system can be net heat positive, net heat negative or can have a zero net heat value. Similar to electricity and gas costing, there exists a change of unit heat cost due to the change of net heat value from positive ( $p_{consume,heat}$ ) to negative ( $p_{supply,heat}$ ).

Figure 6: Characteristic of the heat cost



where:

$p_{supply,heat}$  – cost of supplied heat [€/MWh]

$p_{consume,heat}$  – cost of consumed heat [€/MWh]

Mathematical representation of the heat cost calculation is similar to the aforementioned representations for electricity and gas. According to Fig. 6, two conditions exist:

$$\varepsilon_h \geq p_{consume,heat} k_{kWh2MWh} [P_{h,P2G}(d) - P_{h,REP}(d) - P_{h,IP}(d)] T_{heat} \quad (A1.69a)$$

$$\varepsilon_h \geq p_{supply,heat} k_{kWh2MWh} [P_{h,P2G}(d) - P_{h,REP}(d) - P_{h,IP}(d)] T_{heat} \quad (A1.69b)$$

Where:

$\varepsilon_h$  is a supremum of the cost of heat

$$k_{kWh2MWh} = \frac{1}{1000}$$

is a conversion factor needed for adaption to heat prices that are given in €/MWh.

Charging of the net heating energy consumption is assumed to be done on daily basis ( $T_{heat}=24$  h).

### 1.3.2.3 ASSESSMENT OF THE ELECTRICITY CONSUMPTION FOR METHANE COMPRESSION

Before methane produced by P2G or REP is sent out it needs to be compressed from atmospheric or internal pressure to the pressure level of the gas grid. Using the theory of the adiabatic compression of gases, a general expression is obtained:

$$P_{compression} = 0,0266 \left[ \left( \frac{p_2}{p_1} \right)^{0,23} - 1 \right] P_{gas} \quad (A1.70)$$

where:

$P_{compression}$  = electrical power needed for methane compression [kW]

$p_2$  = methane pressure after compression [bar]

$p_1$  = methane pressure before compression [bar]

$P_{gas}$  = methane flow expressed in power units [kW]

In the case of P2G with IP and REP integration compression (A1.70) can be noted in a simpler way:

$$P_{compression} = k_{comp,atm,inter} P_{gas,P2G} \quad (A1.71a)$$

$$P_{compression} = k_{comp,inter,grid} P_{gas,P2G} \quad (A1.71b)$$

$$P_{compression} = k_{comp,atm,grid} P_{gas} \quad (A1.71c)$$

where different pressure levels are described with:

$$k_{comp,atm,inter} = 0,0266 \left[ \left( \frac{p_{inter}}{p_{atm}} \right)^{0,23} - 1 \right]$$

= coefficient of compression from P2G (atmospheric pressure) to internal pressure of IP, REP [ $kW_{el} / kW_{gas}$ ]

$$k_{comp,inter,grid} = 0,0266 \left[ \left( \frac{p_{grid}}{p_{inter}} \right)^{0,23} - 1 \right]$$

= coefficient of compression from internal pressure of IP, REP to gas grid pressure of IP, REP [ $kW_{el} / kW_{gas}$ ]

$$k_{comp,atm,grid} = k_{comp,atm,inter} + k_{comp,inter,grid}$$

= coefficient of compression from P2G (atmospheric pressure) to gas grid pressure of IP, REP [ $kW_{el} / kW_{gas}$ ]

$p_{inter}$  – internal pressure of IP [bar]

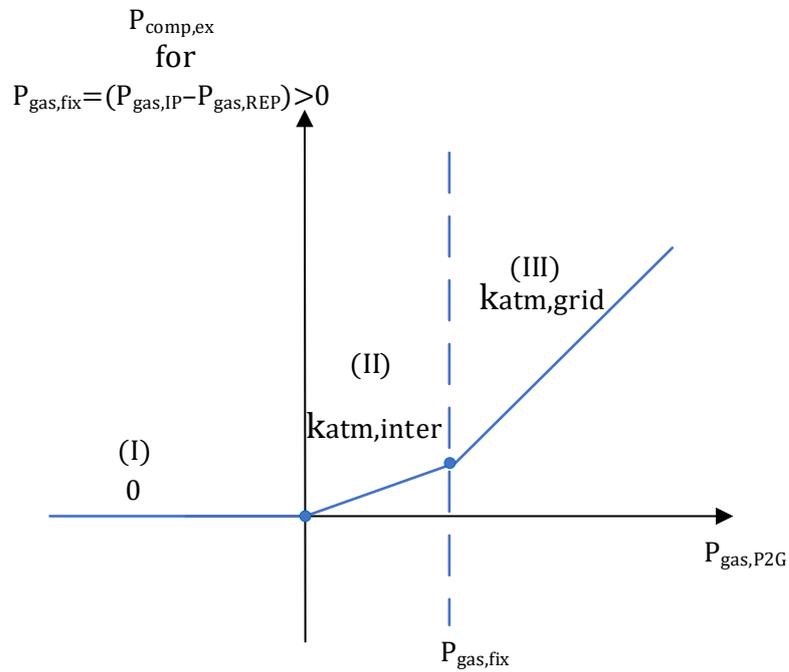
$p_{grid}$  – gas grid pressure [bar]

$p_{atm}$  – pressure of gas from P2G (atmospheric pressure) = 1 bar

Electrical power for methane compression from the P2G hub to the gas grid in excess to the compression power already used within sole REP and IP when the P2G hub is not present,  $P_{comp,ex}$  is assessed in the following analysis.

Two different connection (IP or REP) possibilities are observed. If  $P_{gas,fix} = P_{gas,IP} - P_{gas,REP}$  is positive, compression is determined using the characteristic given in Figure 7:

Figure 7: Compression if  $P_{gas,IP} - P_{gas,REP} \geq 0$



As it is shown in Fig. 7, compression characteristic has three partitions that can be represented with three conditions. Using (A1.70), accurate value of  $P_{comp,ex}$  is obtained when maximum of all three conditions is found:

$$P_{comp,ex} \geq 0 \quad (A1.72a)$$

$$P_{comp,ex} \geq k_{comp,atm,inter} P_{gas,P2G} \quad (A1.72b)$$

$$P_{comp,ex} \geq 0.0266 \left[ \left( \frac{p_{inter}}{p_{atm}} \right)^{0.23} + \left( \frac{p_{grid}}{p_{inter}} \right)^{0.23} - 2 \right] P_{gas,P2G} - k_{comp,inter,grid} P_{gas,fix} \quad (A1.72c)$$

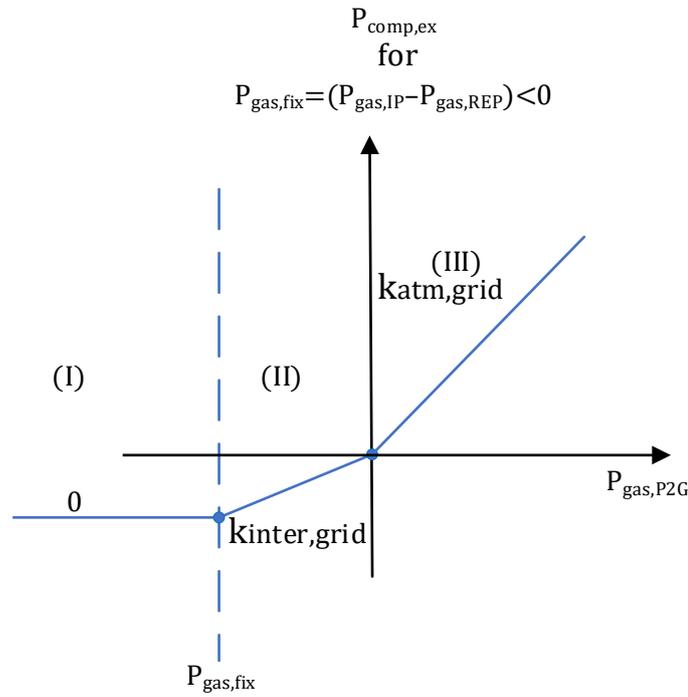
where:

$P_{comp,ex}$

– compression power needed for methane exchange between P2G hub, IP, REP and the grid in excess to the compression power used when P2G hub is not present [kW]

If  $P_{gas,IP} - P_{gas,REP}$  is negative, compression is determined using the characteristic given in Fig. 8:

Figure 8: Power for compression if  $P_{gas,IP} - P_{gas,REP} \leq 0$



Similarly, maximum of each one of the three conditions is needed to obtain the value of  $P_{comp,ex}$ :

$$P_{comp,ex} \geq k_{comp,inter,grid} P_{gas,fix} \quad (A1.73a)$$

$$P_{comp,ex} \geq k_{comp,inter,grid} P_{gas,P2G} \quad (A1.73b)$$

$$P_{comp,ex} \geq k_{comp,atm,grid} P_{gas,P2G} \quad (A1.73c)$$

#### 1.3.2.4 OPERATION COST CALCULATION FOR THE WHOLE PLANT (P2G+REP+IP)

Operation cost of P2G encompasses taking in and providing out of each feedstock and energy carrier during the whole plant (parametrized P2G + the existing REP and IP) exploitation time. To obtain optimal schedule, P2G operation is observed in short time steps (instances) from the beginning to the end of the time horizon. When all unit prices and quantities are included, operation cost can be noted as:

$$C_{\sigma} = \sum_{m=0}^{M-1} [J_{\sigma,el,pow,m}] + \sum_{d=0}^{D-1} [J_{\sigma,BM,dry,d} + J_{\sigma,BM,wet,d} + J_{\sigma,BC,d} + J_{\sigma,heat,d} + J_{\sigma,gas,d} + J_{\sigma,CO2,emiss,d} + J_{\sigma,H2O,grid,d} - J_{\sigma,BC,out,d} - J_{\sigma,H2,out,d} - J_{\sigma,CH4,out,d} - J_{\sigma,O2,out,d} + J_{\sigma,dry,res,d} + J_{\sigma,wet,res,d} + J_{\sigma,GWGS,tar,d}] + \sum_{k=0}^{N-1} [J_{\sigma,el,en}] \quad (A1.74)$$

where:

$M$  = number of months included in the complete time horizon

$D$  = number of slow sampling timesamps (days) included in the complete time horizon

$N$  = number of fast timesamps included in the complete time horizon

Operation cost expression (A1.74) is arranged according to the assessments explained in 1.3.2.1 – 1.3.2.3. Regarding electricity, month period is considered for electrical power operation cost:

$$J_{\sigma,el,pow,m} = p_{\sigma,el,pow} \max\{P_{el,grid}\} \quad (A1.75a)$$

while electrical energy operation cost is calculated for each time step:

$$J_{\sigma,el,en} = \max\{p_{supply,el,en} T_{el} [P_{el,P2G} - (P_{el,REP} - P_{el,IP})], p_{consume,el,en} T_{el} [P_{el,P2G} - (P_{el,REP} - P_{el,IP})]\} \quad (A1.75b)$$

Cost of dry and wet biomass, as well as the cost of biochar are assumed to be constant during one day (24 h). Therefore, dry biomass daily operation cost is:

$$J_{\sigma,BM,dry,d} = \max_{j \in [1,2,\dots,Nsd]} \left\{ \sum_{i=1}^{j-1} p_{i,dry} \dot{M}_{i,dry} T_{day} + p_{j,dry} [\dot{m}_{BM,dry,in} T_{day} - \sum_{i=1}^{j-1} \dot{M}_{i,dry} T_{day}] \right\} \quad (A1.75c)$$

Wet biomass daily operation cost is:

$$J_{\sigma,BM,wet,d} = \max_{j \in [1,2,\dots,Nsw]} \left\{ \sum_{i=1}^{j-1} p_{i,wet} \dot{M}_{i,wet} T_{day} + p_{j,wet} [\dot{m}_{BM,wet,in} T_{day} - \sum_{i=1}^{j-1} \dot{M}_{i,wet} T_{day}] \right\} \quad (A1.75d)$$

Biochar daily operation cost is:

$$J_{\sigma,BC,d} = \max_{j \in [1,2,\dots,NsBC]} \left\{ \sum_{i=1}^{j-1} p_{i,BC} \dot{M}_{i,BC} T_{day} + p_{j,BC} [k_{kg2ton} \dot{m}_{BC,in} T_{day} - k_{day2year} \sum_{i=1}^{j-1} \dot{M}_{i,BC}(d) T_{day}] \right\} \quad (A1.75e)$$

Operation cost for heat is also given for a period of one day:

$$J_{\sigma,heat,d} = \max\{p_{supply,heat} (P_{h,P2G} - (P_{h,REP} + P_{h,IP})) T_{day}, p_{consume,heat} (P_{h,P2G} - (P_{h,REP} + P_{h,IP})) T_{day}\} \quad (A1.75f)$$

Gas operation cost is also considered on the daily scale:

$$J_{\sigma,gas,d} = \max \left\{ p_{supply,gas} \left( (P_{gas,IP} - P_{gas,REP}) - P_{gas,P2G}(d) \right) T_{day}, p_{consume,gas} \left( (P_{gas,IP} - P_{gas,REP}) - P_{gas,P2G} \right) T_{day} \right\} \quad (A1.75g)$$

$$J_{\sigma,CO2,emiss,d} = p_{\sigma,CO2,emiss} M_{CO2} (\dot{n}_{CO2,burn} - \dot{n}_{CO2,store,in}) T_{day} \quad (A1.75h)$$

$$J_{\sigma,H2O,grid,d} = p'_{\sigma,H2} Q_{H2O,grid} T_{day} \quad (A1.75i)$$

$$J_{\sigma,H2,out,d} = M_{H2} p_{\sigma,H2} \dot{n}_{H2,store,out} T_{day} \quad (A1.75j)$$

$$J_{\sigma,BC,out,d} = p'_{\sigma,BC} \dot{m}_{BC,out} T_{day} \quad (A1.75k)$$

$$J_{\sigma,CH4,out,d} = p'_{\sigma,CH4} \dot{n}_{CH4,sell} T_{day} \quad (A1.75l)$$

$$J_{\sigma,O2,out,d} = p'_{\sigma,O2} \dot{n}_{O2,out} T_{day} \quad (A1.75m)$$

$$J_{\sigma,dry,res,d} = p_{\sigma,dry,res} \gamma_{dry,res} \dot{m}_{BM,dry,AD} T_{day} \quad (A1.75n)$$

$$J_{\sigma,wet,res,d} = p_{\sigma,wet,res} \gamma_{wet,res} \dot{m}_{BM,wet,AD} T_{day} \quad (A1.75o)$$

$$J_{\sigma,GWGS,tar,d} = p_{\sigma,tar} k_{TAR} \dot{m}_{BC,GWGS} T_{day} \quad (A1.75p)$$

where:

$p_{\sigma,H2O}$  = price for water from the water grid system [€/m<sup>3</sup>]

$p_{\sigma,CO2,emiss}$  = penalties for CO<sub>2</sub> emission [€/kg]

$p'_{\sigma,H2}$  = selling price of hydrogen (material only; conditioning and transport costs excluded) [€/kg]

$p'_{\sigma,BC}$  = selling price of biochar (only material, transport costs excluded) [€/kg]

$p'_{\sigma,CH4}$   
= selling price of methane for transport (only material, conditioning and transport costs excluded) [€/kg]

$p'_{\sigma,O2}$  = selling price of oxygen (only material, conditioning and transport costs excluded) [€/kg]

$p_{\sigma,dry,res}$  = positive or negative price for residue of dry AD (positive if considered as waste, negative if considered as valuable fertilizer) [€/kg]

$p_{\sigma,wet,res}$  = positive or negative price for residue of wet AD (positive if considered as waste, negative if considered as valuable fertilizer) [€/kg]

$p_{\sigma,tar}$  = cost of management of tar waste from the gasification and water gas shift plant [€/kg]

$M_{CO_2}$  = molar mass of  $CO_2$  =  $44 * 10^{-3}$  [kg/mol]

$M_{H_2}$  = molar mass of  $H_2$  =  $2 * 10^{-3}$  [kg/mol]

All powers, mass and molar rates are average values on the given time interval.

### 1.3.3 ASSESSMENT OF CONNECTION POINT CAPACITIES FOR THE ENTIRE PLANT (P2G+REP+IP)

Electrical, gas and water grid connection capacities for the entire plant configuration (P2G+REP+IP) are to be calculated. As P2G could be added to an existing REP or IP, firstly, capacities of existing REP and IP are provided by the user. Then, according to the OT operation values, possible enlargement of the connection capacity is to be assessed. For the electricity, enlargement capacity is assessed according to the following conditions:

$$P_{el,P2G} + P_{comp,ex} - [P_{el,REP} - P_{el,IP}] - P_{cp,el,exist} \leq \Delta P_{cp,el} \quad (A1.76a)$$

$$-P_{el,P2G} - P_{comp,ex} + [P_{el,REP} - P_{el,IP}] - P_{cp,el,exist} \leq \Delta P_{cp,el} \quad (A1.76b)$$

To reduce calculation burden and add robustness in the parametrized P2G operation, (A1.76a) is adjusted to obtain maximal electricity consumption while (A1.76b) is adjusted to obtain maximal electricity production. Accordingly, to obtain maximal consumption, maxima of all electricity consuming processes are added while processes that produce electricity (CHP and FC) are excluded:

$$\begin{aligned} & \max(P_{el,electrolyzer}) + \max(P_{el,cc}) + \max(P_{el,AD,dry}) + \max(P_{el,AD,wet}) + \max(P_{el,BM,dry2BC}) \\ & + \max(P_{el,BM,wet2BC}) + \max(P_{el,GWGS}) + \max(P_{el,meth}) + \max(P_{el,demin}) \\ & + \max(P_{comp,ex}) + \max\{P_{el,IP} - P_{el,REP}\} - P_{cp,el,exist} \leq \Delta P_{cp,el} \end{aligned} \quad (A1.77)$$

Maximal electricity production is obtained when only maximum of CHP/FC are considered:

$$\max(P_{el,CHP} + P_{el,FC}) + \max\{P_{el,REP} - P_{el,IP}\} - P_{cp,el,exist} \leq \Delta P_{cp,el} \quad (A1.78)$$

From (A1.10), (A1.12a) and (A1.13a) the following expressions for  $P_{el,CHP}$  and  $P_{el,FC}$  can be derived:

$$P_{el,CHP} = \eta_{el,CHP}(1-x)P_{total,CHP/FC} = \eta_{el,CHP}(1-x)k_{CH_4}\dot{m}_{CH_4,CHP/FC} + \eta_{el,CHP}(1-x)k_{BG}\dot{m}_{BG,CHP/FC} + \eta_{el,CHP}(1-x)k_{H_2}\dot{m}_{H_2,CHP/FC} \quad (A1.79a)$$

$$P_{el,FC} = \eta_{el,FC}xP_{total,CHP/FC} = \eta_{el,FC}xk_{CH_4}\dot{m}_{CH_4,CHP/FC} + \eta_{el,FC}xk_{BG}\dot{m}_{BG,CHP/FC} + \eta_{el,FC}xk_{H_2}\dot{m}_{H_2,CHP/FC} \quad (A1.79b)$$

To obtain CHP and FC altogether, (A1.79a) and (A1.79b) are added:

$$P_{el,CHP/FC} = P_{el,CHP} + P_{el,FC} = [\eta_{el,CHP}(1-x) + \eta_{el,FC}x]k_{CH4}\dot{m}_{CH4,CHP/FC} + [\eta_{el,CHP}(1-x) + \eta_{el,FC}x]k_{BG}\dot{m}_{BG,CHP/FC} + [\eta_{el,CHP}(1-x) + \eta_{el,FC}x]k_{H2}\dot{m}_{H2,CHP/FC} = \eta_{el,CHP/FC}k_{CH4}\dot{m}_{CH4,CHP/FC} + \eta_{el,CHP/FC}k_{BG}\dot{m}_{BG,CHP/FC} + \eta_{el,CHP/FC}k_{H2}\dot{m}_{H2,CHP/FC} \quad (A1.80)$$

It could be easily seen that efficiencies within (A1.80) can be summarized in common efficiency parameter:

$$\eta_{el,CHP/FC} = [\eta_{el,CHP}(1-x) + \eta_{el,FC}x] \quad (A1.81a)$$

Similarly, common CHP/FC investment ( $p_{i,CHP/FC}$ ) unit price can be derived from the CHP investment unit price ( $p_{i,CHP}$ ) and FC investment price ( $p_{i,FC}$ ):

$$p_{i,CHP/FC} = [p_{i,CHP}(1-x) + p_{i,FC}x] \quad (A1.81b)$$

Now, using expressions for each of the P2G subunits and maximal values of P2G processes as they are given in chapter in 1.2 as well as (A1.80) the system (A1.77) - (A1.78) is noted as:

$$\frac{E_s}{\eta_{el}}\dot{N}_{H2,store,in} + k_{el,CC}\dot{N}_{CC} + k_{el,AD,dry}\dot{M}_{BM,dry,AD} + k_{el,AD,wet}\dot{M}_{BM,wet,AD} + k_{el,BM,dry,2BC}\dot{M}_{BM,dry,2BC} + k_{el,BM,wet,2BC}\dot{M}_{BM,wet,2BC} + k_{el,GWGS}\dot{M}_{BC,GWGS} + k_{el,meth}\dot{N}_{meth,M} + k_{el,demin}\dot{N}_{H2O,grid} + P_{comp,ex,M} + \max\{P_{el,IP} - P_{el,REP}\} - P_{cp,el,exist} \leq \Delta P_{cp,el} \quad (A1.82a)$$

$$k_{CH4}\eta_{el,CHP/FC}\dot{M}_{CH4,CHP/FC} + k_{BG}\eta_{el,CHP/FC}\dot{M}_{BG,CHP/FC} + k_{H2}\eta_{el,CHP/FC}\dot{M}_{H2,CHP/FC} + \max\{P_{el,REP} - P_{el,IP}\} - P_{cp,el,exist} \leq \Delta P_{cp,el} \quad (A1.82b)$$

where:

$P_{el,P2G}, P_{el,REP}, P_{el,IP}$   
= P2G, REP, IP electrical power at each electricity sampling interval (mean value on the interval) [kW]

$P_{cp,el,exist}$  = existing electrical connection capacity (nominal value) [kW]

$\Delta P_{cp,el}$  = enlargement of the electrical connection capacity [kW]

$P_{comp,ex,M}$  = maximum of all  $P_{comp,ex}$  [kW]

Since all maxima are obtained as separate variables in the optimization problem and since REP and IP profiles are known a priori, it is easy to see that system (A1.82) gives only two inequalities for the optimization problem.

Enlargement of the electrical connection capacity obtained by conditions (A1.82a), (A1.82b) can only be non-negative:

$$\Delta P_{cp,el} \geq 0 \quad (A1.83)$$

For the gas connection, enlargement capacity assessment is based on aggregated hourly transport of gas. Similar to electricity, both positive and negative options are considered:

$$P_{gas,IP} - P_{gas,REP} - P_{gas,P2G} - P_{cp,gas,exist} \leq \Delta P_{cp,g} \quad (A1.84a)$$

$$-(P_{gas,IP} - P_{gas,REP} - P_{gas,P2G}) - P_{cp,gas,exist} \leq \Delta P_{cp,g} \quad (A1.84b)$$

where:

$P_{gas,P2G}, P_{gas,IP}, P_{gas,REP}$  = P2G, IP, REP average gas power in one day (24h) [kWh/h]

$P_{cp,gas,exist}$  = existing gas connection capacity [kWh/h]

$\Delta P_{cp,g}$  = enlargement of the gas connection capacity [kWh/h]

Enlargement of the gas connection capacity obtained by conditions (A1.84a), (A1.84b) can only be non-negative:

$$\Delta P_{cp,g} \geq 0 \quad (A1.85)$$

For the water connection, enlargement capacity is maximum of P2G water grid consumption:

$$\max_{days} Q_{H2O,grid} = \frac{\dot{N}_{H2O,grid}}{k_{H2O}} = \Delta Q_{cp,w} \quad (A1.86)$$

where:

$Q_{H2O,grid}$  = water consumption of P2G in one day (24h) [m<sup>3</sup>/h]

$\Delta Q_{cp,w}$  = enlargement of the water connection capacity [m<sup>3</sup>/h]

### 1.3.4 INVESTMENT COST

Investment cost includes costs of all assembly parts of the P2G hub and costs of additional investments in grid connection points. In the following expression, per unit assembly costs are given as  $p_{i,x}$ . Accordingly, total investment cost is noted:

$$\begin{aligned} C_{invest} = & p_{i,mBM,dry,store} M_{BM,dry,store} + p_{i,mBM,wet,store} M_{BM,wet,store} + p_{i,mBCstore} M_{BC,store} + \\ & + p_{i,dotmBM,dry,2BC} \dot{M}_{BM,dry,2BC} + p_{i,dotmBM,wet,2BC} \dot{M}_{BM,wet,2BC} + p_{i,dotmGWGS} \dot{M}_{BC,GWGS} + \\ & p_{i,dotm,dry,AD} \dot{M}_{BM,dry,AD} + p_{i,dotm,wet,AD} \dot{M}_{BM,wet,AD} + p_{i,CHP/FC} P_{el,CHP/FC} + p_{i,dotnCC} \dot{N}_{CC} + \\ & p_{i,nCO2store} N_{CO2,store} + p_{i,nH2store} N_{H2,store} + p_{i,nO2store} N_{O2,store} + p_{i,H2Ostore} N_{H2O,store} + \\ & p_{i,nCH4store} N_{CH4,store} + p_{i,HE} P_{h,HE,max} + p_{i,electrolyser} P_{el,el,M} + p_{i,dotnMethreactor} \dot{N}_{meth,M} + \\ & \left( p_{i,el,demin} + p_{i,cp,w} \frac{1}{k_{el,demin} k_{H2O}} \right) P_{el,demin,M} + p_{i,Adrain} A_{drain} + p_{i,nSGstore} N_{SG,store} + \\ & + p_{i,nBGstore} M_{BG,store} + p_{i,cp,el} \Delta P_{cp,el} + p_{i,cp,g} \Delta P_{cp,g} + p_{i,comp} P_{comp,ex,M} \quad (A1.87) \end{aligned}$$

In the (A1.87), unit assembly costs “ $p_{i,x}$ ” are multiplied by the maximum values of assembly parts. Those maximums are directly obtained during the optimization process.

Except from  $P_{el,CHP/FC}$  that is calculated according to the (A1.80), the values of all other capacities are obtained using the following expressions:

$$M_{BM,dry,store} = \max(\dot{m}_{BM,dry,in}T_{day}, m_{BM,dry,store}) \quad (A1.88a)$$

$$M_{BM,wet,store} = \max(\dot{m}_{BM,wet,in}T_{day}, m_{BM,wet,store}) \quad (A1.88b)$$

$$M_{BC,store} = \max(\dot{m}_{BC,store,in}T_{day}, \dot{m}_{BC,store,out}T_{day}, m_{BC,store}) \quad (A1.88c)$$

$$\dot{M}_{BM,dry,2BC} = \max(\dot{m}_{BM,dry,2BC}) \quad (A1.88d)$$

$$\dot{M}_{BM,wet,2BC} = \max(\dot{m}_{BM,wet,2BC}) \quad (A1.88e)$$

$$\dot{M}_{BC,GWGS} = \max(\dot{m}_{BC,GWGS}) \quad (A1.88f)$$

$$\dot{M}_{BM,dry,AD} = \max(\dot{m}_{BM,dry,AD}) \quad (A1.88g)$$

$$\dot{M}_{BM,wet,AD} = \max(\dot{m}_{BM,wet,AD}) \quad (A1.88h)$$

$$\dot{N}_{CC} = \max(\dot{n}_{CO_2,store,in}) \quad (A1.88i)$$

$$N_{CO_2,store} = \max(n_{CO_2,store}) \quad (A1.88j)$$

$$N_{H_2,store} = \max(n_{H_2,store}) \quad (A1.88k)$$

$$N_{O_2,store} = \max(n_{O_2,store}) \quad (A1.88l)$$

$$N_{H_2O,store} = \max(n_{H_2O,store}) \quad (A1.88m)$$

$$N_{CH_4,store} = \max(n_{CH_4,store}) \quad (A1.88n)$$

$$P_{heat,HE,M} = \max(P_{heat,HE}) \quad (A1.88o)$$

$$P_{el,electrolyzer,M} = \max(P_{el,electrolyzer}) \quad (A1.88p)$$

$$\dot{N}_{meth,M} = \max(\dot{n}_{CH_4,metH} + \dot{n}_{CH_4,BG}) \quad (A1.88q)$$

$$P_{el,demin,M} = \max(P_{el,demin}) \quad (A1.88r)$$

$$\dot{N}_{CH_4,out} = \max(\dot{n}_{CH_4,out}) \quad (A1.88s)$$

$$P_{gas,P2G,M} = \max(P_{gas,P2G}) \quad (A1.88t)$$

$$N_{SG,store} = \max(n_{SG,store}) \quad (A1.88u)$$

$$M_{BG,store} = \max(m_{BG,store}) \quad (A1.88v)$$

Although referenced costs are given in 3. Determination of coefficients and prices, here are default unit cost values for each one:

$$p_{i,mBM,dry,store} = 10 \text{ [€/kg]}$$

$$p_{i,mBM,wet,store} = 5 \text{ [€/kg]}$$

$$p_{i,mBC,store} = 15 \text{ [€/kg]}$$

$$p_{i,dotmBM,dry,2BC} = 0.6 * 10^6 \text{ [€/kg/s]}$$

$$p_{i,dotmBM,wet,2BC} = 0.7 * 10^6 \text{ [€/kg/s]}$$

$$p_{i,dotmGWGS} = 1 * 10^6 \text{ [€/kg/s]}$$

$$p_{i,dotm,dry,AD} = 21 * 10^6 \text{ [€/kg/s]}$$

$$p_{i,dotm,wet,AD} = 20 * 10^6 \text{ [€/kg/s]}$$

$$p_{i,CHP,per,kW} = 3000 \text{ [€/kWe]}$$

$$p_{i,FC,per,kW} = 5000 \text{ [€/kWe]}$$

$$p_{i,dotnCC} = 8 * 10^4 \text{ [€/mol/s]}$$

$$p_{i,nCO2store} = 0.45 \text{ [€/mol]}$$

$$p_{i,nH2store} = 10 \text{ [€/mol]}$$

$$p_{i,nO2store} = 0.625 \text{ [€/mol]}$$

$$p_{i,H2Ostore} = 0.02 \text{ [€/mol]}$$

$$p_{i,nCH4store} = 1.25 \text{ [€/mol]}$$

$$p_{i,HE} = 100 \text{ [€/kW]}$$

$$p_{i,electrolyser} = 2500 \text{ [€/kW]}$$

$$p_{i,dotnMethreactor} = 4.25 * 10^5 \text{ [€/mol/s]}$$

$$p_{i,el,demin} = 100 \text{ [€/mol/s]}$$

$$p_{i,Adrain} = 2 \text{ [€/m}^2\text{]}$$

$$p_{i,nSGstorage} = 1.25 \text{ [€/mol]}$$

$$p_{i,nBGstorage} = 1.25 \text{ [€/mol]}$$

$$p_{i,comp} = 600 \text{ [€/kW]}$$

Cost of electrical, gas and water connections depend on scale of grid (transmission or distribution) that is used for P2G connection as well as on the particular country of the Danube region.

The OT offers an option to include investment subsidies as a percentage, not only for the overall investment, but also for each individual part. Therefore, final investment cost is reduced depending on the subsidies.

### 1.3.5 DEGRADATION COST

The OT takes into account the degradation of each part of the P2G hub, except for the connections (electrical grid, gas grid, water grid). After the set number of years, it is assumed that parts of the P2G hub need to be replaced, which is the base for the calculation of the degradation cost.

For each P2G assembly part given in (A1.88), degradation factor  $p_{deg,*}$  is calculated as:

$$p_{deg,*} = \frac{1}{N_{lifetime,*}} p_{i,*} \quad (A1.89)$$

where:

$N_{lifetime,*}$  = expected lifetime of the assembly part (given in years) = 20 years (default value)

$p_{i,*}$  = unit cost of assembly part as used in (A1.87)

Total equipment degradation cost is calculated as a sum of all degradation costs:

$$C_{deg} = \sum_* p_{deg,*} \cdot * \quad (A1.90)$$

When calculating the degradation cost, the OT does not include investment subsidies, but the full price of each of the parts.

## 1.4 FORMULATION OF THE MATHEMATICAL PROGRAM FOR OPTIMIZATION

### 1.4.1 OPTIMIZATION PROBLEM

Using previously calculated costs; (A1.74) for operation, (A1.87) for investment, (A1.90) for degradation, the following cost optimization for the plant is formulated:

$$\min \frac{C_{invest}}{N_{Years}} + C_{deg} + C_{\sigma} \quad (A1.91)$$

To complete mathematical problem, minimisation (A1.91) is constrained with the investment pay-off period. Within this pre-set number of years, the plant operation is to satisfy:

$$\frac{C_{invest}}{N_{Years}} + C_{deg} + C_{\sigma} \leq C_{\sigma}(P2G \equiv 0) \quad (A1.92)$$

where:

$N_{Years}$  = maximum payoff period (given in years)

$C_{\sigma}(P2G \equiv 0)$  – operational cost of the plant (A1.74) without P2G operation

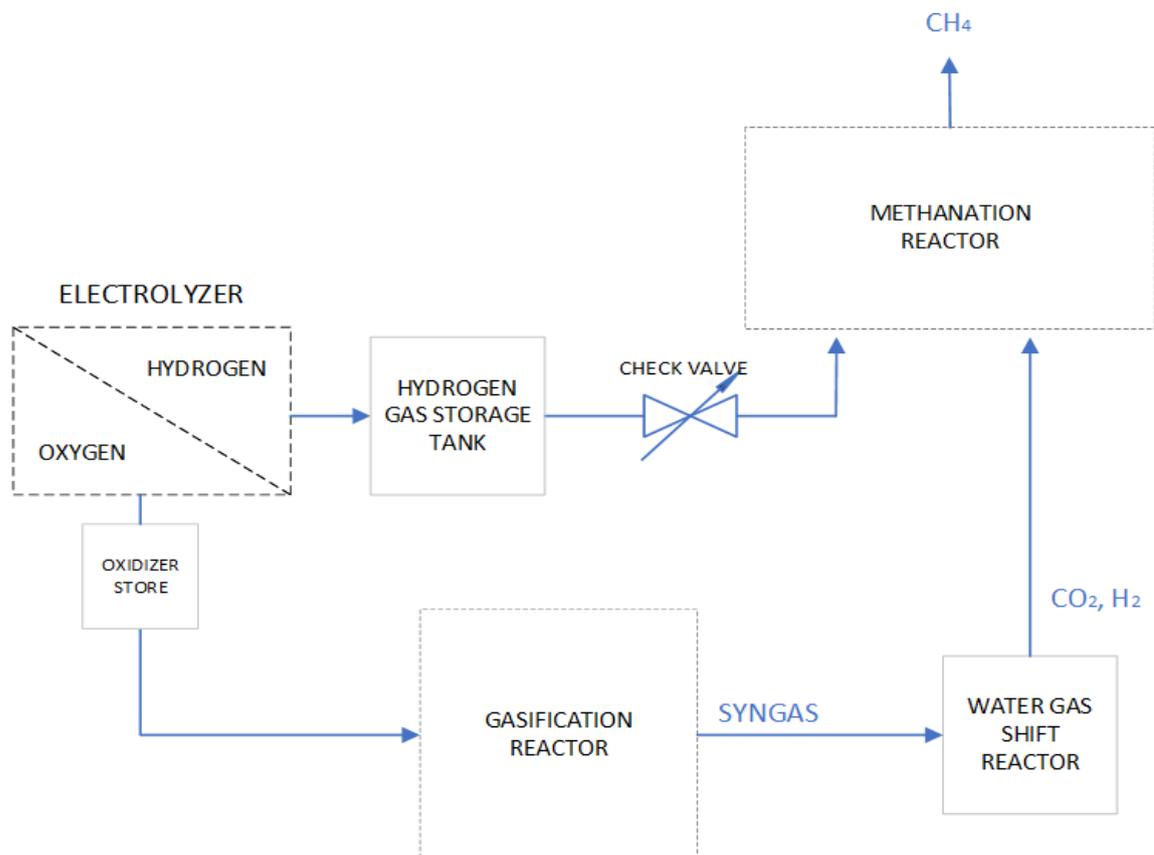
At first, concept modelling equations are to be used to obtain a classical linear dynamic system suitable for an optimization solver. Then, with respect to all mentioned limitations and with the given unit costs and prices, variable manipulation is done to obtain minimization of (A1.91). Finally, result of minimization will give the answer on feasibility of the concept under the given circumstances.

## 2. BIOCHAR BASED POWER TO GAS PLANT

### 2.1 PROCESSES IN BIOCHAR BASED POWER TO GAS PLANT

Biochar power to gas plant comprises several processes. In the Figure 1, gasification (gasifier and water gas shift reactors), electrolysis (electrolyser and hydrogen gas storage) and methanation processes are depicted, as well as their interconnection.

Figure 9: Processes of Biochar Power to Gas Plant



### 2.2 GASIFICATION

Gasification is the oxidation with insufficient oxidizer supply. Instead of producing CO<sub>2</sub> during complete oxidizing (combustion), gasification of the carbon fuel ends up in CO

production. Similarly, gasification of the hydrogen fuel ends up in  $H_2$  production, while combustion leads to  $H_2O$ . During gasification fuel is blown through oxidizer. Usually air, water vapor,  $CO_2$  and oxygen are used as oxidizers. There are many types of gasifier reactors: fixed bed, fluidized bed, entrained flow etc. With different gasifier designs, different models of heat exchange between fuel and oxidizer are obtained. In the first step of gasification, oxygen from electrolysis is used as oxidizer and biochar is used as fuel for syngas production. Temperature of the gasifier is high: between 1000-1500 K [1-2], and according to the literature [3-4] gasification is assumed to be an adiabatic process. In the next step, water gas shift bubble column vessel is used to obtain  $CO_2$  for methanation, from CO.

### **2.3 WATER GAS SHIFT IN BUBBLE COLUMN VESSEL**

Syngas produced in the first step of gasification goes to bubble column vessel where water gas shift reaction, occurs. Temperatures in the bubble column are much lower (400-600 K) than temperatures in the gasifier, which enables a high conversion rate of CO into  $CO_2$ . Water supply is needed to support this reaction.

### **2.4 ELECTROLYSIS**

Power to gas plant uses hydrogen to accomplish an upgrade of hydrocarbon gases. Hydrogen is produced in electrolyser by electrolysis of demineralized water. Electrical energy is to be consumed during this process. The intention is to use low-cost electrical energy for hydrogen production. Due to fluctuation of electrical energy prices on the market, it is possible to use few types [5] of electrolysers. Classical option and the cheapest one is alkaline electrolyser. But there are drawbacks in exploitation of alkaline electrolyser. It is limited by minimum operating power and slow starting performance. There is also ecological issue due to decomposing its electrolyte. Proton exchange membrane (PEM) electrolyser performance is much faster, and it has much wider operating range. There is also solid oxide electrolyser (SOEC) type to be exploited commercially in the future. This one operates at higher temperatures and has a potential to increase the efficiency of electrolysis.

### **2.5 METHANATION**

Biological methanation is a process of methane production and is a key process in P2G plant. This process takes place in methanation reactor in which aquatic solution with microorganisms is formed to enable methane production. There are three major types of methanation reactors: stirred tank reactor, trickle-bed reactor, and bubble column gas-lift reactor. To produce methane, it is necessary to take gaseous carbon. Except from carbon feedstock, methanation reactor takes gaseous  $H_2$ . In biological methanation reactor, each feedstock gas is firstly dissolved in water and then chemical reactions for methane production begin. Solubility of gases, especially solubility of  $H_2$  is usually a bottleneck in this process. So called gas-liquid mass transfer rate depends on

technological details. There are several paths of chemical reactions that lead to methane production. Accordingly, methanogenic potential could be defined as: hydrogenotrophic, acetoclastic, carboxydrotrophic. In this work, bubble column reactor with methanogenic hydrogenesis is considered.

Methanation reaction occurs in the methanation reactor, more precisely in its liquid phase:



Ideal stoichiometric values of reactants are  $H_2 : CO_2 = 4 : 1$ .

### 3. DETERMINATION OF COEFFICIENTS AND PRICES

#### 3.1.1 ASSESSMENT OF ANAEROBIC DIGESTION

Conversion coefficients for AD process are set to the following values:

$$\alpha_{dry} = \text{coefficient of biomass to biochar conversion during dry AD} = 0.07 [6]$$

$$\alpha_{wet} = \text{coefficient of biomass to biochar conversion during wet AD} = 0.05 [6]$$

$$\gamma_{dry} = \text{conversion coefficient of dry biomass mass to biogas amount during AD} = 0.9 [7]$$

$$\gamma_{wet} = \text{conversion coefficient of wet biomass mass to biogas amount during AD} = 0.8 [7]$$

Molar fraction in the biogas:

$$s'_M = \text{molar fraction of } CH_4 \text{ in biogas [8]} = 0.6$$

$$s'_C = \text{molar fraction of } CO_2 \text{ in biogas [8]} = 0.4$$

is used to obtain biogas molar mass:

$$M_{BG} = \text{molar mass of biogas (60\% } CH_4, 40\% CO_2) = 0.027 [\text{kg/mol}]$$

While general knowledge of residues is not common to be known, residues of the AD processes are set to zero values:

$$\gamma_{dry,res} = 0$$

$$\gamma_{wet,res} = 0$$

For the wet AD process, [8] gives data on biogas flow rate of 1851 kg/day together with its electricity and heat consumption of 4 kW and 6,4 kW respectively. From the given data, electricity and heat consumption coefficients can be obtained:

$$k_{el,wet,AD} = \text{electrical coefficient of wet AD} = 186,7 \gamma_{wet} \left[ \frac{\text{kW}}{\left(\frac{\text{kg}}{\text{s}}\right)_{wet,biomass}} \right]$$

$$k_{h,wet,AD} = \text{electrical coefficient of dry AD} = 300 \gamma_{wet} \left[ \frac{\text{kW}}{\left(\frac{\text{kg}}{\text{s}}\right)_{wet,biomass}} \right]$$

Similar coefficients can be used for dry biomass:

$$k_{el,dry,AD} = \text{electrical coefficient of wet AD} = 186,7 \gamma_{dry} \left[ \frac{\text{kW}}{\left(\frac{\text{kg}}{\text{s}}\right)_{dry,biomass}} \right]$$

$$k_{h,dry,AD} = \text{electrical coefficient of dry AD} = 300 \gamma_{dry} \left[ \frac{\text{kW}}{\left(\frac{\text{kg}}{\text{s}}\right)_{wet,biomass}} \right]$$

According to the [9], cost of AD of about 2700 €/kW<sub>e</sub> can be considered. Using the calorific value of biomass, price of dry AD can be calculated:

$$p_{i,dotm,dry,AD} = 21.6 * 10^6 \text{ [€/(kg/s)]}$$

Similar cost value can be used for wet biomass.

### 3.1.2 ASSESSMENT OF BIOMASS2BIOCHAR

Conversion coefficients for BM2BC process are set to the following values:

$$\beta_{dry} = \text{coefficient of biomass to biochar conversion during dry BM2BC} = 0.3 \text{ [10]}$$

$$\beta_{wet} = \text{coefficient of biomass to biochar conversion during wet BM2BC} = 0.2 \text{ [10]}$$

For BM2BC processes, [11] gives electricity consumption that is used to obtain:

$$k_{el,BMdry2BC} = \text{electrical coefficient of dry BM2BC} = 8700 \left[ \frac{\text{kW}}{\left(\frac{\text{kg}}{\text{s}}\right)_{dry,biomass}} \right]$$

and investment cost for dry process is [12]:

$$p_{i,dotm,BMdry2BC} = 0.6 * 10^6 \text{ [€/(kg/s)]}$$

Due to the moisture, investment for wet BM2BC needs to be enlarged while heat import is again not needed.

### 3.1.3 ASSESSMENT OF GWGS

Molar mass of syngas  $M_{SG}$  is calculated using biomass gasification analysis [13] and typical syngas composition after WGS [14]. Syngas mole fraction of  $H_2$  ( $g'_1$ ) and  $CO_2$  ( $g'_2$ ) after WGS is found to be:

$$g'_1 = \frac{3}{5}; g'_2 = \frac{2}{5}$$

Accordingly, molar mass of syngas can be calculated to be:

$$M_{SG} = 0.018 \text{ kg/mol}$$

While there is no significant loss of mass during gasification, mass efficiency of biochar to syngas conversion is assumed to be:

$$\eta_{BC \rightarrow SG} = 0,9$$

while default value of tar content is set to zero:

$$k_{TAR} = 0$$

Needed water supply for gasification alone can be found in [15], while water needed for WGS can be determined according to the stoichiometry of the WGS reaction:

$$k_{H_2O, GWGS} = 0.4075$$

According to [16], stoichiometry number of oxygen in gasification is assumed to be:

$$v_2 \approx 0.2$$

In the [17] efficiency of the GWGS as two stage gasification process is given. Accordingly, sum of electrical and heat energy needed for GWGS could be calculated. As the exact ratio between electricity and heat is not known, coefficients are set to be equal:

$$k_{el, GWGS} = \text{electrical coefficient of GWGS} = 100 \left[ \frac{\text{kW}}{(\text{kg/s})} \right]$$

$$k_{h, GWGS} = \text{heat coefficient of GWGS} = 100 \left[ \frac{\text{kW}}{(\text{kg/s})} \right]$$

Regarding investment cost, using [17] the following value of GWGS is obtained:

$$p_{i, dotmGWGS} = 1 * 10^6 \text{ [€/(kg/s)]}$$

### 3.1.4 ASSESSMENT OF CHP AND FC

Amount of liquid water that can be obtained during FC operation, according to the [18], can be found to be:

$$\eta_{FC,H_2O} = 0.001.$$

Regarding allowed amount of hydrogen in biogas, according to [19] the following value is set:

$$\alpha_{H_2} = 0.2.$$

In the [20] efficiencies and investment cost for CHP as well as investment cost for FC are given. In the [21] efficiency of FC could be found. Accordingly, the following values of efficiencies are obtained:

$$\eta_{el,CHP} = 0,4$$

$$\eta_{h,CHP} = 0,5$$

$$\eta_{el,FC} = 0,5$$

$$\eta_{h,FC} = 0,45$$

Regarding investment costs, the following is obtained:

$$p_{i,CHP,per,kW} = 3000 \text{ [€/kW}_e\text{]}$$

$$p_{i,FC,per,kW} = 5000 \text{ [€/kW}_e\text{]}$$

### 3.1.5 ASSESSMENT ELECTROLYSIS

Although there are various different literature sources, efficiency of electrolyser is set to:

$$\eta_{el,electrolyzer} = \text{efficiency of electrolysis} = 0.7 \text{ [22]}$$

According to the efficiency, heat coefficient of electrolyser is calculated:

$$k_{h,el} = \text{heat coefficient of electrolysis} = 32 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$$

For electrolyser cost, an average value is used:

$$p_{i,electrolyser} = 2500 \text{ [€/kW]}.$$

### 3.1.6 ASSESSMENT OF CARBON CAPTURE

In the [23] Carbon Capture unit, its energy balance and investment cost is given. Accordingly, heat consumption can be calculated to be:

$$k_{h,CC} = \text{heat coefficient Carbon Capture} = 170 \left[ \frac{\text{kW}}{\text{(mol/s)}} \right]$$

Electricity consumption is estimated to be:

$$k_{el,CC} = \text{electrical coefficient of Carbon Capture} = 20 \left[ \frac{\text{kW}}{(\text{mol/s})} \right]$$

Investment cost of Carbon Capture is calculated to be:

$$p_{i,dotnCC} = 8 * 10^4 \text{ [€/(mol/s)]}$$

### 3.1.7 ASSESSMENT OF DEMINERALIZATION

Internet gives few commercial examples of demineralization units. According to the given value of the flow and price of the unit, electricity coefficient and cost parameter can be easily assessed:

$$k_{el,demin} = \text{electrical coefficient of demineralization} = 7.5 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$$

$$p_{i,demin} = 100 \text{ [€/(mol/s)]}$$

### 3.1.8 ASSESSMENT OF METHANATION

Total energy efficiency can be calculated according to the expression given in [24]. Literature [25] gives heat production of the biological methanation reactor. With the known LHV values of input hydrogen and output methane, efficiency value of about 60 percent [26] as well as produced heat power, it is possible to calculate electrical consumption power. Accordingly, the following coefficients are obtained:

$$k_{el,meth} = \text{electrical coefficient of methanation} = 800 \left[ \frac{\text{kW}}{\text{mol/s}} \right]$$

$$k_{h,meth} = \text{heat coefficient of methanation} = 250 \left[ \frac{\text{kW}}{\text{mol/s}} \right].$$

According to the [27], cost of methanation reactor is 500 €/kW<sub>CH<sub>4</sub></sub>. This is used to calculate its cost of about:  $p_{i,dotnMethreactor} = 4.25 * 10^5 \text{ [€/(mol/s)]}$

### 3.1.9 ASSESSMENT OF STORAGES

As it is given in [28], hydrogen storage in P2G application is operating at low pressure. As its price is also estimated in [28], it is easy to obtain cost parameter for hydrogen storage:

$$p_{i,nH2storage} = 10 \text{ [€/mol]}$$

In similar way, costs of other gas storages are obtained:

$$p_{i,nCH4storage} = 1.25 \text{ [€/mol]}$$

$$p_{i,nBGstorage} = 1.25 \text{ [€/mol]}$$

$$p_{i,nSGstorage} = 1.25 \text{ [€/mol]}$$

$$p_{i,nO2storage} = 0.625 \text{ [€/mol]}$$

$$p_{i,nCO2storage} = 0.45 \text{ [€/mol]}$$

### **3.1.10 ASSESSMENT OF COMPRESSION, HEAT EXCHANGER AND DRAINAGE AREA**

According to the internet research and various assumptions, for the rest of the equipment the following investment costs can be assumed:

$$p_{i,comp} = 600 \text{ [€/kW]}$$

$$p_{i,HE} = 100 \text{ [€/kW]}$$

$$p_{i,Adrain} = 2 \text{ [€/m}^2\text{]}$$

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