Deliverable 3.3

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KPA Calculator

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Approvals

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DISCLAIMER OF WARRANTIES

ABBREVIATIONS

BFW	Boiler feed water
CPP	Control process parameter
HPS	High pressure steam
IPS	Intermediate pressure steam
KPA	Key performance attribute
KRI	Key resource indicator
LHV	Lower heating value
LPG	Liquid petroleum gas
LPS	Low pressure steam
M&C	Monitoring and control
MPS	Medium pressure steam
RGC	Raw gas compressor
SH	High pressure steam
SHH	High high pressure steam
SL	Low pressure steam
SLL	Low low pressure steam
SM	Medium pressure steam
TLE	Transfer line exchanger
WP	Work package

EXECUTIVE SUMMARY

This report presents a summary of the work performed under the Task 3.3 "*Development of a KPA calculator"*.

Every productive processes found in an industry own series of parameters (operational conditions, feeding requirements, etc.) that should be fulfilled in order to obtain a desired product. As a result of the work developed in tasks 3.2 and 3.3, included in the Deliverable 3.2, a set of parameters able to ensure that the final product characteristics match to the cost, production rates, quality, safety, resource efficiency expected while minimising the environmental impacts of the considered process (that usually will be required by regulation) have been selected for each of the demo sites. These parameters are known as the *Key Performance Attributes, KPAs.*

Once these KPAs are found, the next step is to develop a system enabling the identification of the values of these KPAs in real time or after running a simulation model to a plant operator or manager. Then depending on the value of the KPAs, the operator or manager would be able to modify the value of the Critical Process Parameters, CPPs, in order to find new working conditions that ensure the correct KPAs values. This system is a *KPA calculator* that must provide the KPA values and whether the values are in a valid range.

The deliverable 3.3 is divided into three parts:

- Description of the characteristics of an easy-to-handle KPA calculator based on MS EXCEL®.
- Description of the functional specifications of the KPA calculator (inputs, outputs and constraints) for the three demo sites associated with the project TOP-REF (FERTINAGRO, DCI and PETROGAL).
- Development of an example of KPA calculator for some processes of these demo sites.

The final aim of this task and deliverable was to define the aim, scope and characteristics that an easy-to-handle KPA calculator should have. In addition, an example of how a KPA calculator based on MS EXCEL® of DCI and PETROGAL's thermal processes and for the overall processes of FERTINAGRO looks like was developed. This KPA calculator example was built from very simplified models and easy equations, so the obtained KPAs values will be very rough.

The use of a KPA calculator can be extrapolated to any industrial sector or facility as a method to ensure that the changes in the working conditions do not affect to the characteristics of the final products. This line of work is also aligned with Key Actions 2.3 (Process monitoring, control and optimization) and 6.1 (Analysis and establishment of efficient technology dissemination methodologies, mechanisms and frameworks) of SPIRE.

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1 INTRODUCTION

The aim of this deliverable linked to the task 3.3 is to define the characteristics of an easy-to-handle KPA calculator based on MS EXCEL®. This task is part of the Work Package 3. One of the main aims of the Work Package 3 (Processes Performance Diagnosis) of the TOP-REF project is to carry out an identification of the main attributes that represent the most relevant constraints and requirements for their respective end and intermediate products. One of the more specific objectives is to break down the product requirement found, in order to determine the KPAs of each process. An additional objective is to stablish the basis for a tool that will be useful as a manner to represent the results of the simulations developed in the Work package 4.

In addition, another aim of the deliverable is to determine the inputs and outputs needed to design a KPA calculator for all the industrial partners in the framework of the TOP-REF project. Because of the inherent characteristic of the KPAs, every industrial facility should have a different KPA calculator because inputs parameters and the KPAs will be different. However, the use of a KPA calculator will help to avoid different ways of calculating the corresponding KPAs within the whole TOP-REF project.

The software MS EXCEL® has been chosen for developing the KPA calculator because of its degree of diffusion and ease of implementation. The KPA calculator provides the input fields for the required data to calculate the KPAs.

Two alternative possibilities have been evaluated: obtaining the information from a mathematical simulation model or from an online monitoring & control system. In both cases, the KPA calculator is intended to gather the required information to calculate and show the values of the KPAs.

In the case of the use of a mathematical model, two additional possibilities can be found: a simple mathematical simulation model integrated in the KPA calculator and an autonomous complex and detailed mathematical simulation model that exports the information to the KPA calculator. In the first case, the mathematical simulation model is simple enough to be included in the KPA calculator. In this case, the KPA calculator will present proper fields to introduce the information required by the simulation model and at the same time will provide the values of the KPAs and whether the values are in the correct range. In the second case, the KPA calculator will use the output of an external mathematical simulation model as an input and just will provide the values of the KPAs and whether they are in range or not.

In the case of being linked to a monitoring and control (M&C) system, the KPA calculator should be able to communicate with the M&C system online and in real time in order to obtain the inputs for calculating the KPAs as in the second case of the use of a mathematical model.

Because those complete and robust mathematical models will be developed during Work package 4 (models are not yet developed), up to now, in this deliverable it is not possible to develop a complete KPA calculator that is able to connect with process models or with a M&C system (related to the Work package 5). Instead of this, three examples of KPA calculators with simple mathematical simulation models integrated in the KPA calculator have been developed:

- A KPA calculator able to simulate the operation of the boiler and the dryer of FERTINAGRO;
- A KPA calculator able to simulate the operation of the boiler that produces the SHH steam used in the steam grid of DCI;
- A KPA calculator able to simulate the operation of one of the gas turbine that produces power to be sold and the operation of the cogeneration boiler fed by the exhaust gases of the gas turbine of PETROGAL.

These mathematical models used for developing the examples are simple enough to show how a KPA calculator works but not enough complete to provide reliable values in order to take decisions about the operation of the plant.

This deliverable 3.3 is divided into three parts:

- Section 3, **Characteristics of a KPA calculator**, where the characteristics that an easy-to-handle KPA calculator based on MS EXCEL® should have are described.
- Section 4, **Inputs, outputs and limitations**, where the schemes to understand the inputs and outputs, and the constraints that can be found of the KPA calculator for each industrial partner are included.
- Section 5, **Examples of application**, where the three examples of KPA calculator, the assumptions and the used models are explained.

2 DEFINITION OF TERMS

Key Performance Attribute: A Key Performance Attribute (KPA) is a variable directly related to the final product of a process, which value must be in a range of values that ensures that the final product is the desired one. The attributes, that are specific for each process and industry, will be linked to the product rate, the product cost, the quality characteristics and its environmental or safety aspects. The KPAs can be divided into two types: Global KPAs (Attributes to be checked of the final product to be sold) and Local KPAs (Attributes of a product that leaves a process and feeds a following one or an interface interaction).
Critical Process Parameter: the Critical Process Parameters (CPPs) are parameters directly related to the KPAs of a process that have a relevant influence on it: KPA = f(CPP1, CPP2,…,CPPn)
Lower Heating Value: a property of a fuel, defined as the amount of heat released by combusting a specified quantity of fuel considering that the water fraction of a combustion process is in vapor state at the end of combustion.

3 CHARACTERISTICS OF A KPA CALCULATOR

The main aim of a KPA calculator is to be able to check whether the values of the KPAs are in an acceptable range. In the case that the values are not adequate, by using the calculator the user could verify if by changing the CPPs or the design of the facilities (not in the case of TOP-REF project, where the aim is to provide non-invasive tool), the values of the KPAs are in this range.

These KPAs will set the boundaries for the variation of the Critical Process Parameters (CPPs). One of the main aims of the industrial activity is trying to balance economical profit and resource efficiency (that will be measured by the KRIs). KPAs will ensure that the optimization of the CPPs won't change the expected productive goods.

One of the most important characteristics that a KPA calculator should own is being easy-to-handle. For this reason the programming of the calculator should be orientated to a visual interface. In the framework of the TOP-REF project, the software MS EXCEL® has been proposed because of being an easy-to-handle and commonly used by all kind of user tool. Similarly, any visual tool able to import information from external sources (files or online M&C system) and to export this information to a visual interface (for example based on Java, visual basic.net or Borland Delphi) would be appropriate.
In the case of MS EXCEL®, the software has a developing tool based on Visual Basic, so it is capable of communicating with online M&C systems or importing/exporting external files obtained from mathematical simulation modeling software (as the used software in the WP4, Aspen Plus® and INOSIM® Professional).

Another important characteristic of a KPA calculator is that the interaction with the user should be basically visual. The final aim of the calculator should be just to show the value of the KPAs and whether the values are within the range defined as acceptable.

In case of working with a KPA calculator with a mathematical model integrated the user will be asked to introduce the information required by the model. Then, once the model had calculated the KPAs, the user will obtain the values and whether they are within the expected range. By changing the required inputs (that can be CPPs of the process) the user can find new working conditions that could lead to better KPAs values. In figure 1 the flux of information is shown in a diagram flow in this case.

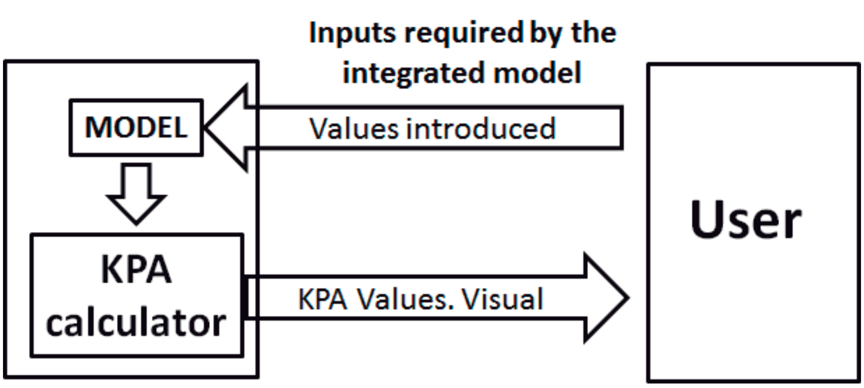

Figure 1: Diagram of the flux of information for KPA calculator linked to a KPA calculator with integrated simulation model

In case of being integrated with M&C system or external mathematical simulation model software, the KPAs calculator shall be able to import the information and then to provide the KPA values.
In this case, the M&C system or the external simulation software will provide the value of the KPAs (or the info required to calculate the value of the KPAs) and the KPA calculator just will show information regarding the characteristics of the product of each process (local KPAs) or the market products (global KPAs). In figure 2 the flux of information of this case is shown.

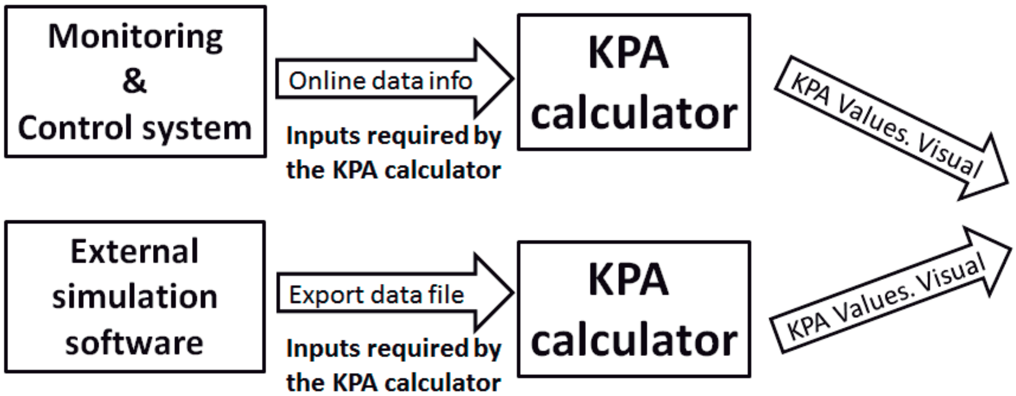

Figure 2: Diagram of the flux of information for KPA calculator linked to M&C system or to external simulation software

Finally, the KPAs calculator should be able to check whether the values of the KPA are within a required range of operation. For this, in both cases, working with an online M&C system or with simulations, the KPA calculator should be adjusted to shown the value and the range and by visual methods to indicate if the value is over, under or in the expected range (by using color scales, alert messages, etc.).

4 INPUTS, OUTPUTS AND LIMITATIONS

Once the KPAs calculator has been analyzed and characterized, it is necessary to define the external information that will be used by the calculator for each industrial demo site. This information will come from an M&C system or from an external mathematical simulation model.

For each industrial application, a scheme based on the information found in the Deliverable 3.2 of the project TOP-REF is included. In this scheme, the inputs, the outputs and the local and global KPAs (interfaces) (according to the subsystems definition) are shown.

4.1 FERTINAGRO's facilities

Figure 3 shows a modification of the subsystem definition developed in the Deliverable 3.2. In this scheme, the inputs and outputs for each subsystem in the case of FERTINAGRO is included. There are two set of inputs (one for the burner and one for the process plant) and also two outputs (one set of local KPAs, the exhaust gases leaving the burner, and one set of global KPAs, related to the market product).

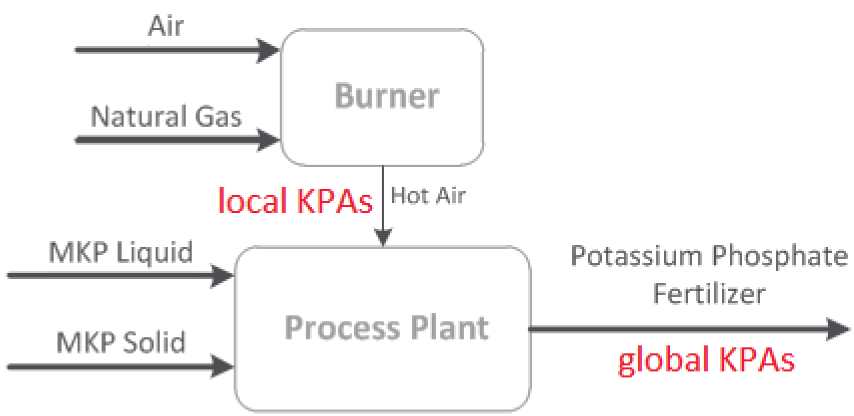

Figure 3: Subsystems of FERTINAGRO fertilizer plant

4.1.1 Local KPAs calculator: hot exhaust air from burner

In the case of FERTINAGRO, the characteristics of the hot air that leaves the burner will be the local KPAs. The burner provides a stream of hot exhaust gases that is used to dry the mixture of wet granules that leaves the mixer. This stream of gases should have a determined temperature and volumetric flow to ensure that the granules that leave the dryer are dry enough.

By the following, a list of the local KPAs for the burner, which should be shown by the KPA calculator, is included. All of these KPAs are local KPAs:

- Volumetric flow rate [m^3N/h] of exhaust gases.
- Temperature [°C] of exhaust gases.
- Composition [vol.-%O_2, N_2, CO_2, H_2O, fuel] of exhaust gases.
- Cost [€/Nm^3] of exhaust gases. This will be calculated by accounting the power for propelling Air, Natural Gas and hot Air and the volumetric flow rate of Natural Gas.

4.1.2 Possible limitations in the burner

The most important parameters in the case of the burner are the Temperature and the volumetric flow rate of hot exhaust gases (hot air). At this moment, there isn't any online monitoring system in FERTIGRANO able to measure the composition of the gases or the volumetric flow rate, but there exist seasonal offline measures according to local environmental regulation.

In the case of a KPA calculator linked to an external mathematical simulation model it is possible, by means of combustion and heat transfer models, to calculate the exhaust gas composition. In the case of a KPA calculator integrated in the current M&C system, additional monitoring system would be necessary.

In order to calculate the cost of the exhaust gases, it will be necessary to know the cost of the Natural Gas and the cost of the electricity for propelling the gases to be implemented in the KPA calculator.

4.1.3 Global KPAs calculator: final market product from process plant

The KPA calculator should receive the following information to show the global KPAs:

- Mass flow rate [kg/h] of final market product.
- Mass flow rate [kg/h] of fines product.
- Mass flow rate [kg/h] of oversized product.
- Amount of water in the final product [%] at the exit of the sieve.
- Final product cost [€/kg]. This cost will be obtained by means of total power consumption [kW] in the plant (minus the power in the burner), the mass flow rate [kg/h] of phosphoric acid, potassium carbonate and potassium dihydrogen phosphate.

The KPA calculator should include information about the electricity and the raw material costs.

4.1.4 Possible constrains for the KPA calculator of the process plant

In the case of global KPAs, the most important parameters are the mass flow rate of product, the amount of water and the cost of the final product. At this moment, there is not any online monitoring system in the facilities able to measure the water content of at the exit of the sieve.

In the case of a KPA calculator linked to an external simulation model it is possible, by means of kinetics and heat and mass transfer models, to calculate the growing process of the granules and the water content. In the case of a KPA calculator integrated in the current M&C system, additional monitoring functions would be necessary to obtain the amount of water in the granules.

In the cost calculation of the final product, it will be necessary to know the price of the electricity for the whole plant and the prices of the raw materials. This price should be updated in the KPA calculator.

4.2 DCI's facilities

In figure 4, it is possible to see a simplification of DCI's production plant. It is divided into two main subsystems: the process plant and the utility system with several interactions between their interfaces.

Four main blocks of information should be contained in the KPA calculator of DCI: the boiler, the steam grid, the cracking furnaces and the fractionation section. For thus, four set of outputs (local and global KPAs) will be obtained. The attributes of the steam, exhaust gases and hydrocarbons leaving the cracking furnaces, the SHH steam leaving the boiler and the steam and electricity leaving the steam grid will be local KPAs. On the other side, the attributes of the Ethylene and Propylene leaving the fractionation section and the condensate leaving the steam grid will be global KPAs.

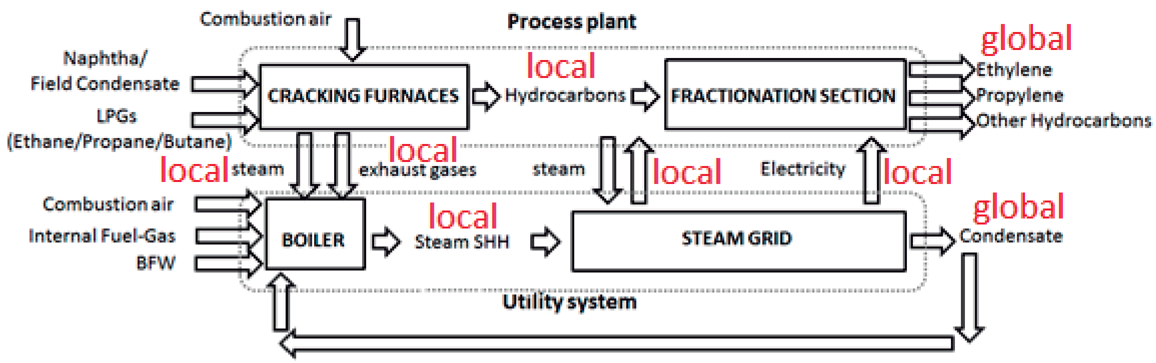

Figure 4: Subsystems of DCI process

4.2.1 Local KPAs calculator

In the case of DCI it is necessary to configure a KPA calculator that should be able to provide the key attributes of the outputs of the cracking furnaces, the boiler and the steam grid that correspond to local KPAs.

In this section, component by component, the list of the required information by the KPA calculator is included.

Boiler:

In the case of the boiler, the KPA calculator shall be able to provide information about:

- Volumetric flow rate [m^3N/h] of SHH steam.
- Temperature [°C] of SHH steam
- Pressure [bar] of SHH steam.
- Cost [€/Nm^3] of SHH steam. In order to calculate the cost of the SHH steam, it will be necessary to provide the cost of the steam and exhaust gases leaving the cracking furnaces, the volumetric flow rate and the cost of the Internal Fuel-Gas, the volumetric

flow rate and the cost of the BFW and the condensate water and the power and cost of the electricity for propelling all of them to the boiler.

The cost of the electricity, BFW, Internal Fuel-Gas, steam from cracking furnaces, exhaust gases and condensate water should be introduced in the KPA calculator. The price of the Internal Fuel-gas, the steam and the exhaust gases from the cracking furnaces and the price of the condensate water can (and will be in the task 3.4) be calculated by means of thermoeconomic analysis.

In this case, the outputs of the boiler are local KPAs for the steam grid.

Steam grid:

In the case of the steam grid, this sub-system will provide power and heat to the fractionation section. There are mainly two inputs for the steam grid (the SHH steam produced in the boilers and the steam entry at different pressure levels from the process plant) but several outputs among the whole fractionation section.

In this case the output of the boilers (local KPAs) is already calculated in the KPA calculator but information about the different inlets of steam at the different pressure levels is additionally required.

In the case of DCI, there exist four additional different levels of pressure in addition to the SHH that can be introduced in the steam grid from the fractionation section or from external sources (supplier or different neighboring industrial facilities).

For the steam grid, the KPA calculator must be able to provide information about:

- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of SHH steam from the steam grid to the process plant (Large Machines: RGC, C_2 compressor and C_3 compressor)
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of SH steam from the steam grid (extraction of C_2 compressor) to the process plant (Large Machines: RGC, C_2 compressor and C_3 compressor)
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of SM steam from the steam grid (extraction from RGC) to the process plant (Large Machines: RGC, C_2 compressor and C_3 compressor)
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of SL steam from the steam grid to the process plant (Large Machines: RGC, C_2 compressor and C_3 compressor)
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of SLL steam from the steam grid to the process plant (Large Machines: RGC, C_2 compressor and C_3 compressor)
- Mechanical power [kW] to the fractionation section process plant for the 3 Large Machines: RGC, C_2 compressor and C_3 compressor.

The steam grid will supply the steam and the mechanical power to the fractionation section. According to the KPA definition in the Deliverable 3.2, all of the outputs of the steam grid are local KPAs but the condensate water that is a global KPA.

Cracking furnaces:
The final purpose of the cracking furnaces is to obtain a mixture of hydrocarbons that will be fed to the fractionation section. These furnaces are fed by naphtha, field condensate, propane and butane that react by obtaining the heat from the combustion of fuel gas (mainly methane and hydrogen) coming internally downstream from the process (by-product of the cracking reaction) and SHH saturated steam from TLEs located at the outlet of the cracking furnaces.

The list of local KPAs to be obtained by means of the KPA calculator is:

- Volumetric or mass flow rate [Nm^3/h or kg/h], composition [%], power for propelling [kW] and cost [€/kg] of hydrocarbons.
- Volumetric or mass flow rate [Nm^3/h or kg/h], power for propelling [kW] and cost [€/kg] of exhaust gases.
- Volumetric or mass flow rate [Nm^3/h or kg/h], power for propelling [kW] and cost [€/kg] of steam.

All of the outputs of the cracking furnaces will be KPAs for the boiler and the fractionation section. In addition in order to obtain the costs of the hydrocarbons, exhaust gases and steam, it will be necessary to implement, the price of the electricity and the price and the flow rate of the naphtha, field condensate, propane, butane and internally produced fuel-gas in the KPA calculator.

4.2.2 Possible constrains for the local KPA calculator

In a similar manner, component by component, a list of possible constraints or limitations that could be found during the KPA calculator development will be described.

Boiler:
The most important attributes in the case of the boilers are the temperature, pressure and volumetric flow rate of SHH steam. In the facilities of DCI there is online instrumentation that is able to measure in real time those KPAs. In the case of a KPA calculator linked to a simulation model, it is possible, by means of combustion and heat transfer models, to calculate the SHH steam produced.

To calculate the cost of the SHH steam it will be necessary to know the cost of the internal fuel-gas, the electricity, the BFW, the steam and the exhaust gases from cracking furnaces and the cost of the condensate water. The BFW and the electricity are supplied by external sources, but the rest is internally produced and it is possible to find some issues for determining their values. In this case it is possible that previous calculations based on thermoeconomic analysis should be implemented in the models or in the KPA calculator.

Steam grid:
In the case of the steam grid, it is possible to model the steam flow rate at different pressures, in order to maximize the usefulness of the steam but the minimum requirements of volumetric flow rate, temperature and pressure of the steam should be also provided. In this case the KPA calculator basically will require and provide the same values.

In order to obtain the costs, it is possible that previous calculations based on thermoeconomic analysis should be implemented in the models or in the KPA calculator.

Cracking furnaces:
The most important parameters in this case will be the temperature, and the composition of the mixture of hydrocarbons. In the facilities of DCI there is online instrumentation that is able to measure in real time most of those KPAs. In the case of a KPA calculator linked to a simulation model, it would be possible, by means of the kinetic, combustion and heat transfer models, to calculate the production rate of hydrocarbons, steam and exhaust gases.

4.2.3 Global KPAs calculator

In the case of DCI two subsystems will produce global KPAs: the fractionation section and the steam grid. By following, the list of Global KPAs to be obtained by means of the KPA calculator and the possible limitations are included:

Steam grid:

- Mass flow rate [kg/h], temperature [°C], pressure [bar] and cost [€/kg] of condensate water coming from Large Machines (RGC, C_2 compressor, C_3 compressor and process equipment – heat exchangers, etc.)

Fractionation section:
The fractionation section is responsible for the marketable products. This subsystem is fed by the mixture of hydrocarbons that leaves the cracking furnace and the steam (5 levels of pressure) and power imported from the steam grid.

- Mass flow rate [kg/h], temperature [°C], purity [vol.- or wt.-%] and cost [€/kg] of ethylene
- Mass flow rate ([kg/h], temperature [°C], purity [vol.- or wt.-%] and cost [€/kg] of propylene

The outputs of the fractionation section and the condensate flow are global KPAs.

4.2.4 Possible limitations of the Global KPA calculator

As in the case of other subsystems linked in cascade to previous subsystems, the final cost of the outputs would require the use of thermoeconomic analysis in order to include the cost of different sequential processes. A complete development of the methodology is included in the Deliverable 3.1 and will be applied to the industrial demo sites in the Task 3.4.

In the case of a KPA calculator linked to a simulation model it is possible, by means of separation and compression models, to obtain the outputs of the fractionation section. Regarding the M&C system of DCI, in their facilities there is instrumentation enough to obtain the KPAs.

4.3 PETROGAL's facilities

In figure 5 a simplified scheme of the PETROGAL's production is shown. In PETROGAL's facilities it is possible to find two main blocks: the process plant and the utility system as well as several interactions between their interfaces.

Four different and three identical subsystems should be contained in the KPA calculator of PETROGAL: the gas turbines, the boilers, the cogeneration boilers, the steam grid and the production processes for the plants 1 (atmospheric distillation), 2 (fluidized catalytic cracking) and 3 (hydrocracking). According to that definition, seven set of outputs (local and global KPAs) will be obtained.

The attributes of the final product obtained from the plants 1 to 3 and the condensate will be Global KPAs, meanwhile the rest of outputs of the analyzed blocks will be local KPAs. Because of the great amount of intermediate products and the variability (substances and purity) of the final product of the plants 1 to 3, a generic KPA calculator has been developed.

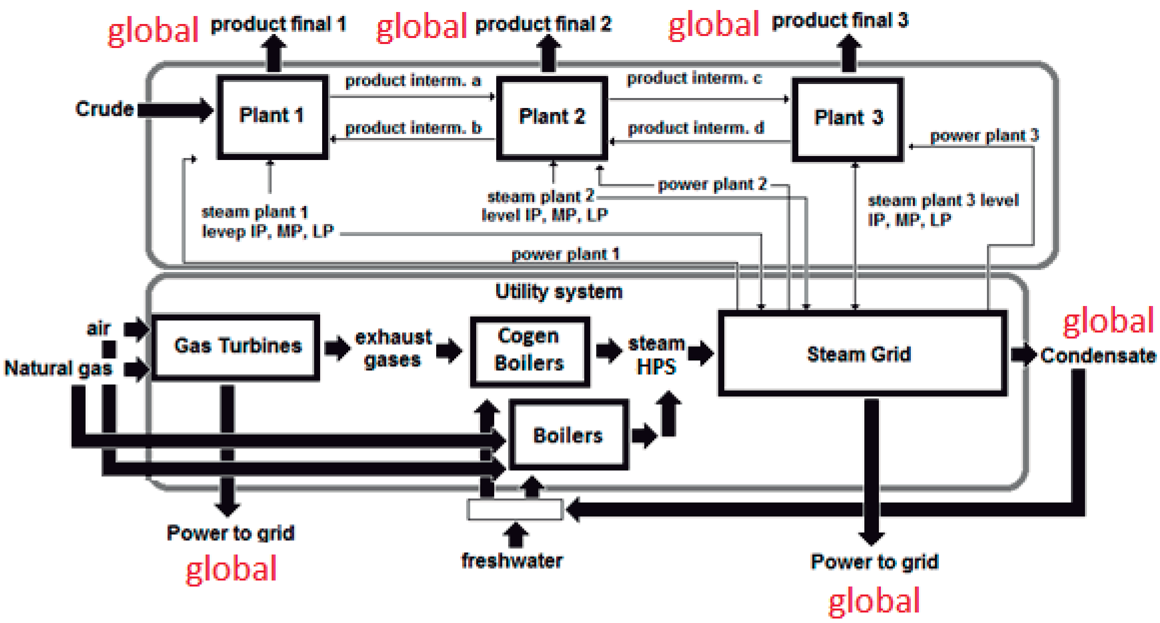

Figure 5: New subsystems definition for Petrogal process

4.3.1 Local KPA calculator

In the case of PETROGAL the local KPAs calculator will calculate the key performance attributes of the gas turbines (but the power to grid), the cogeneration boilers, the regular boilers, the steam grid (but the power to grid and the condensate) and the intermediate products of the plants 1 to

3. As in the previous cases, the local KPAs calculator should include information about the KPAs and the range.

In this section, component by component, the list of local KPAs and the possible limitations to obtain the values is included.

Gas turbines:
The gas turbines (twin turbines) are responsible for one of the marketable products of the facilities of PETROGAL: electric power. In addition the exhaust gases of the turbines will feed the cogeneration/regeneration boiler in order to produce HPS steam. The characteristics of the exhaust gases will be considered as local KPAs meanwhile the electric power will be a Global KPA.

The KPA calculator should be able to provide the value of:

- Volumetric flow rate [Nm^3N/h], temperature [°C], pressure [bar] and cost [€/Nm^3N] of exhaust gases. The cost of the exhaust gases will be obtained by accounting the power and the cost for propelling the natural gas and the air and the volumetric flow rate and the cost of the natural gas. These costs will be introduced in the KPA calculator in order to obtain the cost.

Cogeneration/Regeneration boilers:
The cogeneration boilers (two twin boilers) are one of the responsible for producing HPS steam by using the exhaust gases of the gas turbine and the BFW (condensate and fresh).

The KPA calculator should be able to provide the value of:

- Volumetric flow rate [Nm^3/h], temperature [°C], pressure [bar] and cost [€/Nm^3] of HPS steam.

In order to obtain the cost of the HPS steam it will be necessary to know the volumetric flow rate of exhaust gases and its costs, the mass flow rate and the cost of BFW and condensate water and the electric power and electricity cost for propelling all the intervening raw materials.

Boiler:
In the case that there is not enough production of HPS steam, regular boilers are used. These regular boilers are fed by natural gas, a mixture of fresh BFW and condensate water (as the cogeneration/regeneration boiler) to produce HPS steam.

In the case of the boiler, the KPA calculator will obtain the same KPAs than in the case of the cogeneration/regeneration boiler:

- Volumetric flow rate [Nm^3/h], temperature [°C], pressure [bar] and cost [€/Nm^3] of HPS steam.

In this case it is necessary to account the flow rate and the price of the natural gas fed to the boiler in addition to the flow rate and the cost of the BFW and condensate water.

Steam grid:

In the case of PETROGAL, the steam grid is fully connected (at different pressure levels) to the three productive process plants. At every level, there is transfer of steam between the plants and the steam grid and vice versa. In addition, the electricity consumption in the plants is fed by the electricity production that takes place in the steam grid and the system is even able to produce electricity to that can be sold to the national electrical grid.

Because of this interconnection, the KPA calculator (steam grid part) of PETROGAL will contain several inputs. As in the case of DCI, a KPA calculator linked to a simulation model, the volumetric or mass flow rate [Nm^3/h or kg/h], the pressure [bar] and the temperature [°C] of each steam pressures levels are required. In the case of a monitoring and control system, the same information will be necessary.

The steam grid will supply the steam and the mechanical and electrical power to the plant sections 1 to 3. The list of local KPAs for the steam grid is:

- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of HPS steam from the steam grid to the plants 1, 2 and 3 and from the plants to the steam grid.
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of MPS steam from the steam grid to the plants 1, 2 and 3 and from the plants to the steam grid.
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of IPS steam from the steam grid to the plants 1, 2 and 3 and from the plants to the steam grid.
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of LPS steam from the steam grid to the plants 1, 2 and 3 and from the plants to the steam grid.
- Electrical power [kW] to the plants 1 to 3.

In the case of the steam grid, all the outputs will be local KPAs but the electrical power (for the case of excess electrical power) that is fed to the grid and the condensate water that will be global KPAs.

Plants 1, 2 and 3:

The last part of the KPA calculator for the PETROGAL facility will correspond to the productions plants 1, 2 and 3. These plants are practically identical in terms of replicability (regarding the KPA calculator). The three plants will require flow rates of steam at each pressure levels and flows of electrical power from the steam grid to the plants.

These productive plants will also introduce steam at every pressure levels into the steam grid, will produce intermediate product (a, b, c and d) and market product (1, 2 and 3). The main difference between the three plants is that only the first plant is fed by crude oil.

Regarding the local KPAs the calculator should provide information about:

- Mass flow rate [kg/h], temperature [°C], composition [vol.- or wt.-%] and cost [€/kg] of sub-products a, b, c and d.
- Volumetric or mass flow rate [Nm^3/h or kg/h], temperature [°C], pressure [bar] and cost [€/kg] of HPS, MPS, IPS and LPS steam send from the plants 1, 2 and 3 to the steam grid.

In order to evaluate the costs, the KPA calculator will need:

- Mass flow rate [kg/h] and cost [€/kg] of crude feed in the plant 1.
- Volumetric or mass flow [Nm^3/h or kg/h] and cost of the HPS, MPS, IPS and LPS steam consumed in the plants 1, 2 and 3.

4.3.2 Possible limitations of the Local KPA calculator

In a similar manner, component by component, a list of possible constraints or limitations that could be found during the KPA calculator development will be described.

Gas turbines:

In the case of a KPA calculator linked to a simulation model it is possible, by means of combustion and heat transfer models, to calculate the exhaust gas composition and temperature and the power production. In the case of the gas turbines, in the case of PETROGAL it would be possible to monitor online the KPAs so, no major limitations are found.

Cogeneration/Regeneration boilers:

In the case of the cogeneration boiler, the introduction of two inputs that are linked to the output of different subsystems (steam grid and gas turbine) implies that the price of condensate water and the price of the exhaust gases should be calculated by using process integration diagnosis tools as thermoeconomic analysis. In the facilities of PETROGAL there is an M&C system able to provide all the information required in the KPA calculator. In the case of a KPA calculator linked to a simulation model it would be possible, by means of heat transfer models, to calculate the volumetric flow rate, temperature and pressure of the HPS steam.

Regular boilers:

In the case of the regular boilers, the introduction of an input linked to the output of different subsystems (steam grid) implies that the price of condensate water should be calculated by using thermoeconomic analysis or any other integrated approach. In the facilities of PETROGAL there is an M&C system able to provide all that information required in the KPA calculator. In the case of a KPA calculator linked to a simulation model, the use of combustion and heat transfer models with the aim of calculating the volumetric flow rate, temperature and pressure of the SHH steam will be studied.

Steam grid:

As in the case of DCI, it is possible to model the steam flow at different pressures, in order to maximize the usefulness of the steam. Anyway, the KPA calculator basically asked and provides the same values. In order to obtain the costs, it is possible that previous calculations based on thermoeconomic analysis should be implemented in the models or in the KPA calculator.

Plants 1, 2 and 3:

There are several constraints in the case of PETROGAL. The first one is the complete interconnection of the three productive plants and the steam grid at every level of pressure and matter transfer. In addition, the market products of the plants can vary over time.

Another constraint is that most of the inputs and the outputs of the KPA calculator will refer to the same information. In addition it is easy to calculate the cost of the final market products by accounting the cost in fuels and the production of market product, but it will be necessary to apply the thermoeconomic analysis to the overall plant, in order to calculate the cost of the internal streams and the introduction of these costs in a KPA calculator could present difficulties.

4.3.3 Global KPA calculator

In the case of PETROGAL three subsystems can produce global KPAs: the gas turbines, the steam grid and the productive plants 1, 2 and 3. By following, the list of Global KPAs to be obtained by means of the KPA calculator and the possible limitations are included:

Gas turbines:

- Power Production [kW] sold to the grid.

Steam grid:

- Mass flow rate [kg/h], temperature [°C], pressure [bar] and cost [€/kg] of condensate water.
- Electrical power [kW] to the grid.

Productive plants 1, 2 and 3:

- Mass flow [kg/h], composition [%] and cost [€/kg] of market product 1, 2 and 3. The list of possible products that can be obtained in these plants are:
  - Propane: plants 1 and 2
  - Butane: plants 1 and 2
  - Naphtha: plants 1 and 3
  - Jet fuel: plants 1 and 3
  - Fuel oil: plants 1 and 2
  - Gasoline: plants 2 and 3
  - Gasoil: plant 2
  - Propylene: plant 2

4.3.4 Possible limitations of the Global KPA calculator

As in the case of other DCI, the use in cascade of outputs from previous subsystems will cause the final cost of the outputs to be calculated by means of tools analogous to thermoeconomic analysis in order to include the cost of different sequential processes.

In addition, in the case of PETROGAL, each plant does not produce products for the market. It produces products for storage that then are blended to obtain the products for the market. The composition of each blend changes daily, depending on the type of crudes and the type and quantities of intermediate products that are produced with each crude mix. The price of each intermediate product change with the properties obtained in each day and with the price of this product in the international market. As it can be seen, the variables are KPAs but it will be difficult to obtain a set of range values.

5 EXAMPLES OF APPLICATION

Once the characteristics and outputs (and possible constraints) of the KPA calculator of each industrial production plant of the TOP-REF project are described, an example of the application of the KPA calculator for each plant will be shown.

In the examples developed, the KPA calculators are linked to a mathematical simulation model integrated in the KPA. Because of the complexity of simulating some chemical processes (as separation column, cracking furnaces and compete steam grids) by using simple linear regressions or easy equation models in MS EXCEL®, the examples of KPA calculator are mostly related to the thermal processes of the utility subsystems related to the facilities of the uses cases considered within TOP-REF.

It is important to remark that it is not necessary to implement any simulation model into a KPA calculator and that in the proposed examples the simulation models have been implemented in order to see how a KPA calculator should work.

5.1 KPA calculator example for FERTINAGRO

In the case of the KPA calculator of FERTINAGRO, both subsystems, the burner and the process plant, are included.

In figure 6 it is possible to see the example of KPA calculator implemented for FERTINAGRO.

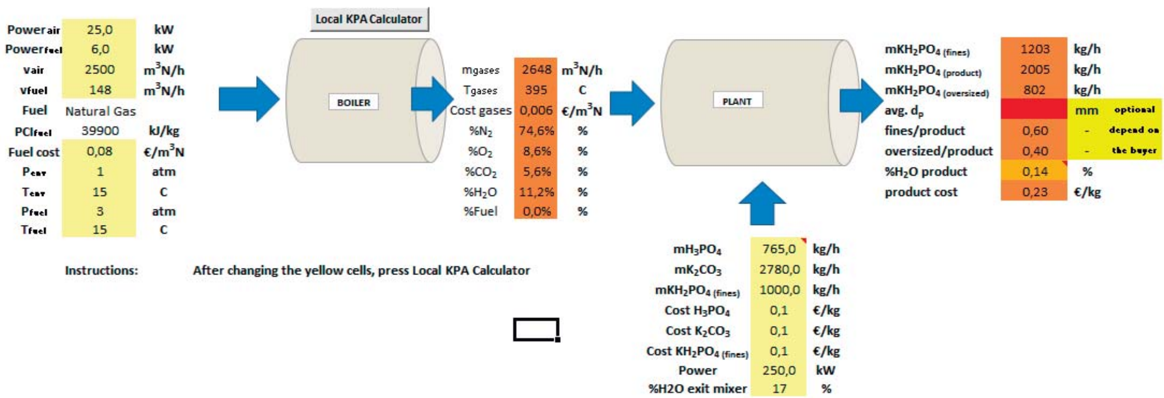

Figure 6: Example of KPA calculator for FERTINAGRO.

As it can be seen, the KPA calculator is divided into two parts with two inputs and two outputs: the burner and the process plant. In order to use the KPA calculator, the user must fulfil the light yellow cells and then click on the *"Local KPA Calculator"* button. The mathematical model included in the MS EXCEL® file will calculate the outputs of the boiler and the process plant.

For the final KPA calculator, the MS EXCEL® file should be able to import the external information to fulfill the light yellow cells (instead of the user) from an M&C system or from an external mathematical simulation model. The results will be shown in the orange cells.

5.1.1 Assumptions and limitations of the example KPA calculator

The assumptions taken to develop the simplified model were the following:

- The composition of the exhaust gases and the temperature at the exit of the burner have been obtained by using the ***solver*** tool included in MS EXCEL® in order to solve the matter and energy balance around the burner.
- The natural gas composition has been assumed as 100% of CH_4 and the combustion reaction has been considered as stoichiometric and complete according to the equation $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ and using the ideal gas model (with c_p variable vs temperature)
- The boiler presents irradiation losses according to the ambient temperature and assuming that the temperature of the boiler's wall is 180ºC (measured by a thermographic camera during a working period). With this assumption, the heat losses in the boiler are close to 30%.
- The pressure of the gases at the exit of the boiler is 1 atm.
- For the fines, oversized and target distribution of size of the market product a 30/20/50 %.-wt distribution was assumed because it is no possible to known the particle size distribution without a kinetic model. For this reason it is not possible to know the average size of granule (in red).
- The water content of the final product has been calculated by using an experimental correlation obtained from measures taken during the setting up of the plant. The obtained correlation is:

$$\%H_2O\ product = \%H_2O\ mixer - \left(\frac{Tgases - Tproduct}{\alpha}\right)$$

  Where $\%H_2O\ product$ is the amount of water at the exit of the dryer, $\%H_2O\ mixer$ is the water content at the exit of the mixer, T_{gases} is the temperature of the exhaust gases, Tproduct is the temperature at the exit of the dryer (assumed constant and equal to 85ºC) and α is an experimental value in a range of 14 – 21 with an average (and used) value of 18.5.
- The cost of the exhaust gases has been calculated by accounting the gases production, the price of the natural gas and the price of the electricity (set to 0.10€/kWh for the example)

Regarding the limitations, in order to use the KPA calculator "FERTINAGRO KPA calculator.xls", it is necessary to install the "solver tool" in a MS EXCEL® v. 2010 or higher.

5.2 KPA calculator example for DCI

In the case of the KPA calculator of DCI, only the boiler that produce the SHH steam has been included.

In figure 7 it is possible to see the example of KPA calculator implemented for DCI.

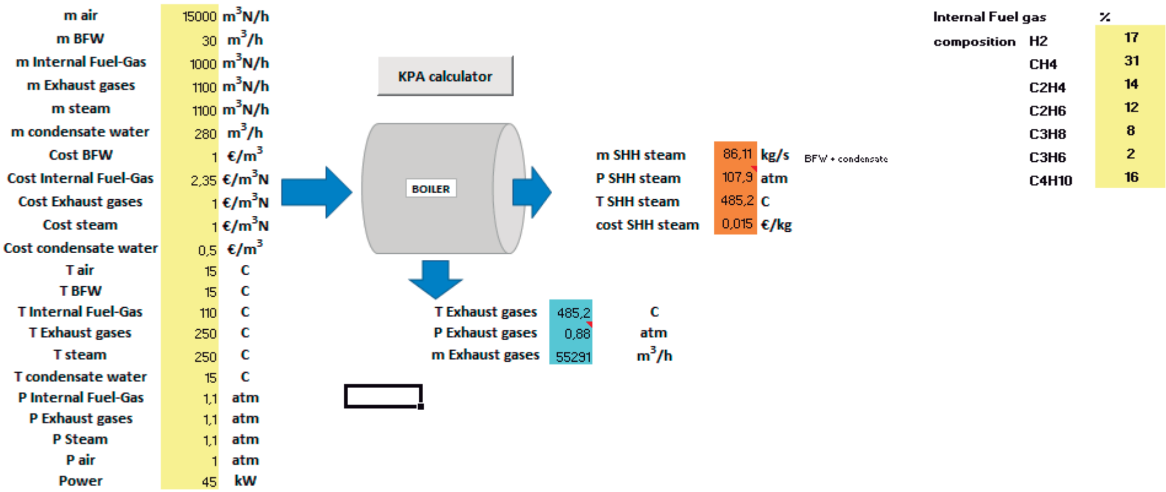

Figure 7: Example of KPA calculator for DCI.

The KPA calculator is just divided into one part with one input and two outputs: the SHH steam and the exhaust gases of the boiler. In order to use the KPA calculator, the user must fulfil the light yellow cells and then click on the "*KPA Calculator*" button. The mathematical model included in the MS EXCEL® file will calculate the output of the boiler.

5.2.1 Assumptions and limitations of the example KPA calculator

The assumptions taken are:

- The temperature of the exhaust gases has been set equal to the temperature of the SHH steam.
- The temperature of the SHH steam has been obtained by using the tool solver included in MS EXCEL® by solving the matter and energy balance.
- The composition of the exhaust gases leaving the boiler has been obtained assuming stoichiometric and complete combustion of the internal fuel according to the following equations by using ideal gas model with c_p variable with temperature:
    - $H_2 + 1/2O_2 \rightarrow H_2O$
    - $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
    - $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$
    - $C_2H_6 + 7/2O_2 \rightarrow 2CO_2 + 3H_2O$
    - $C_3H_6 + 9/2O_2 \rightarrow 3CO_2 + 3H_2O$
    - $C_3H_8 + 8O_2 \rightarrow 3CO_2 + 4H_2O$
    - $C_4H_{10} + 13/2O_2 \rightarrow 4CO_2 + 5H_2O$
- The composition of the exhaust gases from the cracking furnaces has been set as 57 vol.-%H_2O and 43 vol.-%% CO_2.
- A pressure drop of 20% has been assumed in the boiler.
- A heat loss of 20% has been considered in the boiler.
- The cost of the SHH steam has been calculated by accounting the steam production, the price of the internal fuel-gas, the prices of the exhaust gases, the price of the steam exhausted and the price of the electricity (set at 0.10€/kWh as example).

- The pressure of the SHH steam has been set to 108 bar.

Regarding the limitations, in order to use the KPA calculator “DCI KPA calculator.xls”, it is necessary to install the “solver tool” in a MS EXCEL ® v. 2010 or higher.

5.3 KPA calculator example for PETROGAL

In the case of the KPA calculator of PETROGAL, one of the gas turbines and one of the heat recovery (cogeneration) boilers have been included.

In figure 8 it is possible to see the example of KPA calculator for PETROGAL that is going to be implemented.

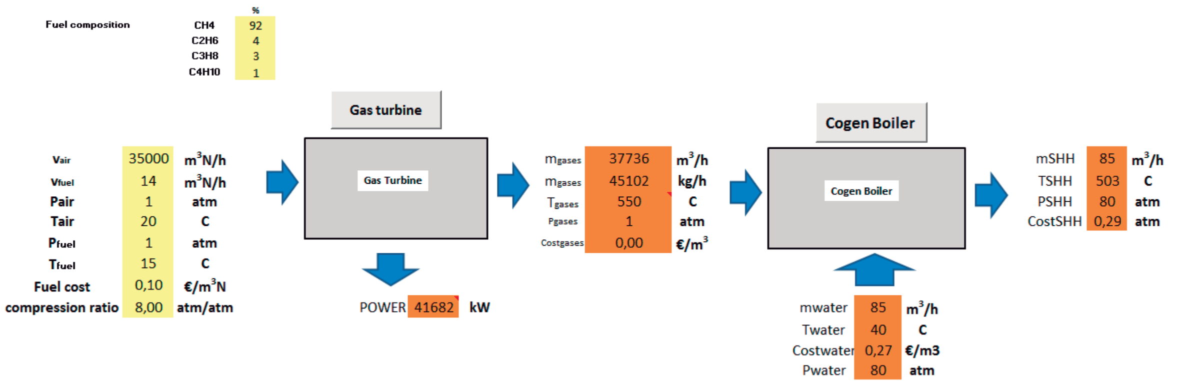

Figure 8: Example of KPA calculator for PETROGAL.

The KPA calculator is divided into two parts with two inlets and two outputs: the gas turbine and the cogeneration boiler. In order to use the KPA calculator, the user must fill the light yellow cells and then click on first the “*gas turbine”* button followed by the “cogen boiler” button. The mathematical models included in the MS EXCEL® file will calculate the output of the gas turbine and the cogeneration boiler.

5.3.1 Assumptions and limitations of the example KPA calculator

The assumptions taken in order to develop the simplified models are:

- The temperature of the exhaust gases of the gas turbine has been obtained by using the tool solver included in MS EXCEL® by solving the mass and energy balance.
- The gas turbine cycle has been solved considering the Brayton cycle with a value of gamma (polytrophic constant) equal to 1.4.
- The composition of the exhaust gases leaving the gas turbine has been obtained assuming stoichiometric and complete combustion of the fuel according to the following equations by using ideal gas model with temperature-dependent specific heat capacity.
    - $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
    - $C_2H_6 + 7/2O_2 \rightarrow 2CO_2 + 3H_2O$
    - $C_3H_8 + 8O_2 \rightarrow 3CO_2 + 4H_2O$

  - $C_4H_{10} + 13/2O_2 \rightarrow 4CO_2 + 5H_2O$
- An isentropic efficiency of 80% is considered in the turbine and the compressor.
- A temperature of 550ºC is set at the exit of the turbine according to the specifications of PETROGAL.
- A pressure of 80 bar is set for the HPS steam.
- An exhaust gases temperature at the exit of the cogeneration boiler of 120ºC and 20% of heat losses are assumed.
- The cost of the HPS steam has been calculated by accounting the steam production, the price of the fuel and the price of the electricity (set at 0.10€/kWh as example).

Regarding the limitations, in order to use the KPA calculator "PETROGAL KPA calculator.xls", it is worth to highlight again that it is necessary to install the "solver tool" in a MS EXCEL® v. 2010 or higher.

6 IMPACT OVER SPIRE ROADMAP AND INDUSTRIAL PERFORMANCE

One of the main goals of SPIRE is to define guidelines and actions that would lead to a drastic reduction of the environmental footprint while the competitiveness of the industries is increased. Basically the concept should be "doing more with less". This premise will necessarily group resource efficiency actions. In addition, every industry has the power to modify the control parameters that could affect the productivity and efficiency of their processes. On the other hand, it is still necessary to ensure the quality, environmental, production rate and costs of the products and by-products.

The KPAs calculator can be integrated on any M&C system or be the visual interface of any mathematical simulation model system as a manner to check that the changes on the working conditions do not produce discordance in the characteristics of the final products.

The KPAs calculator is aligned with several Key Actions of the SPIRE roadmap:

- Due to its capacity of evaluating the changes on the CCPs, the use of the KPA calculator is aligned with the Key Action 2.3 (Process monitoring, control and optimization).
- The standardization of the use of KPAs calculators in M&C and simulation model systems will lead to establish more efficient technology dissemination methodologies, mechanisms and frameworks (Key Action 6.1).

Regarding the impact on the industrial performance, the KPA calculator can help the industrial processes manager of any industry to identify whether the changes of working conditions are leading to final market products and by-products with the proper and expected characteristics in terms of cost, production rates, quality, safety, resource efficiency and the environmental impacts.

7 CONCLUSIONS

In this report, the aim, scope and characteristics that an easy-to-handle KPA calculator should have, have been included.

For each industrial demo site, the list of inputs and outputs and the possible limitations that can be found in the implementation of a KPA calculator are included.

In addition, an application example of a KPA calculator based on MS EXCEL® of FERTINAGRO, DCI and PETROGAL and the MS EXCEL® files have been carried out and explained. These KPA calculator examples have been built with simplified models.

It is necessary to highlight that in the case of being linked to a simulation model, the KPA calculator would work in a batch process (because a previous run of a simulation model is needed in order to fill the cells with the required info), meanwhile when it is integrated with an M&C system, the calculator can work online in a continuous mode.

The KPA calculator will be the appropriate tool to check if the value of the KPAs is within the expected range or not in the framework of the TOP-REF project. Once the models and the monitoring and control systems are perfectly linked (as a result of WP4 and 5), the development of a more complex KPA calculator according to the characteristics defined in this report will be possible for the TOP-REF demo sites.