

# Optimal integration of renewable based processes for fuels and power production: Spain case study

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## Abstract.

In this work we propose a framework for the optimal integration of renewable sources of energy to produce fuels and power. A network is formulated using surrogate models for various technologies that use solar energy, photovoltaic, concentrated solar power or algae to produce oil, wind technology, biomass based syngas to ethanol, methanol, FT-liquids and thermal energy, hydroelectric power and waste based power plant via biogas production. The optimization model is formulated as an MILP that allows determining the optimal selection of technologies to meet a certain demand; sustainability and CO<sub>2</sub> emissions are also considered. The network is applied to evaluate process integration at different scales, from province to country level, and including uncertainty in sources availability. The solution suggests the use of hydropower and oil production, while bioethanol and biodiesel plants are allocated close to fuel demand points such as large population areas. Up to 20% of fuels and total power can be substituted with the current technology and with 1% area usage. It is possible to reach 50% substitution with renewables using 20% area with the availability and efficiency of current processes.

Keywords: Wind power; Solar Energy; Biomass; Waste; Process integration; CO<sub>2</sub>

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## 1. Introduction

Concern on global warming and the increasing demand for energy have increased the potential for renewables to enter the energy mix. Among them, hydropower, wind, solar and biomass are the most commonly used. While biomass is a raw material than can somehow be stored for a certain period of time, and hydropower can be regulated [1], solar and wind energy are more difficult to handle [2]. Currently battery systems do not have the capacity to store large amounts of power [3]. To meet a certain demand of power and fuels, and mitigate the effect of the availability of renewable sources, several alternatives are available such as thermal cycles [4], chemicals production, i.e. hydrogen or methane [5] or hydro-storage [1]. Over the last years, plant integration of renewable resources has been considered for this purpose. First and second generation bioethanol production processes were integrated [6] to make use of the excess of energy when processing lignocellulosic biomass to provide energy for ethanol dehydration. Not only biomass types, but different energy sources have also been integrated such as the facility that combines solar concentrated power and biomass for maintaining the power production capacity over time [7]. Martín and Davis [5] evaluate the integration of solar wind and power for the production of methane, synthetic natural gas. Prasad et al. [8] evaluate the integration of solar and wind energy for power production to mitigate the lack any of the sources. Martín and Grossmann [9] integrate solar, wind and biomass to capture CO<sub>2</sub>, and hybrid systems are also presented in the recent literature [10]. The design of most of the facilities involving renewables is subjected to the variability in the energy sources and that of the electricity price [2]. This variability affects the utilization of the units of the process, not only wind turbines and solar panels, but also the number of electrolyzers in operation and process units. Some units may remain idle or partially idle for certain periods of time representing an investment in units that is not used to their full capacity. Therefore, resource variability determines the investment in expensive units. However, the design problem involves multiperiod optimization under uncertainty. These kinds of problems have been addressed before in the literature [11]. Grossmann and Sargent [12] included the uncertainty in the information within process design. Later, Halemane and Grossmann [13] describe the problem of flexible process design. Both concepts have regained attention with the inclusion of renewables in the energy mix. In the integration of methanol via hydrolytic hydrogen and algae based oil [9], the problem is formulated in such a way that it exploits the operation of the plant to reduce the problem size. Martín [14] present a methodology to address

the design and monthly operation of plants using renewable sources for the production of methanol from CO<sub>2</sub> hydrogenation. Surrogate models are developed, not only for the process units, but also for the cost of the process sections so as to be able to include uncertainty in solar and wind into the design decisions. Recent examples show the integration of hydro and photovoltaics [15].

However, large scale demand such as at regional or country level requires the integration of resources at local or greater scale, a problem that represents a technical challenge [16]. Some studies [17,18] present overviews regarding integration possibilities as a perspective for the combination of different sources of energy. In order to help make those decisions, process system engineering has the tools to compare sources, technologies and locations in search of the optimal use of natural resources for renewable power and fuels production. Large scale integration of resources to control production capacity is challenging due to the problem size and its mathematical complexity, together with the fact that that renewables feature seasonal and daily variation. Most of the studies either focus on biofuels supply chain design for different regions such as Europe [19], the US [20] or Canada [21], or electric power supply and grid operation based on the unit commitment problem [22], considering market prices [23] even including stochastic behavior of the variables [24], in particular applied to small regions [25]. In the case of the power sector, heat is also typically included in the analysis [26]. However, electric power is most of the times produced by using a fuel that may be synthesized such as methane or Fischer Tropsch fuels. Therefore, both supply networks are linked and must be addressed simultaneously. So far both have been designed independently due to the fact that they are areas that are studied by different communities.

In this work we extend the analysis of the generation of biofuels and power using renewable sources by integrating the two networks that traditionally have been developed as independent entities. However, they are linked by the common use of raw materials for the production of chemicals, fuels and power as well as the possibility of storing power in the form of chemicals with the aim of meeting the corresponding demands by making the most of the availability of different resources. In this sense, the integration is more flexible since chemicals can be used to store energy as well as hydropower. Furthermore, solar and wind variability are considered to evaluate the effect on the process integration. The paper is organized as follows. Section 2 presents the technologies considered for the network. In section 3 we describe the model. We have divided the processes in subsections so that the intermediates can be

stored or used in various different processes such as syngas to hydrogen, ethanol or methanol. Section 4 presents results of the integration of renewables over time and under uncertainty, and the application of the network in a multi area system so as to evaluate the production of power and fuels to meet the demand of regions and countries. Finally, section 5 draws some conclusions.

## **2. Process network description.**

We consider a large number of renewable raw materials including biomass, lignocellulosic and waste, wind, solar and water. These sources are currently the basis for renewable based power and fuels in most countries because of their availability and transformation capabilities. Lignocellulosic biomass can be biochemically processed to bioethanol [27] or thermally transformed into syngas [28]. Syngas is a versatile building block that can be further used to produce power, hydrogen [7], ethanol [28], synthetic Fischer Tropsch (FT) liquids [29], methanol [9] or simply thermal energy [7]. Wind is used for power production [30], and solar energy can be transformed into power using PV panels [31] or mirrors, using Concentrated Solar Power (CSP) technologies. In this last case refrigeration systems are required and two alternatives are typically evaluated, namely, wet [32] or dry [33] cooling. Power can also be produced using hydropower facilities. When there is an excess of power produced, we can pump up water so that dams are used to store power too in the form of potential energy. Furthermore, waste can also be used to produce biogas and with it, power, using a gas and a steam turbine [34]. Alternative systems to store the excess of power produced can be the production of hydrogen via water electrolysis, and with it, methanol [14] or methane [30]. While methane can further be used in a gas turbine [34], methanol is used for oil transesterification in the production of biodiesel. Algae are also grown consuming CO<sub>2</sub>, and with it, produce biodiesel [35]. As we can see, renewables are fully interdependent and the integration is the natural step forward in the analysis. In the following subsection we describe the processes that have proved to be promising in the transformation of the above mentioned renewable raw materials into fuels, intermediate chemicals and power based on previous work.

### **2.1.-Wind energy**

The electricity is generated in a wind farm, consisting of a number of turbines, as a function of the wind velocity over time. The wind turbine investment costs are around 1500 €/kW [36].

## 2.2.-Solar energy

### 2.2.1.-PV solar

Solar photovoltaic panels are used to transform solar energy into power. The installation cost ranges from 1,700 to 4,000 \$ per kW installed [37], with a target of 1000 \$/kW [38].

### 2.2.2.-Concentrated Solar Power.

A CSP facility consists of three parts (see Figure 1): the heliostat field including the collector and the molten salts storage tanks, the steam turbine, and the cooling system. The tower collects the solar energy, heats up a transfer fluid, and produces steam for a regenerative Rankine cycle. The steam is generated in a system of three heat exchangers where water is heated up to saturation, and then evaporated using the total flow of molten salts. A fraction of the molten salts is used to superheat the steam before it is fed to the first body of the turbine. The rest are used for the regenerative part of the Rankine cycle. Both flows of salts are used to evaporate the water that has been condensed from the exhaust of the turbine. In the second body of the turbine, part of the steam is extracted at medium pressure and is used to heat up the condensate. The rest of the steam is finally expanded to an exhaust pressure, condensed and recycled. We evaluate the use of cooling towers, whose operation requires water [32], or air cooler condensers with an A-frame design [33].

Special attention is paid to the cooling system. Either wet or dry cooling are common technologies. The use of wet cooling consumes fresh water. When air coolers, typically A-frames, are used, a fraction of the power produced is required to run the fans. The amount of power or water required to condense the exhaust steam from the turbine depends on the ambient conditions.

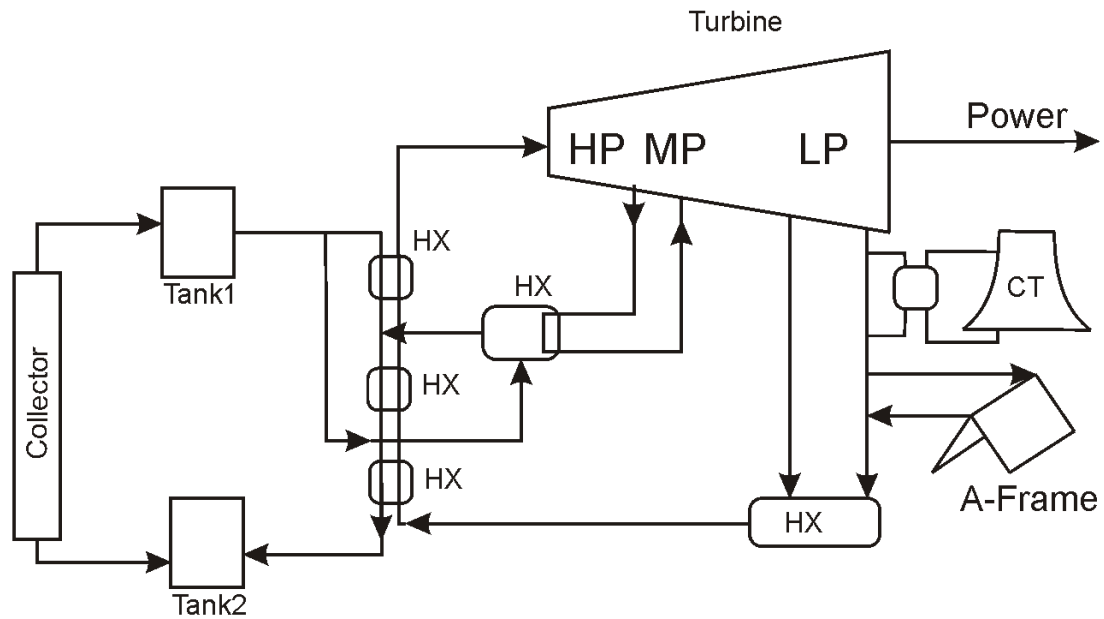


Figure 1.- Concentrated solar power facility. HX: Heat Exchanger; CT: Cooling tower. HP: High pressure. MP: Medium pressure;

### 2.3.-Hydropower

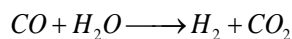
Small-scale hydropower facilities are normally designed to use river flows, otherwise dams are built to store water and use its potential energy to produce power. The idea is to couple the system with pumps so that, if there is an excess of energy, water is accumulated at a high elevation to store energy in the form of potential energy. The investment costs of large (>10 MWe) hydropower plants range from \$1750/kWe to \$6250/kWe. It is very site-sensitive, with a typical figure of about \$4000/kWe (US\$ 2008). The investment costs of small (1–10 MWe) and very small ( $\leq 1$  MWe) hydro power plants (VSHP) may range from \$2000 to \$7500/kWe and from \$2500 to \$10,000/kWe, respectively, with average costs of \$4500/kWe and \$5000/kWe. Operation and maintenance (O&M) costs of hydropower are between 1.5% and 2.5% of investment cost per year. The resulting overall generation cost is between \$40 and \$110/MWh (typical \$75/MWh) for large hydropower plants, between \$45 and \$120/MWh (typically, \$83/MWh) for small plants, and from \$55 to \$185/MWh (\$90/MWh) for VSHPs [39].

## 2.4.-Biomass

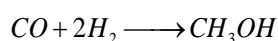
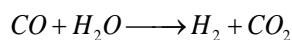
### 2.4.1.-Lignocellulosic

**Gasification of lignocellulosic biomass** at high temperature, 850-1000 °C, yields a mixture of carbon monoxide and hydrogen, syngas, see Figure 2. Raw syngas is produced in the gasifier using steam and oxygen as fluidification agents. Before further use, a train of clean up stages is required. First, it has to be processed to remove hydrocarbons by means of a reforming stage using steam. Next, solids are to be removed using either a scrubber or a filter system. Subsequently, its composition may need to be adjusted for the proper H<sub>2</sub> to CO ratio, and finally sour gases, CO<sub>2</sub> and H<sub>2</sub>S, must be removed to avoid catalyst poisoning. Syngas is a very versatile raw material for producing chemicals such as hydrogen, methanol, ethanol or more complex ones such as Fischer – Tropsch liquids.

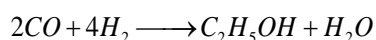
-The production of hydrogen is based on the well known water gas shift reaction where steam is used to drive the equilibrium to the production of hydrogen. In situ recovery of hydrogen is possible using membrane reactors [7]



-The mechanism for producing methanol or ethanol is based on a Fischer-Tropsch type of synthesis. The production of methanol is governed by the following set of reactions that take place at 200°C and 50 bar [9]. The purification of the products typically consists of the separation and recycle of the unconverted gases and the dehydration of the methanol using a distillation column or molecular sieves.

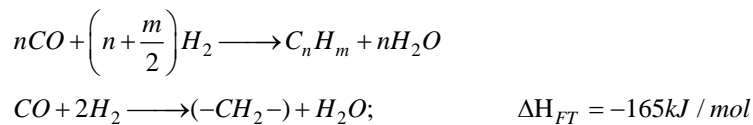


-Ethanol production consists of allowing the carbon chain to grow a little further. Therefore, a part from ethanol, methanol, propanol and butanol are also produced. The reactor operates at 300°C and 68 bar, where the desired reaction is shown below. After the recovery of the unreacted gases and its recycle, a sequence of distillation columns is required to obtain flue grade ethanol [28]



-FT-Liquids production: The idea is to grow the carbon chain from the radical -CH<sub>2</sub>- by constantly adding CO to the previous piece on the surface of the catalyst. The production of a particular chemical is based on controlling the growth and the termination of the chain. Thus, diesel substitutes are typically

produced by operating the reactor at 30 bar and 212 °C. The gas products can be used as fuel. Next, the two-phase liquid mixture is separated to remove the aqueous phase, while the organic phase is sent to an atmospheric distillation column. In order to increase the yield to fuels, the heavy components are broken down using hydrocracking, and the mixture is fed to the same distillation column used for the separation of the mixture obtained in the reactor [29].



The production of methanol, ethanol and FT-liquids generate thermal energy, but most importantly in the case of FT-liquids, a flue gas is produced that can also be used to produce heat [40].

We can also use syngas directly as a fuel to produce thermal energy in a furnace or power, using a gas turbine [7]. Figure 2 shows a block diagram of the process and the alternative uses of syngas. Further information can be found in previous papers [7,9,28,29].

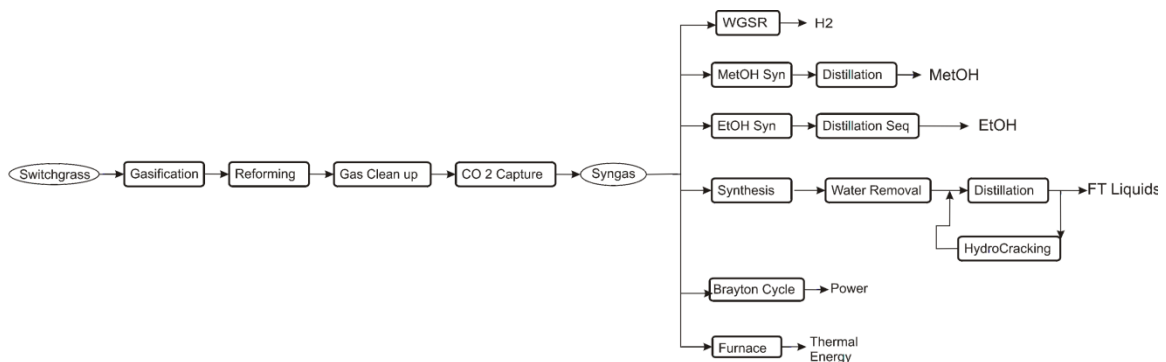
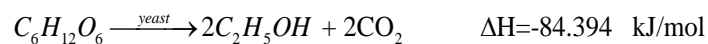
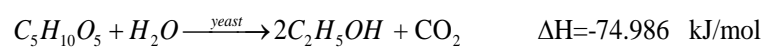


Figure 2.- Gasification based products diagram

**Fermentation:** Switchgrass is pretreated at 180 °C and using a solution of 0.5% sulphuric acid in water so that the structure of the grass is broken down. Next, enzymatic hydrolysis follows at 50°C the pre-treatment to obtain fermentable sugars, mainly xylose and glucose. Ethanol is obtained by fermentation of the sugars at 38°C under anaerobic conditions following the reactions below and reaching a concentration of 6-12% in water due to its poisonous effect in the enzymes.





In order to reach fuel quality ethanol, water must be removed from the water-ethanol mix. A three effect distillation column is used to remove most of the water before the final dehydration using molecular sieves [27]. The lignin obtained as a byproduct is used to provide energy for the process and the excess can be used within the network. Figure 3 shows the scheme of the process.

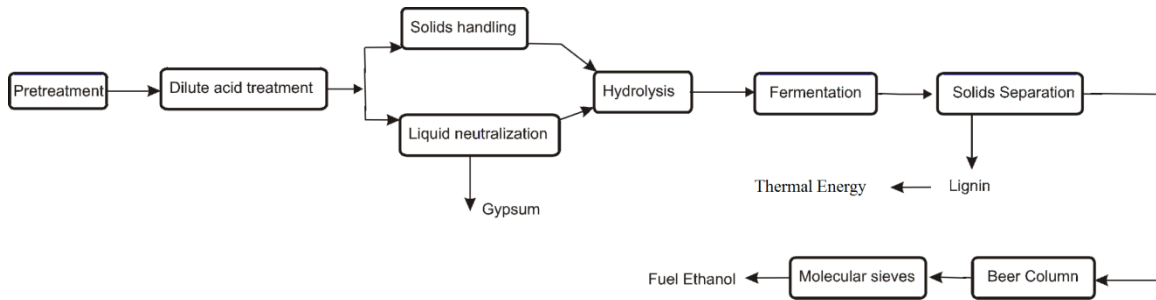


Figure 3.- Biochemical process to second generation bioethanol

#### 2.4.2.-Waste: Biogas

Anaerobic digestion is a biological process performed by many classes of bacteria on a large number of biomass types to produce biogas at 35-55°C depending on the type of bacteria. The largest biogas production yield takes place at 55°C using thermophilic ones. The digestion as such consists of four steps: hydrolysis, acidogenesis, acetogenesis, and methanogenesis. The actual biogas composition, from 50-70% in methane and 30-40% CO<sub>2</sub>, with small amounts of N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>S and NH<sub>3</sub> depends on the raw material, as well as the yield from biomass to biogas. The biogas must be cleaned from H<sub>2</sub>S and traces of ammonia using adsorbent beds operating at 50°C and 25°C and 4.5 bar, respectively, before being used to produce power. The CO<sub>2</sub> present in the gas can also be removed using pressure swing adsorption (PSA) at 4.5 bar and 25°C. The upgraded gas is used in a gas turbine. The high temperature of the exit gases make them useful for the production of steam, and a steam turbine can be used to enhance the power production of the facility [34]. The exhaust of the steam turbine must be cooled down. The same cooling technologies as for the CSP plants can be used.

#### 2.4.3.- Algae

Algae are a rich raw material with a high yield compared to other biomass sources [41]. Its composition as biomass consists basically of carbohydrates (starch), lipids, and proteins. There are a number of options to grow the algae. We can distinguish between raceway ponds (circular, tanks, paddlewheel raceways) or photo reactors (airlift, tubular, bag cultures). The first ones are simple civil

engineering structures with small depth that are filled with water where the algae grow using CO<sub>2</sub> or other carbon source and nutrients [42]. The algae growth depends on the solar incidence and the carbon intake. Another option is the use of photoreactors. The design of this equipment is more complex to allow solar energy to reach the algae. Oil has to be extracted from the algae biomass. The extraction consists of the use of mechanical action and solvents. The solvent is recovered using a distillation column and the oil sent to the next stage. The production of biodiesel from oil is based on the transesterification reaction of the oil with alcohols. The transesterification is an equilibrium reaction between the oil and alcohols. For economic reasons, methanol has been used for a long time. From the technical point of view, it provides high yield to biodiesel, fatty acid methyl ester (FAME), and quick reaction times. The excess of alcohol used to drive the equilibrium to products is recovered in a distillation column whose bottoms operate below 150°C to avoid glycerol decomposition. If heterogeneous catalyst is used, no washing stage is needed, and a simple liquid-liquid separator allows recovering the glycerol phase from the biodiesel phase. Biodiesel is purified in another distillation column that operates under vacuum to avoid biodiesel decomposition, which occurs above 250°C. Figure 4 shows the block diagram from algae to biodiesel [35]

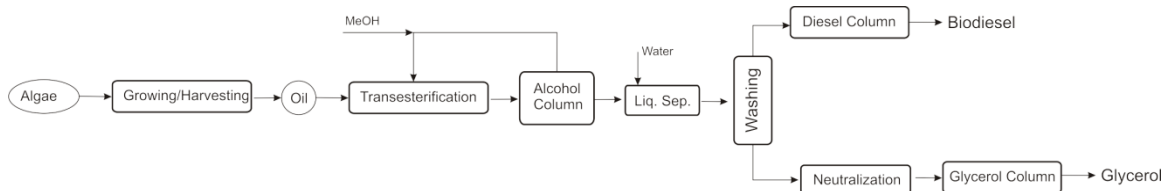


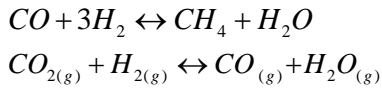
Figure 4.- Block diagram fro biodiesel production

## 2.5.-Chemicals from power

Electric power can be used to produce hydrogen, which is a promising energy carrier. It can also be used to produce hydrocarbons from CO<sub>2</sub>. The process consists of an electrolyzer, an oxygen purification section, a hydrogen processing section, and the synthesis part as seen in Fig 5. Both gas phases from the electrolyzer must be dehydrated. The oxygen stream is cooled down to condense water at 25°C. Next, molecular sieves are used to dehydrate the stream before compression and storage. The hydrogen stream also requires oxygen removal. A deoxo reactor operating at 90°C is used, and the dehydration stage is located downstream the deoxo reactor since it produces water. The hydrogen is now mixed with CO<sub>2</sub> taking in consideration that in order to avoid carbon deposition on the catalyst, a proper ratio of reactants is

required. Then, the gas phase is adjusted to the optimal operating conditions required by the reactor using a compressor and a heat exchanger [30].

The production of methane [31] takes place following the well know methanation reactions at 370°C and 30 bar. The unconverted gases and the water produced are separated and recycled.



Recently methanol [14] has also been produced. The reactions are similar to the ones presented above for the use of syngas, as well as the purification stage as seen in Figure 5. While methanol can be further used in the transesterification of the oil, the methane can be used to produce power using a system consisting of a gas turbine whose exhaust gas is fed to a steam turbine [33]

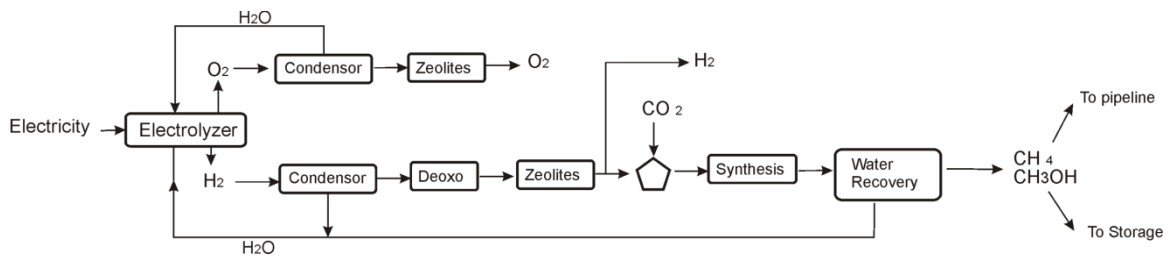


Figure 5.- Block diagram for power to chemicals

### 3. Modelling approach

#### 3.1.-Network modeling

The processes involved in the network, and described in the previous section, are shown in Figure 6. Table 1 provides further information on the transformation stages of the renewable sources into power and intermediates until final products, identifying the technologies with the nomenclature PX for easy reference to Figure 6.

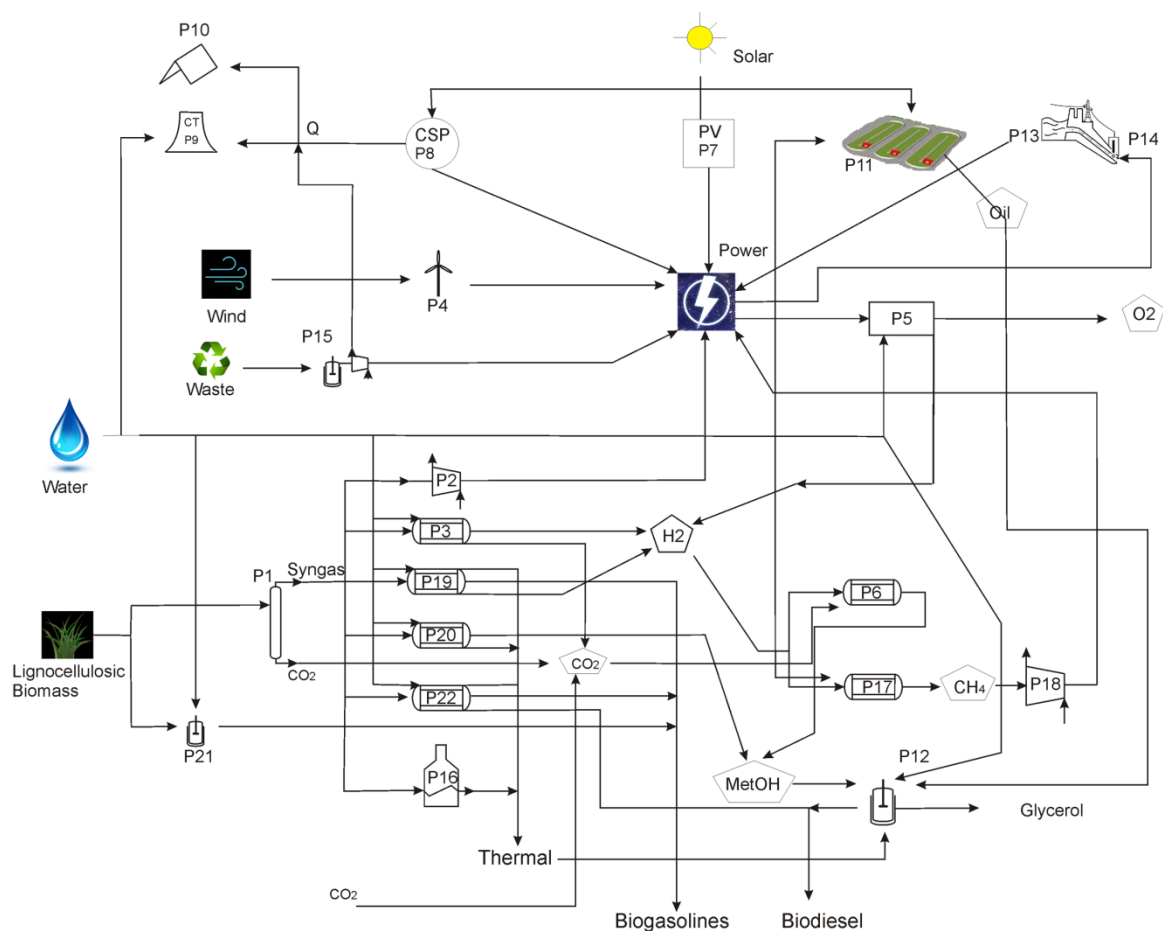


Figure 6.- Renewable base network for power and transportation fuels production. P1: Biomass gasification; P2: Syngas Brayton cycle; P3: Hydrogen production; P4.- Wind turbine farm; P5: Electrolyzers; P6: Methanol production from CO<sub>2</sub>; P7: Photovoltaics; P8: Concentrated solar power; P9: Wet cooling towers; P10: A frame cooling system; P11: Algae ponds; P12: Oil transesterification; P13: Hydropower; P14: Hydropower storage; P15: Anaerobic digestion and power production; P16: Biomass based thermal energy; P17: Methane production from CO<sub>2</sub>; P18: Methane based gas turbine; P19: Bioethanol production from syngas; P20: Methanol production from syngas; P21: Bioethanol production hydrolysis; P22: FT liquids production.

Table 1.- Set of raw materials, transformation technologies and main products

The network is formulated by sections instead of complete processes. For instance, biodiesel production, represented in Figure 5, consists of oil production and the transesterification section. Thus, P11 refers to oil production from solar energy and CO<sub>2</sub> while P12 represents the transesterification section, see Figure 7.

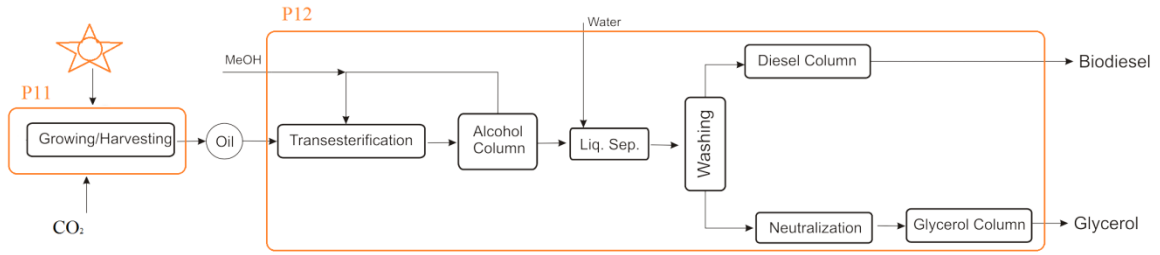


Figure 7.- Modelling approach for process network development.

Each of the sections is modeled as black boxes considering inputs and outputs following the principles in previous work [14]. For each of the sections a main input is identified. This variable, a mass or an energy flow, has been used as the reference to compute the operation of that process, as well as the production of a product, or a number of products, or the needs that are required for it to operate. The main input for the different units is as follows: for wind, its velocity (m/s); for solar, the incidence (kWh/m<sup>2</sup>d), for biomass, waste and water the flow in a period in kg or m<sup>3</sup> per second available. Thus, the input-output black box models are characterized by conversion and feed factors,  $K_i$  and  $Q_i$ , which have been computed out of detailed optimization models described in section 2. Revisiting our example in Figure 7, for P11, the main input is solar energy and produces oil. Apart from the main input, any process also consumes other raw materials or utilities. In the production of biodiesel, P12, apart from the main feed oil, the principal raw material, methanol and thermal energy are also required. Thus, the sections models are written as follows:

$$\begin{aligned} \text{Prod}_i(\text{process}, t) &= K_i \cdot \text{In}(\text{process}, t) \quad \forall t, i \in \{\text{Raw materials}, \text{Wind}, \text{Solar}, \text{Heat}\} \\ \text{Feed}_j(\text{process}, t) &= Q_j \cdot \text{In}(\text{process}, t) \quad \forall t, j \in \{\text{Raw materials}, \text{Heat}\} \end{aligned} \quad (1)$$

The models of each one of the individual processes can be found in the supplementary material along with the tables for coefficients  $K_i$  and  $Q_i$ . The aim of the network is to substitute power and fuels demand. For the case of power, an energy balance accounts for the power generated by the various technologies and that consumed internally, eq. (2)-(3). Note that the aim is not to use fossil based resources, and therefore any power or thermal energy that the processes require must be produced internally in the network and sometimes in the same spot such as the case of the need for thermal energy.

$$\text{Power}_{\text{gen}}(t) = \sum_{\text{process}} \text{PowerP}(\text{process}, t) \quad \forall t, \text{process} \in \{2, 4, 7, 8, 13, 15, 18\} \quad (2)$$

$$\text{Power}_{\text{use}}(t) = \sum_{\text{process}} \text{PowerP}(\text{process}, t) \quad \forall t, \text{process} \in \{5, 10, 14\}$$

$$\text{Power}_{\text{gen}}(t) - \text{Power}_{\text{use}}(t) \geq \text{DemandP}(t) \quad \forall t \quad (3)$$

Power demand actually depends on the holiday periods and larger consumption is expected during winter, December-January, July-August, and Easter. Thus, with respect to the annual average, we assume the following normalized profile in the 12 months:

[1.1, 1, 0.9, 0.85, 0.95, 1, 1.1, 1.2, 1, 0.85, 0.9, 1.15].

The same profile is used for gasoline and diesel

The biogasoline produced corresponds to the production of ethanol via process P19 or P21 or the green gasoline from the FT process, P22. However, since the energy content in ethanol is lower than that in gasoline, we correct the production by a factor,  $\gamma$ , equal to 1.5, assuming the same density for both.

$$\text{Biogasoline}_{\text{prod}}(t) = \frac{1}{\gamma}(\text{Production}(\text{P21}, \text{Out1}) \cdot \text{Biomass}_{\text{use21}}(t) + \text{Production}(\text{P19}, \text{Out1}) \cdot \text{Syngas}_{p19}(t) + \text{Production}(\text{P22}, \text{Out1}) \cdot \text{Syngas}_{p22}(t)) \quad \forall t \quad (4)$$

Similarly, the renewable diesel produced is that obtained from biodiesel as well as that from the FT process. However in this case the correction factor between diesel and biodiesel is almost 1, thus we assume it to be 1.

$$\text{Biodiesel}_{\text{prod}}(t) = \text{Production}(\text{P12}, \text{Out1}) \cdot \text{Oil}_{\text{use}}(t) + \text{Production}(\text{P22}, \text{Out2}) \cdot \text{Syngas}_{p22}(t) \quad \forall t \quad (5)$$

Biodiesel requires thermal energy to operate. It has to be produced internally in the same province as that where the transesterification takes place. There are some technologies that produce thermal energy as byproduct, such as ethanol, methanol and FT fuels production, P19-P22, or we can produce it directly by burning syngas, P16.

$$\text{ThermalE}(\text{P12}, t) \leq \text{ThermalE}(\text{P19}, t) + \text{ThermalE}(\text{P20}, t) + \text{ThermalE}(\text{P16}, t) + \text{ThermalE}(\text{P21}, t) + \text{ThermalE}(\text{P22}, t) \quad \forall t \quad (6)$$

Among the various products and intermediates, we allow storage of hydrogen, methane or methanol. For the first month we do not assume any initial storage. From that point on, a mass balance at each time period is formulated between the stock, the produced amount and the one used. We also assume that the  $\text{CO}_2$ , as a raw material, is either produced in the production of syngas or hydrogen from biomass, or can be imported from a fossil source,  $\text{CO}_{2,\text{fossil}}$ . The  $\text{CO}_2$  is used to produce methanol or synthetic methane via hydrogenation.

$$\text{CO}_{2,\text{Fossil}}(t) + \text{CO}_{2,\text{P1}}(t) + \text{CO}_{2,\text{P3}}(t) \geq \text{CO}_{2,\text{P11}}(t) + \text{CO}_{2,\text{P17}}(t) + \text{CO}_{2,\text{P6}}(t) \quad \forall t \quad (7)$$

There is an area limitation for the installation of PV panels, mirrors and ponds. Initially we establish it to be 1% of the area available. We assume that the turbines do not require this area. The complete model is described in the supplementary material. Similarly, water consumption by processes must be available locally. The complete model can be found in the supplementary material for reference.

### 3.2.-Cost correlations

The investment cost of each one of the processes or sections has been estimated using only the units involved in the sections that have been selected. It is based on the units cost as described in previous papers [28]. The units cost is estimated as a function of the mass or energy flow that they process. The factorial method is used to compute the investment cost of the section of the facility. The method and the correlations are found in [28].

The production cost of each section does not consider intermediates as a cost, since these costs correspond to the sum of the production costs of each of the stages from the actual raw materials, biomass, solar energy, wind energy, etc to the chemical. Thus, each section comprises the cost of operating that section including utilities. Thermal energy is produced within the network. Since we need steam in most cases, we still consider the cost of the steam since we need to transform the thermal energy generated into the proper steam used at each stage

The process has to handle the largest of the flows over time. Thus, we define design variables that will also determine the investment cost as follows:

$$\text{FlowD} \geq \text{Flow}(t) \quad \forall t \quad (8)$$

For the cost correlations we have two types of models, linear and piecewise linear:

#### Linear correlations

The only raw material that we actually pay for is biomass and it is assumed at a cost of \$50/t. The rest is produced internally, and the waste used to produce biogas, we provide treatment for it. Thus, the cost for these sections, P1-P8, P10-P11, P13-P22 is given by eqs. (9)-(10). The coefficients in the equations can be found in the supplementary material, Table 3S.

$$\text{Cost}_{\text{Invest}}(\text{Process}) = \alpha_1 \cdot \text{DesignVar} + \beta_1 \text{YProc}(\text{Process}); \quad (9)$$

$$\text{Cost}_{\text{Prod}}(\text{Process},t)=\alpha_P \cdot \text{DesignVar}(\text{Flow}) + \beta_P Y_{\text{Proc}}(\text{Process}); \quad (10)$$

### Piecewise linear approximations

For a number of facilities either the investment cost P9, P11, P16, P18, or both the investment and the production costs, P12 & P19 are nonlinear. Therefore, a piecewise linear approximation is developed for prespecified capacities,  $\gamma$ . The cost correlations are then written as piecewise linear approximations as given by eqs. (11)-(14). Table 4s in the supplementary material shows the discretization points.

$$\text{Design}_{\text{Variable}} = \sum_{\gamma} D_{\text{in}}(\gamma) \cdot \lambda_{\text{Process}}(\gamma); \quad (11)$$

$$1 = \sum_{\gamma} \lambda_{\text{Process}}(\gamma) \quad (12)$$

$$\lambda_{\text{Process}}(1) \leq Y_P(1)$$

$$\lambda_{\text{Process}}(\gamma) \leq Y_P(\gamma - 1) + Y_P(\gamma) \quad (13)$$

$$\sum_{\gamma} Y_P(\gamma) = 1$$

$$\text{CostP}(\text{Process}) = \sum_{\gamma} \lambda_{\text{Process}}(\gamma) \cdot \text{Cost}_E(\gamma) \quad (14)$$

Further details of the cost correlations can be found in the supplementary material.

The objective function is that given by the operating cost, eq. (15). The production cost is given by unit of time, thus, it is multiplied by the duration of the period,  $\tau_t$

$$\text{Cost} = \sum_{\text{Process}} \sum_t \text{Cost}_{\text{Prod}} \tau_t + \frac{1}{3} \text{Cost}_{\text{Invest}} \quad (15)$$

The model is extended to a network but applying it to particular regions in a geographic area. Thus, each of the variables will have another index, the region. As a result, Eq. (15) is also extended to consider transportation cost among regions. We consider distances computed from the longitude and latitude of the allocations. Furthermore, variables accounting for the transportation of intermediates and products are included. We consider that biogasoline, biodiesel, hydrogen, methane, oil, and methanol can be transported at a given cost from one region to another in need. Power can also be transmitted, but we neglect its cost.

### 3.3.- Environmental metrics

#### 3.3.1.-CO<sub>2</sub> mitigations

Apart from the economic objective function, we would like to evaluate the CO<sub>2</sub> mitigation of each of the networks to compare the effect of size and transportation on the CO<sub>2</sub> emissions. We use eq. (16) to



compute the mitigation of CO<sub>2</sub> since, within the networks, we do not allow any thermal energy, intermediate or power to be produced using fossil fuel but from renewable resources. See Table 2 for the coefficients.

Table 2.- CO<sub>2</sub> emissions [43-47]

$$\begin{aligned}
 \text{Enviromental} = & \sum_{\text{zone}} \sum_{\text{Process}} \sum_t (CO_{2,\text{fossil}} - CO_{2,\text{renew}})_{\text{mitigated}} \cdot \text{EnergyGen}(t, \text{zone}, \text{Process}) - CO_{2,\text{Water}} \cdot \text{Water}(t, \text{zone}, \text{Process}) \\
 & + CO_{2,\text{Used}}(t, \text{zone}, \text{Process}) - \sum_{\text{zone}} \sum_{\text{zone}} \sum_t \sum_i CO_{2,\text{emission,trans}} d(\text{zone}, \text{zone}) \cdot M_i(t, \text{zone}, \text{zone})
 \end{aligned} \tag{16}$$

### 3.3.2-Sustaniability metric

When considering processes, there are three pillars that evaluate their sustainability. So far we have discussed two, economic and environmental. However, there is a third item which is related to the social impact. Recently a new metric has been developed [48], RePSIM, that includes all three. We use this metric to evaluate the sustainability of the network at different scales since the location of production facilities affect not only cost but to the wealth generated across the map. The metric is given by eq. (17):

$$\text{RePSIM} = -P + (M + B - F - \text{RM} - E - W) \cdot C_{\text{CT}} - I \cdot (C_{\text{Annual}}) + \text{JS} + (F \& F_A + F \& F_B) \tag{17}$$

where

B: CO<sub>2</sub> mitigated due to the production of a byproduct (kg CO<sub>2</sub>/yr):

C<sub>Annual</sub> Annual coefficient

C<sub>CT</sub> : Carbon tax (€/kg)

E : CO<sub>2</sub> generated or mitigated due to Energy consumption/production (kg CO<sub>2</sub>/yr)

F: CO<sub>2</sub> generated due to fertilizers production (kg CO<sub>2</sub>/yr):

F&F: Burden due to the impact of a raw material in the food industry \$/yr

I : Investment (€).

JS: Impact of the investment in the jobs generated (€/yr)

M: CO<sub>2</sub> mitigation by substitution of fossil resources by renewable ones kg CO<sub>2</sub>/yr)

P: Production costs (€/yr)

RM: CO<sub>2</sub> produced in the generation of a Secondary Raw material (kg CO<sub>2</sub>/yr)

W: CO<sub>2</sub> generated due to water consumption (kg CO<sub>2</sub>/yr)

### 3.4.-Problem formulation

Two different types of problems are solved. The first one is the design of deterministic integrated networks of renewable technologies. The problem is formulated as follows:

$$\begin{aligned}
 \min \text{Cost} = & \sum_{\text{Process}} \sum_t \text{Cost}_{\text{Prod}} \cdot \tau_t + \frac{1}{3} \text{Cost}_{\text{Invest}} \\
 \text{s.t} & \\
 \text{Network constraints} & \begin{cases} h(d, x(t), t) = 0 \\ g(d, x(t), t) \leq 0 \end{cases} \quad \forall t
 \end{aligned} \tag{F1}$$

d: Design variables

x: Operating flows

t: Period

The constraints are the mass and energy balances modeling each of the processes as well as the demand for fuels and power; see supplementary material. We use also as constraints the sustainability metrics. This formulation (F1) is applied to a province, section 4.1, and then extended to two larger scales, region and country level by including the transportation and transmission of fuels and power, (F1'), is applied in section 4.3 where index  $i$  represents each one of the locations. Thus, the network model presented in the supplementary material is applied to each one of the locations. Transportation of fuels and transmission of power is included as a cost too.

$$\min Cost = \sum_j \sum_{Process} \sum_t Cost_{Prod} \cdot \tau_t + \frac{1}{3} Cost_{Invest} + \sum_i C o s t_{Transportation}(i, j) \cdot d(i, j)$$

*s.t*

$$\text{Network constraints} \begin{cases} h(d, x, t, i) = 0 \\ g(d, x(t), t, i) \leq 0 \end{cases} \quad \forall t, i \quad (F1')$$

Goods exchange:  $m_{ij}(d, x(t), t) \leq 0$

d: Design variables  
x: Operating flows  
t: Period

Again, the constraints correspond to the mass and energy balances modelling each of the processes; see supplementary material.

The second type of application is the extension of (F1) to the design of process networks under uncertainty (F2). Solar, wind and demand are uncertain variables that affect the network design in terms of selection of technologies and inventory. The problem is formulated as a two-stage stochastic optimization problem (see section 4.2) where  $\theta_s$  represents scenario  $s$  for uncertain parameter  $\theta$ . For each of the uncertain parameters, three scenarios are considered with low, medium and high probability. We apply the formulation to the same province as F1 and only at province level for this case of study.

$$\min Cost = \frac{1}{3} Cost_{Invest} + \sum_s p(\theta_s) \sum_{Process} \sum_t Cost_{Prod}(\theta_s) \cdot \tau_t$$

*s.t*

$$\text{Network constraints} \begin{cases} h_s(d, x(\theta_s), t, \theta_s) = 0 \\ g_s(d, x(\theta_s), t, \theta_s) \leq 0 \end{cases} \quad \forall t, s \quad (F2)$$

d: Design variables  
 $x(\theta_s)$ : Operating flow for scenario  $s$   
t: Period  
 $\theta_s$ : Stochastic parameter for scenario  $s$ .

We annualize the cost of the investment using 1/3 [49]. In this work we aim at process integration and therefore a time period of months has been considered. Control and scheduling will be part of further work.

#### 4. Results and discussion

Data for the model does not only include process data, but also weather and demand data. The total amount 251,749 millions of kWh is distributed per region as a function of the number of inhabitants [50]. The same is true for the consumption of fuels. Spain consumes around 632 kg/s of diesel and 124 kg/s of gasoline [51]. We assume that 1% of the area can be devoted to solar panels, mirrors and/or ponds. Lignocellulosic biomass is already there, either because it is the residue of the agricultural industry, or it grows in the area. Water availability for hydropower is based on assuming that the current capacity can be expanded by 25% [52]. Typically the installed capacity is several times that produced regularly. That power is available to be used and distributed in the different regions by the number of habitants. Wind is determined from monthly maps [53]. Waste is computed by the amount generated per animal and the census of the Spanish government [54]. Solar irradiation is from the AEMET atlas [55]. Biomass resources are obtained considering three sources either forest residue [56], the straw that is not used by cattle [57] or perennial miscanthus [58]. We assume that the availability is evenly distributed over the year and over provinces based on their area with respect to the region.

We divide the presentation of results into two levels. First province level, which aims at the development of process integration for individual regions. We take advantage of the formulation and the information available to compare the effect of uncertainty in the renewable resources, wind, solar and biomass, in the evaluation of their use on the investment and the sustainability of the solution. The second level shows interconnection between provinces. In this case we compare two sizes, a region, since in Spain these regions have their own government, and the entire country. This second set is evaluated only as a deterministic problem where we use average values for wind velocities, solar and biomass availabilities. The aim is to evaluate the scalability of the model and the advantages of a larger integration, as well as the distribution in the use of resources when a more heterogeneous area, in terms of resources availability, is considered. For instance, the South of Spain shows large solar availability while to the North, larger lignocellulosic reserves are available.

#### 4.1.- Province scale.

This section evaluates the integration of technologies so that a particular small region, a province, operates on its own resources. In a second step, the effect of the uncertainty in the availability of the major renewable resources on the selection of technologies and the installation cost is considered. Note that biomass availability and its cost are not independent. Therefore, we use biomass variability as uncertain variable together with solar and wind availability and power demand.

##### 4.1.1.- Optimal deterministic multiperiod process integration.

We select one location with the characteristics shown in Table 3. Electricity is estimated by the total power required per inhabitant and the people living in that region. We assume that power, gasoline substitution and diesel substitution changes throughout the year depending on the holidays period as presented above and the weather. For instance, a larger amount of fuels is required in summer due to holiday season as well as in winter, because of the weather. We use the trends of Spain for that since the solar and wind velocities correspond to allocations in the South of Spain.

We apply the network to analyze the province level in Almeria in order to determine the optimal integration of renewable technologies to meet the electricity demand, and cover 20% of the gasoline and diesel demand of the local population over 12 time periods (months). The problem size of the multiperiod MILP is 1269 eqs. 985 var and 54 discrete variables. It was solved in less than 1 CPU min with CPLEX 12.6, in an Intel core i7 machine running Windows 10. Table 3 shows the main weather data for this location.

Table 3.- Input data for process integration

The renewable based network of technologies consists of 100 turbines and electrolyzers as well as 16551 ponds. We require  $2.9 \cdot 10^6$  m<sup>2</sup> of area for PV panels and  $1.610^7$  m<sup>2</sup> is used by the ponds. Electric power is produced using solar energy, PV panels, and wind turbines. Part of the power is used to produce hydrogen that is intended to produce the methanol needed for the transesterification of the oil. Diesel substitutes are only produced using this technology Thermal energy is also required to produce biodiesel. This type of energy is either produced together with ethanol from biomass via hydrolysis, or directly by burning biosyngas. By using this network 2.8 t/s CO<sub>2</sub> are avoided by the substitution of the fossil sources for electricity and fuels by renewables ones. The environmental metric reports a positive value of  $3.8 \cdot 10^8$

€/y. The high demand of diesel and its direct dependence on solar energy, results in the need to store oil along the year to be used during winter (see Figure 8). Figure 9 shows the consumption of water and CO<sub>2</sub> from fossil source used by the network over time. The investment required for the optimal economic solution is 3.4 billion €.

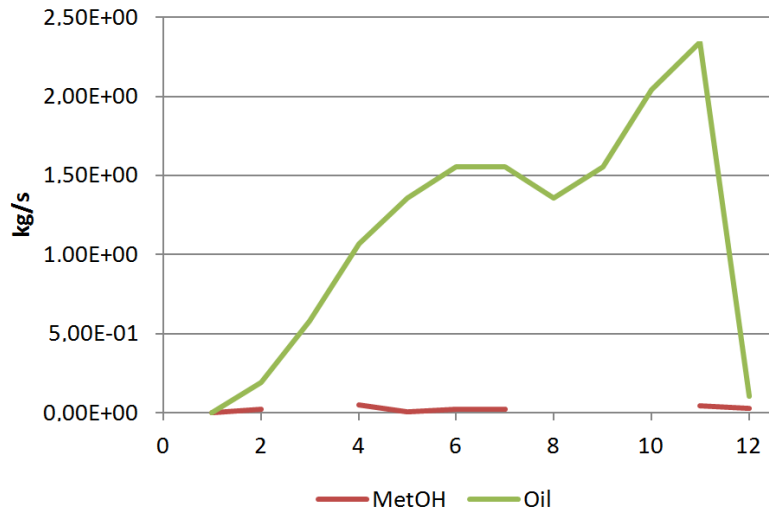


Figure 8.- Availability of stored chemicals over time

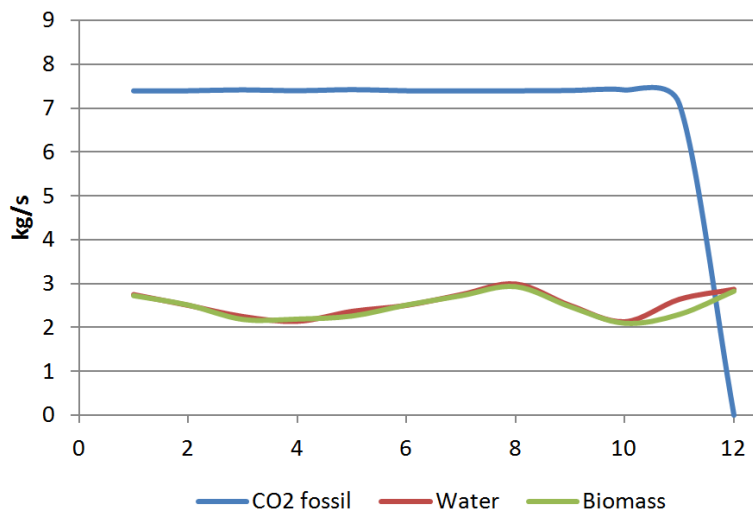


Figure 9.- Use of utilities and materials

4.1.2.- Optimal stochastic multiperiod process integration.

For the same province, Almería, we solve a two-stage stochastic programming model considering that power demand, solar, biomass and wind availability are uncertain. Note that biomass cost is directly related to its price. Therefore we do not consider biomass price as uncertain. For each of the parameters we consider three scenarios with a probability of low, medium and high. 81 scenarios per month are considered

for the 4 uncertain parameters. The aim is to determine the optimal integration of renewable technologies to meet the electricity demand, and cover 20% of the gasoline and diesel demand of the local population over 12 months. The problem size of the MILP formulation is 90,527 eqs. 66,265 var and 54 discrete variables that was solved with CPLEX 12.6, in an Intel core i7 machine running Windows 10, requiring 10 min CPU time.

We require 100 electrolyzers, 100 wind turbines and 18505 ponds.  $4.17 \cdot 10^6$  m<sup>2</sup> of solar PV panels and the rest of the area is used by the ponds. Figures 10 and 11 summarize the monthly average operation. Oil is stored over time so as to produce biodiesel for the months that have lower solar incidence. Process water consumption as well as biomass are consumed regularly, while CO<sub>2</sub> is mostly consumed during the first months of the year to produce the oil that is stored, and its consumption decreases by the end of the period. Compared to the deterministic solution, there is a larger investment of 4.0 billion €, so as to have flexibility in the operation. This is the result of the additional production of hydrogen from biomass and the addition of hydropower as well as the production of methane to be stored as a mean to store the punctual excess of power. Finally, the substitution of fuels is performed with bioethanol via hydrolysis of biomass and algae based, as well as with biomass based FT fuels.

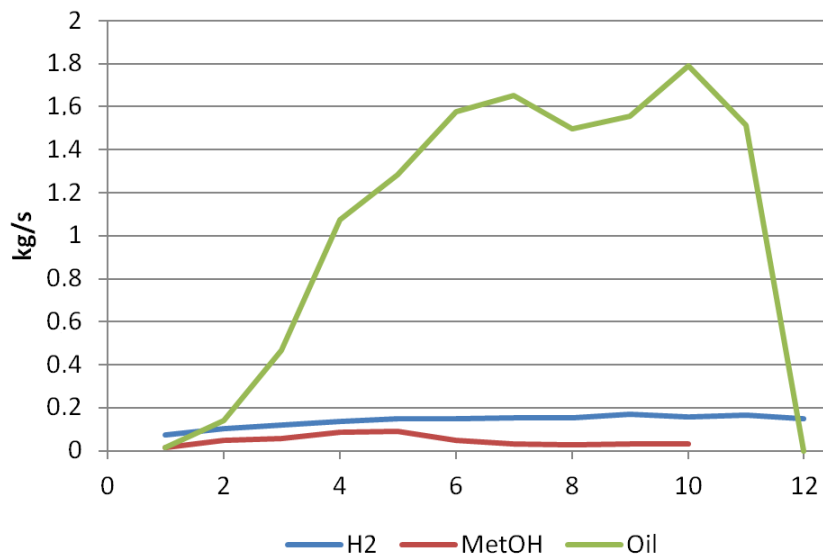


Figure 10.- Availability of stored chemicals over time under uncertainty

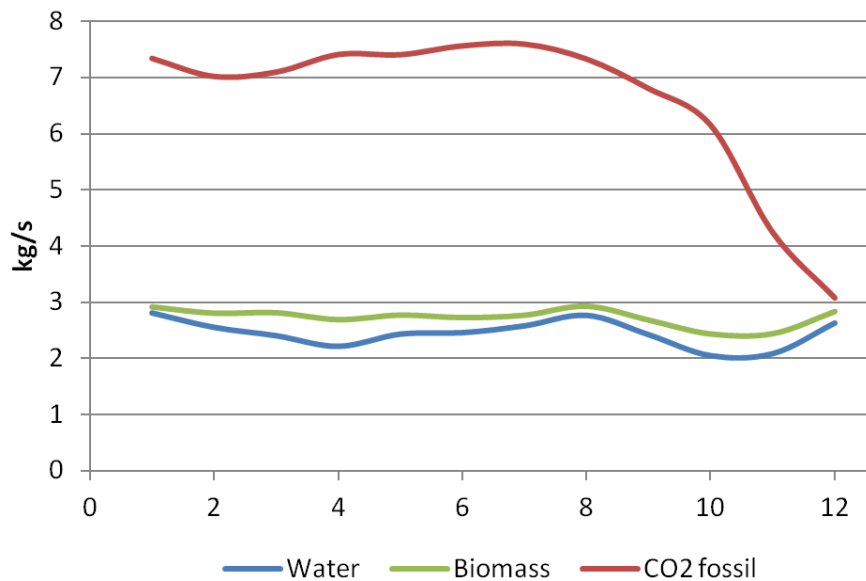


Figure 11.- Use of utilities and materials under uncertainty

This system is not only more robust, but it also shows larger positive RepSIM value of  $4.0 \cdot 10^8$  vs  $3.8 \cdot 10^8$  €/y. However, there is a slight reduction in the CO<sub>2</sub> mitigated, 2.7t/y of CO<sub>2</sub> vs 2.8t/y in the previous case, due to the duplication of technologies. In terms of the technologies selected, the system does not use biosyngas to produce power, but it produces hydrogen that is accumulated as a buffer.

#### 4.2.-Multiregional integration.

In this section we evaluate two integration levels deterministically, regional and national, in order to show the changes in the selection of technologies when a more integrated plan is in place, as well as to present how the problem scales in our attempt to reach the European level.

##### 4.2.1.-Small region (Andalucía)

The further step is to apply the model to a region of several provinces. We select Andalucía. It consists of 8 provinces, including the one used as individual case study above, Almería. It is located at the South end of Spain and it is characterized by high solar energy availability, and a couple of regions such as Almería and Cádiz, with high wind velocity. The idea is to apply the model of the network for each of the regions and determine transfer of intermediates and final products so as to meet the demand of each region. We add transportation costs for the liquids and gases based on the distance between every two locations.

Power, on the other hand, is assumed to be transmitted with no loss for free. In principle all the transfers are available, and the cost is based on the distance and the amount shipped will define which ones to use.

Again, we determine the optimal integration of renewable technologies to meet the electricity demand and cover 20% of the gasoline and diesel request of the local population. The problem size becomes 15,043 eqs. 18,795 var and 432 discrete variables and was solved with CPLEX 12.6, in an Intel core i7 machine running Windows 10, requiring 1min CPU time. The technologies selected to meet the power demand and to reach 20% fuel substitution, are presented in Figure 12. Each symbol represents a facility of a corresponding technology. Only the number of panels, ponds or the wind turbines are represented with one symbol for whichever number is required. The actual numbers are commented in the text for simplicity of the figure. The substitution of fossil based fuel and energy by renewable sources results in environmental disadvantages with respect to the province level, reporting a lower value in CO<sub>2</sub> mitigation, 2t/s, mainly due to transport. Furthermore, the RePSIM metric shows a positive value,  $4.0 \cdot 10^9$  €/y. The investment required to establish such a network over the 8 provinces region adds up to 40 billion €.

Hydropower is selected for all locations, providing a technology to store the excess of power when needed. Ethanol is produced from biomass hydrolysis in all the provinces except for province 7. This facility also produces thermal energy that is required for biodiesel production. Methanol is produced in the same provinces as those that produce biodiesel since it is required for oil transesterification, and transport is not recommended due to its cost. Only Huelva, province 5, does not produce biodiesel but it produces oil. Solar energy is used in the southeast, provinces 1 and 4, Almería and Cádiz, and only province 1 is selected for the installation of a wind farm of 100 wind turbines. As a result, the major producers of power are these two regions, see Figure 12. Biodiesel and biogasolines production is quite distributed, and most of the regions produce a fair amount of products reducing the transportation needs. Even though the production is distributed, provinces 2, 8 and 7 are the major producers of biodiesel.



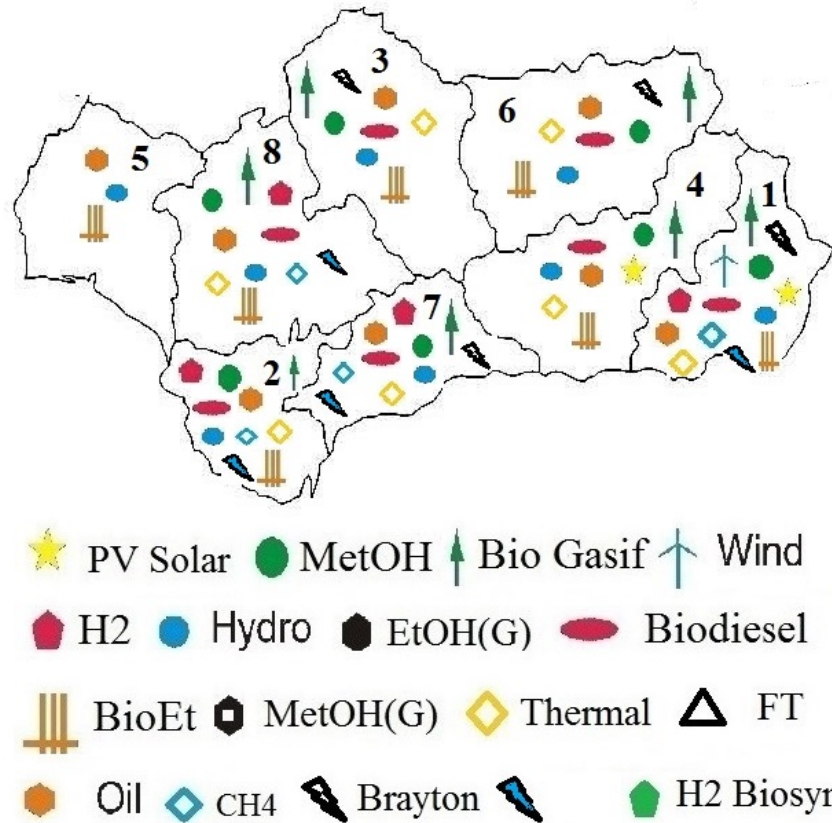


Figure 12.- Allocation of technologies in a region  
 1:Almería;2: Cádiz; 3: Córdoba; 4: Granada; 5: Huelva; 6: Jaén, 7: Málaga; 8: Sevilla.

The full profiles of the production of biodiesel, biogasolines power, methanol hydrogen and water can be seen in Figure 13. The production of liquid fuels is quite steady over time. Only a certain degree of oscillation can be seen in provinces 1,5 and 6 in the case of biodiesel. In the case of biogasolines substitutes, it is not that constant and we can see how provinces 2 and 1 & 6 are opposite in the production profiles showing a large profile in summer in Cadiz, province 2, while provinces 1 and 6 reduce their production over these months. In case of power, province 4 is the major producer and focusses its production over summer so that is mostly responsible for all power production. Province 1 complements region 4 during winter time. We see that the production of hydrogen and methane reaches a steady state from May onwards, actually, the storage of energy in the form of these two is quite obvious.

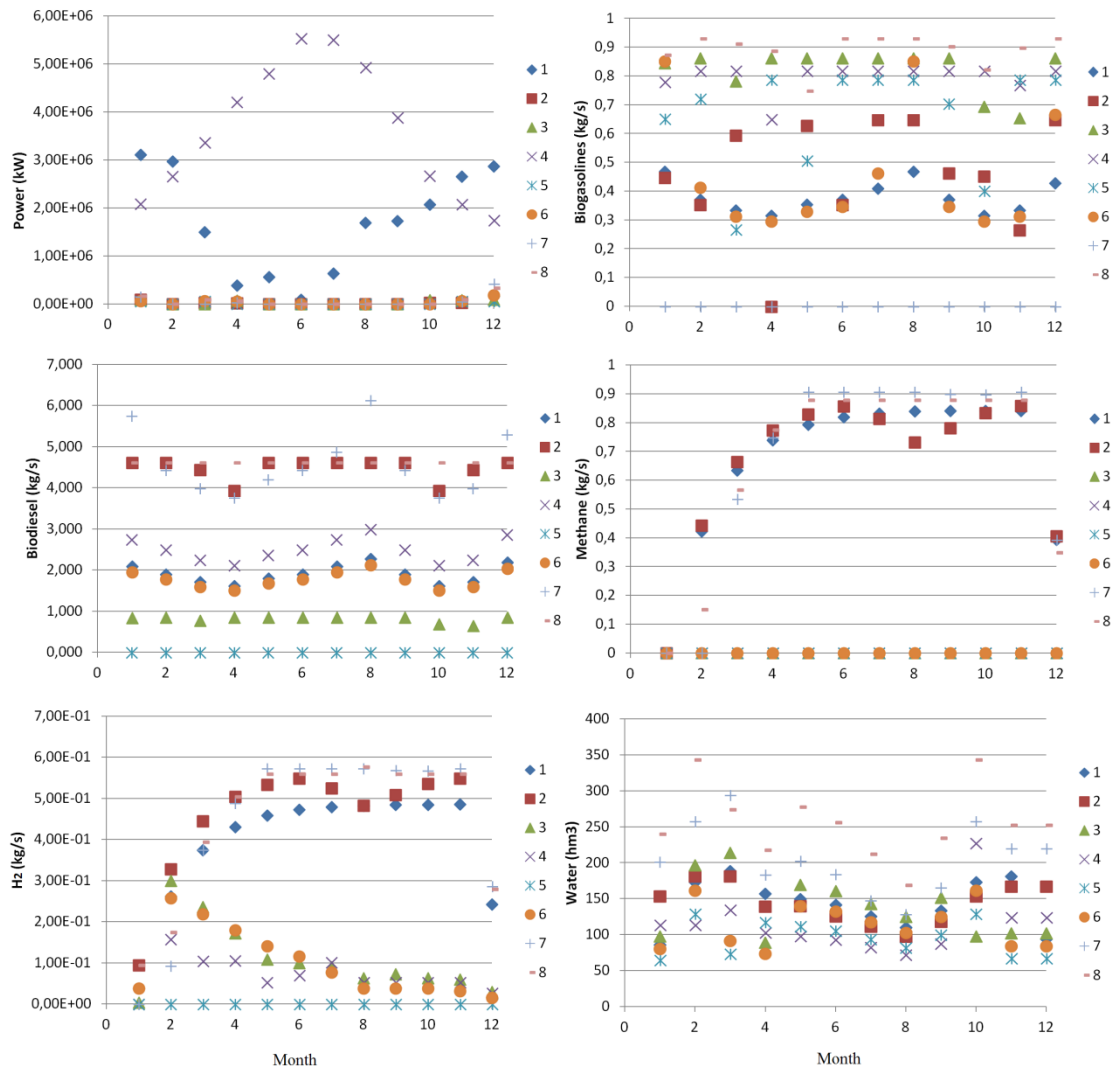


Figure 13.-Operation of the network.  
 1:Almería;2: Cádiz; 3: Córdoba; 4: Granada; 5: Huelva; 6: Jaén, 7: Málaga; 8: Sevilla.

The distributed production shown reduces the transportation of goods as seen in Figure 14. During the first month of the operation, there is quite a few transports of goods, mostly power, but also biogasolines. Province 7 receives gasoline. As it can be seen, typically province 7 is a net importer of gasoline over the year. Power is transferred from 1 and 4 to reach three where it is distributed. This pattern, as well as that of biogasoline, is common along the year; see April, July and October as representative months of the various seasons. The transported goods decrease over the year, see April. Solar energy increases allowing larger production of biodiesel and power. The increased demand during summer, see July as an example month, also increases the transport of gasoline, while fall is characterized by power, hydrogen as power storage, and a small amount of biogasoline transport.

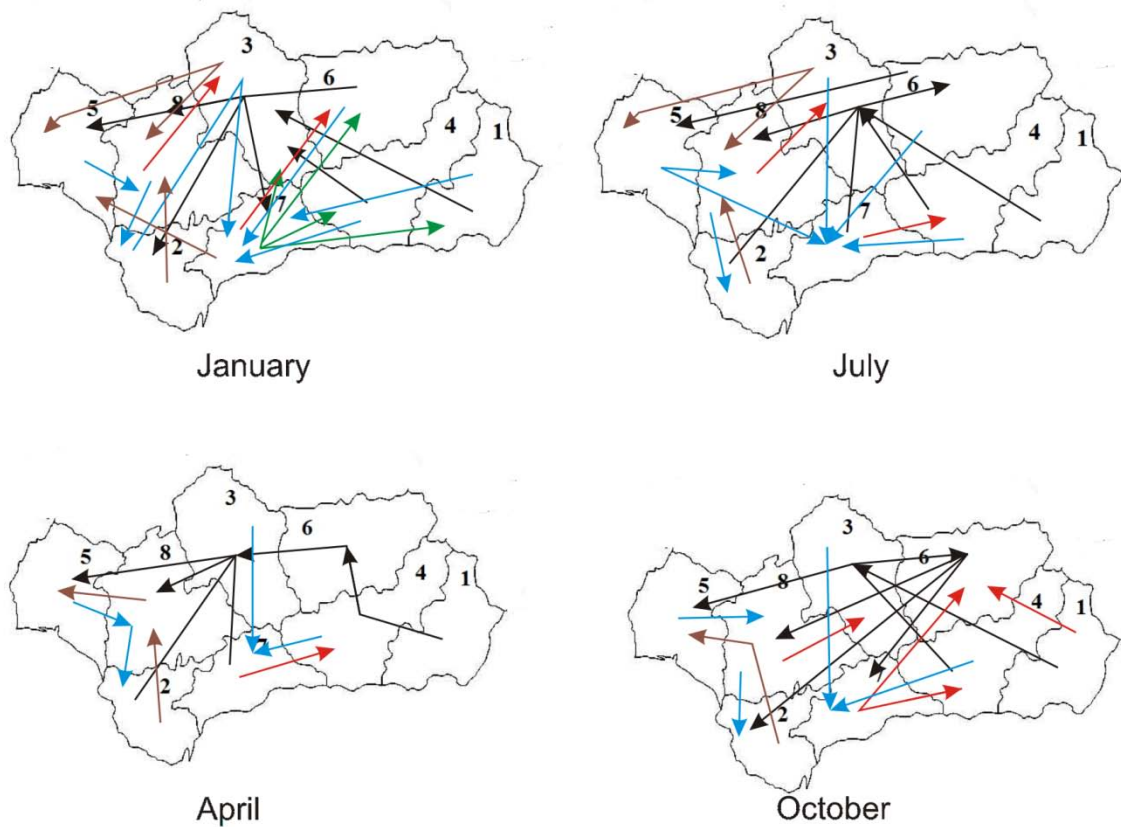


Figure 14.- Flows of mass and power in Andalucía (Black: Power ; Red: H<sub>2</sub>, Green: Methanol, Blue Gasoline, Biodiesel: Brown)

1:Almería;2: Cádiz; 3: Córdoba; 4: Granada; 5: Huelva; 6: Jaén, 7: Málaga; 8: Sevilla.

#### 4.2.2.-Country scale case of study: Spain.

Finally, we apply the optimal renewable based technology selection to the entire country, Spain. The same assumptions as for the smaller region still hold, as well as the source for the data. A total of 47 provinces are selected in the peninsular area. Again, we determine the optimal integration of renewable technologies to meet the electricity demand, and cover 20% of the gasoline and diesel demand. The problem size for the deterministic case becomes 240,596 eqs. 419,478 var and 2,538 discrete variables. It was solved with CPLEX12.6, in an Intel core i7 machine running Windows 10, requiring 25 min. We focus on minimizing the cost, but we also include results on the sustainability of the network. Figure 15 shows the optimal distribution of technologies across Spain for meeting the power demand, and reaching 20% of the fuels substitution. As in the case of the smaller region, each symbol represents a facility of the corresponding technology. Again, only the number of panels, ponds or the wind turbines are represented

with one symbol for whichever number is required. The actual numbers are commented in the text for simplicity of the figure.

The first comparison is with the smaller region presented in section 4.2.1, see Figures 12 and 15. It can be seen that the solution spreads the use of resources reducing the concentration of technologies in provinces such as 1,3,4,5. Bioethanol is no longer produced in almost all provinces. At the national level, biogasolines are no longer produced only using biomass hydrolysis, but gasification also plays a role for the production of not only bioethanol, but also methanol. At any scale, hydropower is recommended, but at national level no methane is used to store power. Biodiesel is no longer produced in provinces 1,3,4 since larger production centers are suggested at the national level. Comparing the south region in Figure 12 with Figure 15, we also identify other differences in the selection of technologies. For instance, solar energy is more widely used when the national scale is analyzed and provinces 1,2,4,6-8 use PV, together with 17 and 19. In the case when evaluating Andalucía alone, only province 1 uses PV panels. The reason may be the need to meet the demand of biodiesel since ponds already use a large area.

At the national level, areas of more concentrated use of technologies correspond to those with higher demand such as Madrid, Barcelona, Seville, Vasque Country and the Mediterranean coast, mostly to reduce transportation. Analyzing in more detail the solution at the national level, we start by the substitution of gasoline. Gasoline substitution is mostly accomplished by bioethanol produced from hydrolysis of biomass. Provinces that produce ethanol via hydrolysis are 3,4,11-12, 21,27,30,34-37, and 42. As it can be seen in Figure 16, the major producers of biogasoline substitutes are provinces 12, 13. A number of provinces produce between 2 and 3 kg/s of substitutes, in all cases these are typical facilities sizes in the biofuels industry. Most of the provinces produce a small amount, almost for self production. Gasification based ethanol is only used in a few provinces such as 2,7, 10, 23, 41, 46,47. The provinces rarely coincide with the ones that produce biodiesel. Provinces 2, 7 and 37 produce both ethanol and biodiesel even though ethanol is produced via hydrolysis in province 37 and via gasification in the other two. Biodiesel is produced across the territory in provinces such as 2,6,7,8,9,10,15,16,18,23, 25,26,32,33,37,41,46,47. In Figure 17 we see that the major producers of biodiesel are provinces 15, 26 and 33. We can also see that medium size facilities, producing from 2 to 9 kg/s follow the profile of the demand, with an increase in the production during summer. The pattern corresponds to the possibility of serving it across the country, but close to the

centers of larger consumption. Oil is locally produced in the same provinces as biodiesel, as well as methanol. Only few locations at the coast, provinces 20, 21, 30, 35 and 38 produce oil on its own. Taking a closer look, these provinces are situated in between provinces that produce biodiesel. Since biodiesel requires thermal energy, typically biomass is also used to produce the thermal energy required in the same province. FT liquids production can be seen in provinces 6,9, 14,16, 22, 24 and 33. These regions produce mostly biodiesel substitutes but a small amount of gasoline as byproduct of the FT process.

Figure 18 shows the production of power. We see that it follows the seasonality and it is focused on a few provinces such as 1,2,4, 17 and 19, corresponding to the ones with large solar availability. For the provinces that produce electric power using wind turbines, 100 wind turbines are installed at each one of the locations selected for that technology. The Mediterranean coast and the center of the peninsula use wind as power source. Note that wind turbines are already installed in central Spain, somehow validating the results obtained by the model. In the case of solar panels, as presented above in comparison with a smaller size region analysis, provinces 1,2,4,6-8 use PV. In all cases the area available for them is used. Note that the area available is distributed between ponds, panels and mirrors. In terms of ponds, there are only three locations producing oil that do not use the maximum number of 50000 ponds, 2, 7 and 17. Water availability is quite regular in all provinces, with minimum in summer and maximum in March, see Figure 19. With large availability we can find only a few ones, 10,11, 23, 20, 20, 32, 33, 37 and 40. However, the possibility of storing energy using dams, suggest the use of hydropower plants all over the territory.

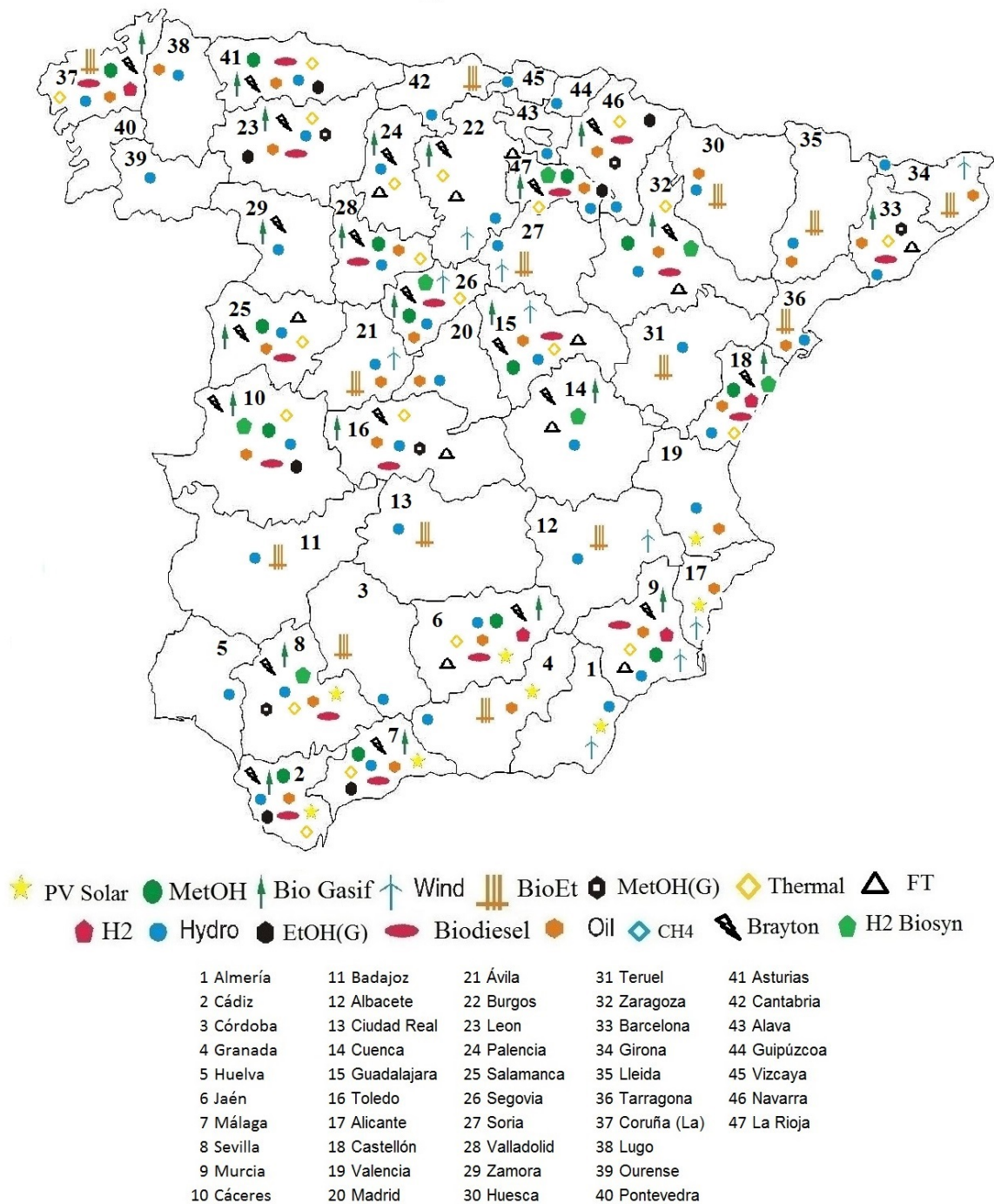
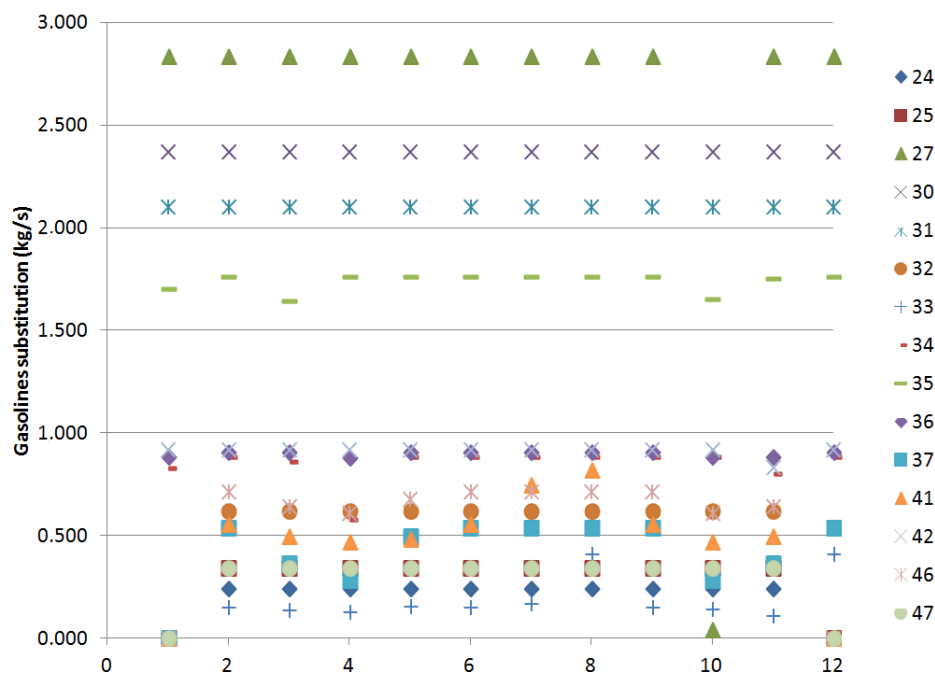
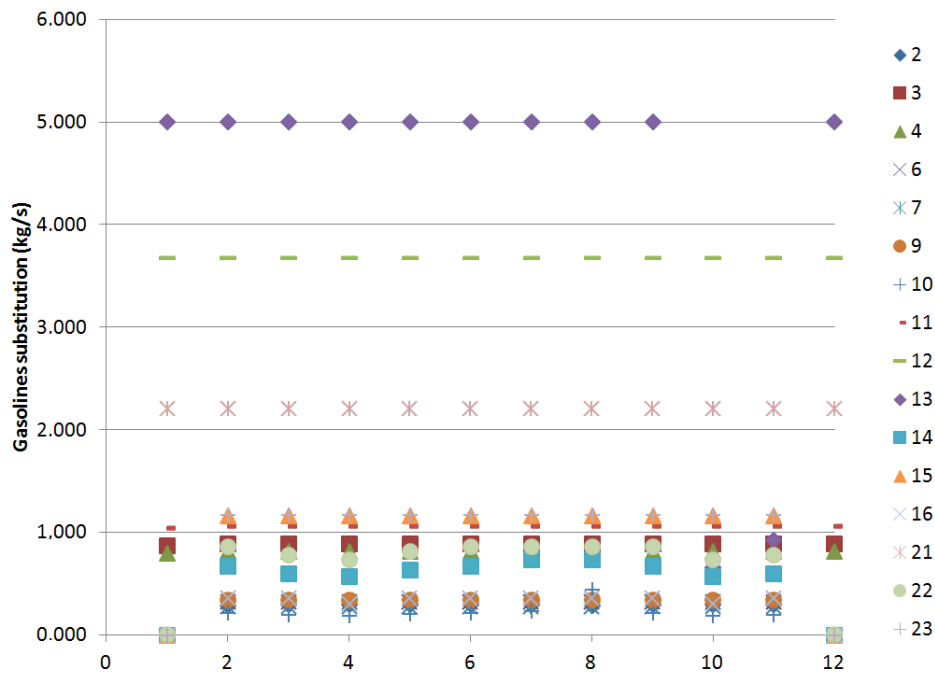


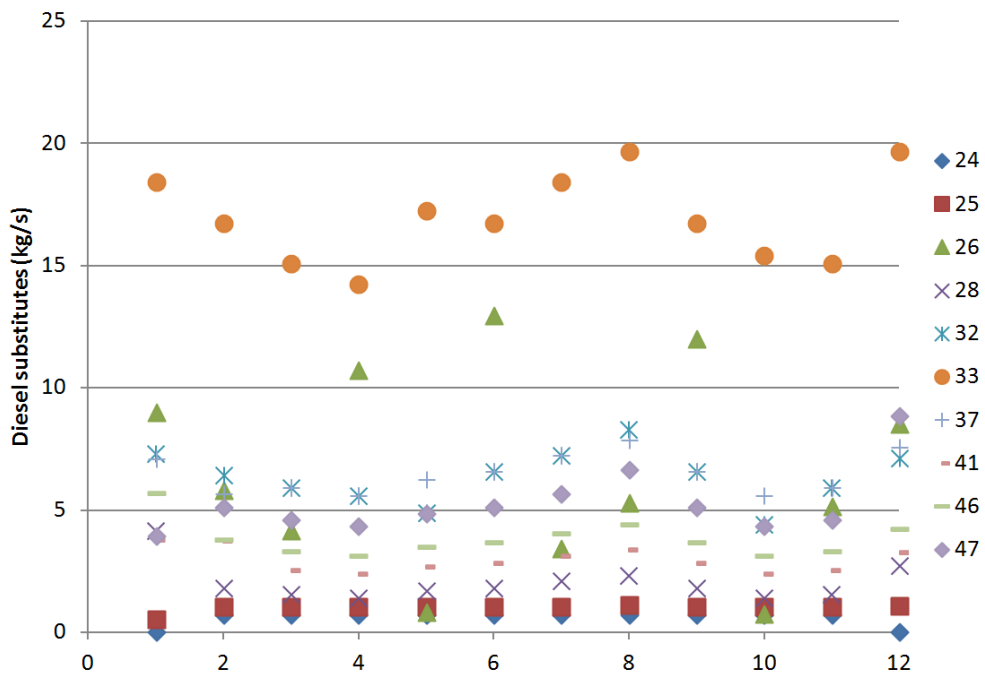
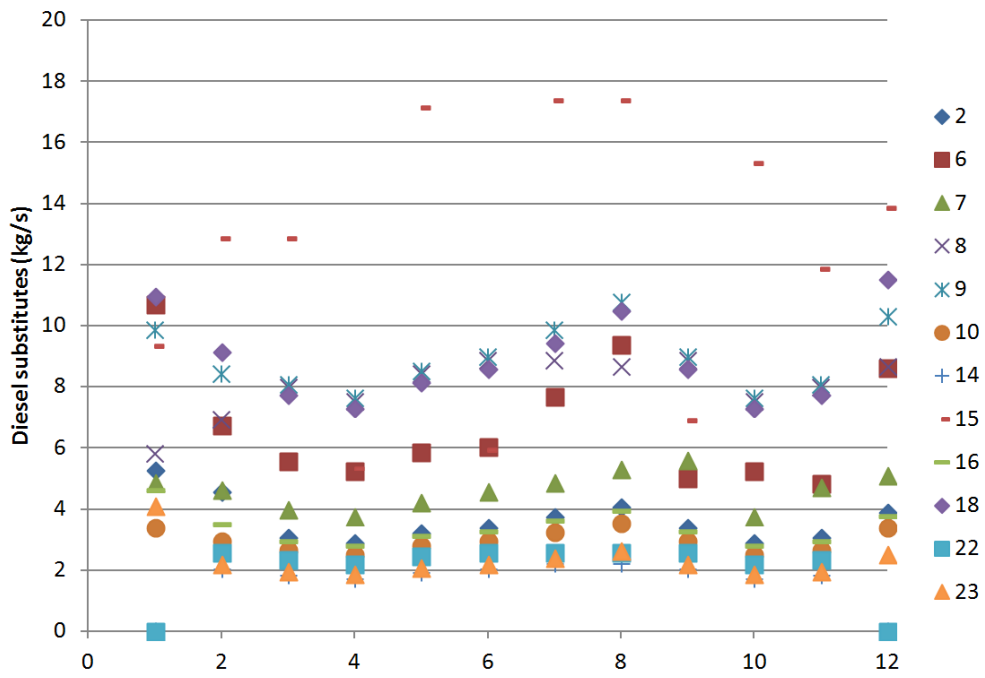
Figure 15.- Allocation of technologies across Spain



Month

1 Almería	11 Badajoz	21 Ávila	31 Teruel	41 Asturias
2 Cádiz	12 Albacete	22 Burgos	32 Zaragoza	42 Cantabria
3 Córdoba	13 Ciudad Real	23 Leon	33 Barcelona	43 Alava
4 Granada	14 Cuenca	24 Palencia	34 Girona	44 Guipúzcoa
5 Huelva	15 Guadalajara	25 Salamanca	35 Lleida	45 Vizcaya
6 Jaén	16 Toledo	26 Segovia	36 Tarragona	46 Navarra
7 Málaga	17 Alicante	27 Soria	37 Coruña (La)	47 La Rioja
8 Sevilla	18 Castellón	28 Valladolid	38 Lugo	
9 Murcia	19 Valencia	29 Zamora	39 Ourense	
10 Cáceres	20 Madrid	30 Huesca	40 Pontevedra	

Figure 16.- Biogasolines production



Month

1 Almería	11 Badajoz	21 Ávila	31 Teruel	41 Asturias
2 Cádiz	12 Albacete	22 Burgos	32 Zaragoza	42 Cantabria
3 Córdoba	13 Ciudad Real	23 Leon	33 Barcelona	43 Alava
4 Granada	14 Cuenca	24 Palencia	34 Girona	44 Guipúzcoa
5 Huelva	15 Guadalajara	25 Salamanca	35 Lleida	45 Vizcaya
6 Jaén	16 Toledo	26 Segovia	36 Tarragona	46 Navarra
7 Málaga	17 Alicante	27 Soria	37 Coruña (La)	47 La Rioja
8 Sevilla	18 Castellón	28 Valladolid	38 Lugo	
9 Murcia	19 Valencia	29 Zamora	39 Ourense	
10 Cáceres	20 Madrid	30 Huesca	40 Pontevedra	

Figure 17.- Biodiesel prouction



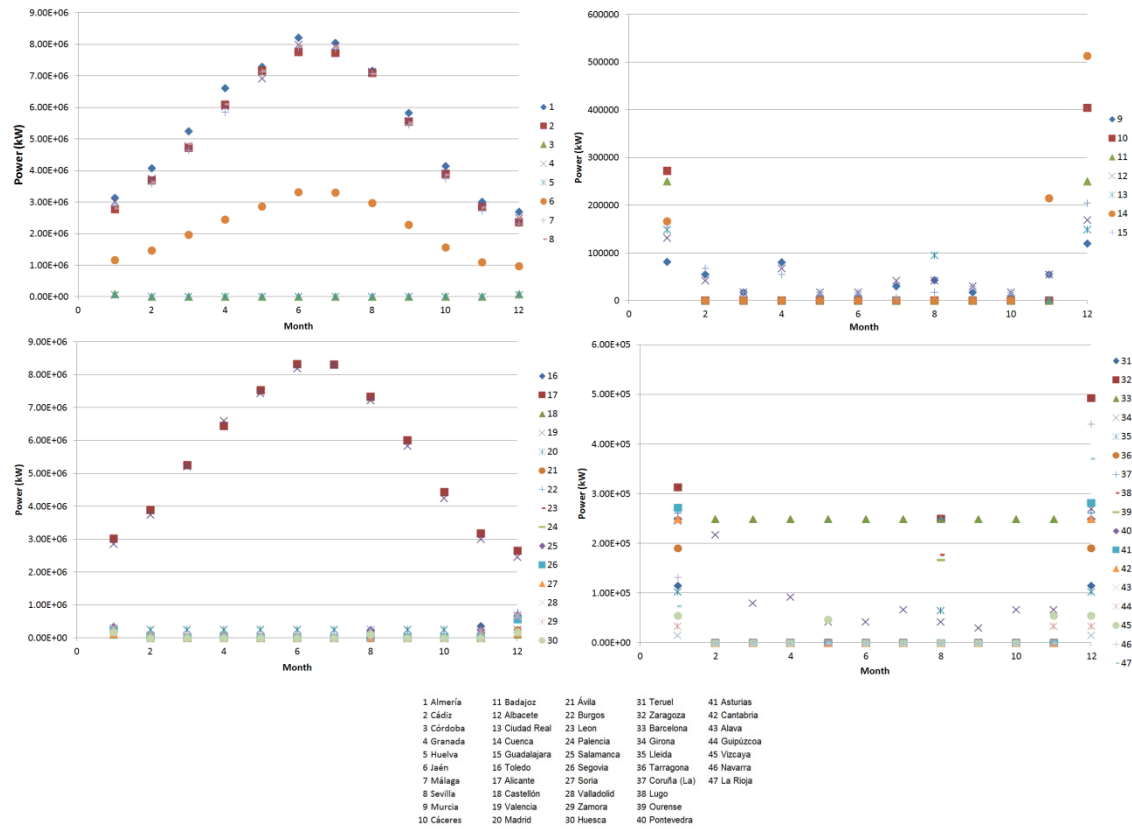


Figure 18.- Electric Power production in different locations

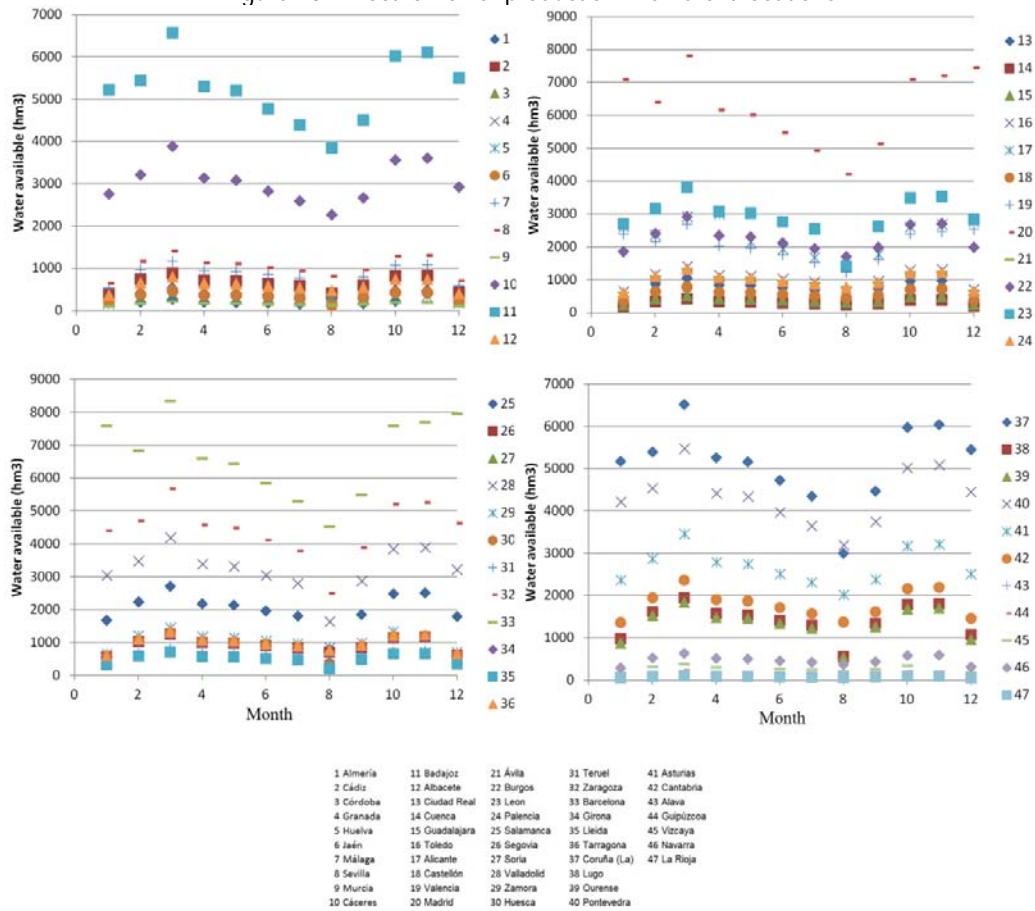


Figure 19.- Water availability

The investment for the network becomes 189 billion euros. Since dams are already built in Spain, hydropower could have eliminated them from the cost. However, for us to decide on the best integration, we decided to consider decisions from grassroots. In terms of environmental comparison with previous cases we see that while the RepSIM value is positive,  $1.9 \cdot 10^{10}$  €/y and higher than before, CO<sub>2</sub> is actually mitigated  $1.2 \cdot 10^5$  kg CO<sub>2</sub>/s, even considering the transportation of fuels.

If we go a step forward, with the current yields of the biomass and the technologies, it is not possible to reach full substitution of biofuels. Therefore, we call here for a more efficient growth of biomass so as to reach the goal of full renewable plants, as well as the need to further integration with Europe. Another important consideration is the use of cars and their efficiency. Recent trend of hybrid or electric cars, at least for urban areas, can help reach full renewable fuels and power systems. Thus, we focus on reaching 50% by using 10% area for ponds and solar capturing devices (PV panels and mirrors). Figure 20 shows the selection of technologies for 50% liquid fuel substitution. The first thing to note is the fact that the solution is not incremental with respect to the previous one. Apart from the fact that there are a larger number of production facilities using a biochemical path to ethanol, it is important to mention that solar energy is reduced to only province 7, since the area is required for biodiesel production in ponds. This means that to increase the production of fuels is not that we add a few more biofuel production facilities, but a new production system is required. The production of biodiesel results in the fact that typically in the same province, oil, methanol and thermal energy are produced, since all are required to obtain biodiesel. However, apart from the provinces that produce biodiesel in both scenarios, 20% and 50% fuel substitution, some provinces change the production scheme from biodiesel to bioethanol when a larger fuel substitution is required, i.e. province 25 or 46, or on the other direction, province 3 abandon bioethanol production to focus on biodiesel. Some others incorporate facilities to produce both types of substitutes. It is also true that there is a common structure, such as the need for hydropower across the territory and the use of wind power in the same provinces as the previous scenario. Therefore, the substitution of fossil based fuel and power has to be carried out following a strategic plan over time. Actually, the cost to reach 50% liquid fuels substitution only represents an increase of 1% higher cost than the base case scenario, 192B€. The sustainability of the solution is similar, in terms of the use of the RepSIM metric,  $1.9 \cdot 10^{10}$ . However, the

mitigation of CO<sub>2</sub> decreases slightly due to the larger transportation of the fuels to reach the consumption sites, 1.1·10<sup>5</sup> kg CO<sub>2</sub>/yr.

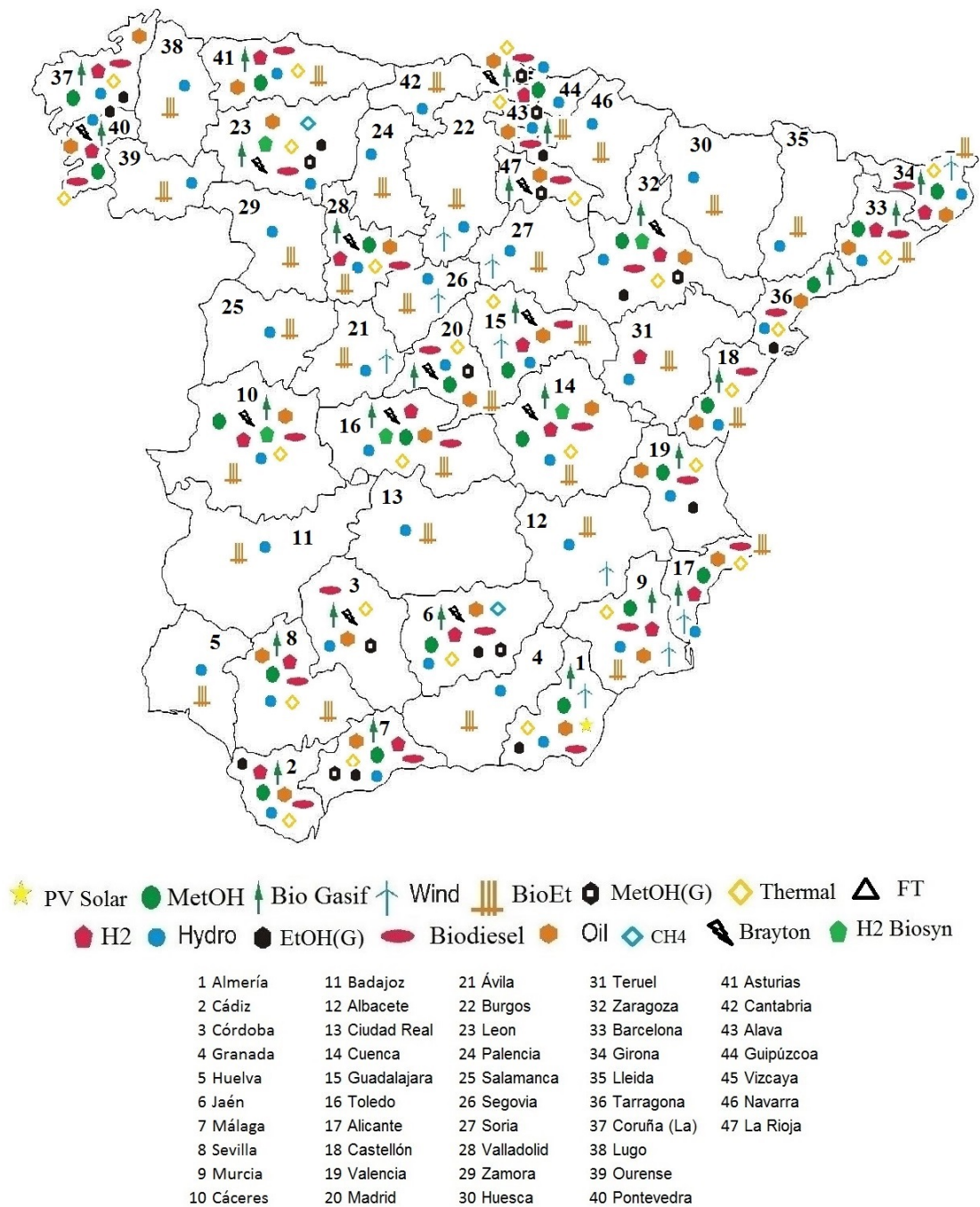


Figure 20.- Solution for renewable technologies to reach 50% fuels substitution and 100% renewable power

## 5. Conclusions

In this work we have proposed a framework for the optimal integration of renewable sources of energy for fuels and power production. We developed surrogate models for various technologies that

include solar energy, PV solar, CSP or algae to produce oil, wind technology, biomass based syngas to ethanol, methanol, FT-liquids and thermal energy, hydroelectric power and waste based power plant via biogas production. The deterministic and the two-stage stochastic programming models allow determining the optimal selection of technologies to meet certain demand. Cost objective functions and environmental metrics are used.

We have evaluated the integration in a small region (Almería) and added the effect of the uncertainty in the availability of solar, wind, biomass and power demand on the solution. As expected, the solution under uncertainty yields higher cost, but it yielded a more robust operation by using a larger number of energy sources. Later, we extended the application to a region, Andalucía, and to an entire county, Spain. The results for the deterministic cases show that for a region the technologies are concentrated, and most of the areas require most of the technologies. However, if a larger area is considered, the technologies are in general more spread out. Concentration of technologies can be found in the areas with larger demand, big cities such as Madrid, Barcelona, Bilbao and Seville. The substitution of fossil based fuels and power is limited by the resources available. It is possible to reach 50% substitution of fossil fuels by using 10% area, but the limitations in biomass availability prevent achieving complete substitution of fossil fuels.

The proposed framework can easily be applied to any other regions, providing a tool to evaluate the use of renewable resources and provide informed decisions on how to locate technologies from a certain basis.

## 6. Nomenclature

$A_i$ : Area of unit  $i$  ( $m^2$ )

$A_{Region}$ : Area of the zone evaluated ( $m^2$ )

$B$ :  $CO_2$  mitigated due to the production of a byproduct ( $kg\ CO_2/yr$ ):

$Biodiesel_{prod}(t)$ : Biodiesel produced in period in a particular zone ( $kg/s$ )

$Biomass_{av}(t)$ : Available biomass in a month ( $kg/s$ )

$Biomass_{use_P}$ : Consumption of biomass in period by process  $P$  ( $kg/s$ )

$Biogasoline_{prod}(t)$ : Renewable substitutes of gasoline in process ( $kg/s$ )

$C_{Annual}$ : Annual coefficient

$C_{CT}$ : Carbon tax ( $€/kg$ )

$CH4_P(t)$ : Methane produced in period ( $kg/s$ )

$CO_{2fossil}(t)$ : Flow of  $CO_2$  from fossil fuels used ( $kg/s$ )

$CO_{2P}(t)$ : Flow of  $CO_2$  used or produced in process  $P$  ( $kg/s$ )

$Cost_E$ : Fixed parameter of cost for the piecewise linear approximation (MM€ or MM€/y)

$Cost_{Invest}$ : Investment cost (MM€)

$Cost_{Prod}$ : Production costs (MM€/s)

$E$ :  $CO_2$  generated or mitigated due to Energy consumption/production ( $kg\ CO_2/yr$ )

F: CO<sub>2</sub> generated due to fertilizers production (kg CO<sub>2</sub>/yr)  
 F&F: Burden due to the impact of a raw material in the food industry \$/yr  
 H<sub>2available</sub>: Hydrogen available in a region (kg/s)  
 H<sub>2electro</sub>: Hydrogen produced in a single electrolyzer (kg/s)  
 H<sub>2P</sub>: Flow of H<sub>2</sub> used or produced in prices P (kg/s)  
 I : Investment (€).  
 JS: Impact of the investment in the jobs generated (€/yr)  
 M: CO<sub>2</sub> mitigation by substitution of fossil resources by renewable ones kg CO<sub>2</sub>/yr)  
 MetOH(t): Methanol produced in a zone in period (kg/s)  
 MetOH<sub>avail</sub>(t): Methanol available in a zone in period (kg/s)  
 NPond<sub>Desing</sub>: Number of ponds in a zone to be built  
 N<sub>turbine</sub>: Number of wind turbines in a zone to be installed  
 N<sub>electro</sub>: Number of electrolyzers in a zone to be installed  
 O<sub>2P</sub>: Oxygen produced in electrolysis (kg/s)  
 Oil<sub>Prod</sub>(t): Oil produced in a particular region in period (kg/s)  
 P: Production costs (€/yr)  
 Power<sub>gen</sub>(t): Power generated in the network in period (kW)  
 Power<sub>use</sub>(t): Power used by the network in period (kW)  
 PowerP(t, process): Power produced or consumed by process in period (kW)  
 Q<sub>P</sub>(t): Cooling required by process p in period (kW)  
 RepSIM: Renewable metric (€/y)  
 RM: CO<sub>2</sub> produced in the generation of a Secondary Raw material (kg CO<sub>2</sub>/yr)  
 Solar (t) Solar incidence (kWh/m<sup>2</sup> d)  
 Syngas(t): Syngas produced (kg/s)  
 Syngas<sub>Procrss</sub>(t): Syngas consumed by process in period (kg/s)  
 t: Period (month)  
 ThermalE(per, Process) : Thermal energy produced or consumed in period by process (kW)  
 W: CO<sub>2</sub> generated due to water consumption (kg CO<sub>2</sub>/yr)  
 Waste<sub>in</sub>(t) : Consumption of waste in period (kg/s)  
 Waste<sub>avail</sub>(t) : Waste available in period (kg/s)  
 Water(t, Process) : Water consumed in period by process (kg/s)  
 Water<sub>avail</sub>(t, Process) : Water available in period (kg/s)  
 xxxD=Desing<sub>Variable</sub> : Design variable for a particular process.  
 Y<sub>proc</sub>(process): Binary variable for the existence of a process  
 Y<sub>P</sub>: Binary variable for the piecewise linear approximation  
 Z: Objective function (€/s)

ε: Small parameter  
 λ<sub>Process</sub>: Variable for piecewise linear approximation

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Table 1.- Set of raw materials, transformation technologies and main products

Raw material	Technologies (I)	Technologies (II)	Products	
Wind	Wind farm (P4)		E. Power	
Solar	PV (P7)		E. Power	
	CSP (P8)	Wet cooling (P9) Cooling tower	E. Power	
		Dry Cooling (P10) A Frame	E. Power	
	Algae Growing (P11)	Transesterification (P12)	Biodiesel	
Biomass	Biochemical Path (P21)		Bioethanol/Heat	
	Syngas (P1)	Brayton cycle (P2)	Power	
		(WGSR) (P3)	Hydrogen→	
			Methanol (P6)	→Biodiesel
			Methane (P17)	E. Power (P18)
		Methanol (P20)	→Biodiesel	
		Ethanol (P19)	Ethanol/Heat	
		FT-Liquids (P22)	Diesel/Gasoline	
		Thermal Energy (P16)	Heat	
Waste	Biogas Power (P15)		Power	
Water	Hydropower (P13)	Power storage(P14)	Power	

Table 2.- CO2 emissions [31]

<i>Process</i>	<i>CO<sub>2</sub> (gCO<sub>2</sub>/kWh)<sup>[31]</sup></i>	<i>Water consumption</i>	0.30 kg CO <sub>2</sub> / m <sup>3</sup> [32]
Biomass	14-35	<i>Ethanol Prod</i>	28(gCO <sub>2</sub> /MJ) <sup>[33] [34]</sup>
PV	48	<i>Biodiesel Prod</i>	24 gCO <sub>2</sub> /MJ) <sup>[35]</sup>
CSP	27		
Wind	12		
Hydropower	24 (2200 Max)		
Biogas	11		
Coal	820		
Gas	490		

Table 3.- Input data for process integration

Month	Wind Vel (m/s)	Solar (kWh/m <sup>2</sup> d)	Biomass Av (kg/month)	Waste (kg/month)	Power demand (kW)	Biogasoline demand Kg/s	Biodiesel demand Kg/s
1	8	2.88	8203052	1.11E+08	477325	0.41	2.11
2	7	3.80	8203052	1.11E+08	433932	0.37	1.91
3	7.5	4.91	8203052	1.11E+08	390539	0.34	1.72
4	9.5	6.19	8203052	1.11E+08	368842	0.32	1.62
5	7.5	6.88	8203052	1.11E+08	412235	0.35	1.81
6	10	7.71	8203052	1.11E+08	433932	0.37	1.91
7	8	7.60	8203052	1.11E+08	477325	0.41	2.10
8	7.5	6.77	8203052	1.11E+08	520718	0.45	2.29
9	8.5	5.46	8203052	1.11E+08	433932	0.37	1.91
10	6.5	3.88	8203052	1.11E+08	368842	0.32	1.62
11	7	2.85	8203052	1.11E+08	390539	0.34	1.72
12	9.5	2.41	8203052	1.11E+08	499025	0.43	2.19