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Optimal allocation of energy sources in hydrogen production for sustainable deployment of electric vehicles

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ABSTRACT

We analyze the use of hydrogen as a fuel for the automotive industry with the aim of decarbonizing the economy. Hydrogen is a suitable option for avoiding pollutant gas emissions, developing environmentally friendly technologies, replacing fossil fuels with clean, renewable energies, and complying with the Paris Agreement and Glasgow resolutions. In this sense, renewable energies such as wind, solar, photovoltaic, geothermal, biomass, etc. can be used to produce the necessary hydrogen to power vehicles. In this way, the entire process from hydrogen production to its consumption as fuel will be 100% clean. If we are to meet future energy demands, it is necessary to forecast the amount of hydrogen needed, taking into account the facilities currently available and new ones that will be required for its generation, storage, and distribution.

This paper presents a process for optimizing hydrogen production for the automotive industry that considers the amount of hydrogen needed, the type of facilities from which it will be produced, how the different sources of production are to be combined to achieve a competitive product, and the potential environmental impacts of each energy source. It can serve as a frame of reference for the various actors in the hydropower and automotive industries so that more efficient designs can be planned for the gradual introduction of hydrogen fuel cell vehicles (HFCVs).

The methodology implemented in this paper sets an optimization problem for minimizing energy production costs and reducing environmental impacts according to the source of energy production. The EU framework with respect to the decarbonization of the economy, the percentages of the different types of energy sources used, and the non-polluting vehicle fleet in the automotive sector will be considered.

1. Introduction

Electric vehicles (EVs) and hydrogen fuel cell vehicles (HFCVs) have emerged in recent times as new drivers for the paradigm shift in the transportation industry because of climate change impacts and intergovernmental mitigation policies (Shin et al., 2019). In this sense, a set of key actions to address climate change mitigation, adaptation, and finance were achieved in the Paris Agreement and Glasgow resolutions COP26 (UN, 2015, 2021). However, their potential greenhouse gas (GHG) emissions depend on how the electricity or hydrogen is produced (Wang et al., 2019; Grosjean et al., 2012). They represent different eco-friendly technological alternatives to traditional vehicles (Gupta et al., 2022; McLeay et al., 2022) that will be future competitors within the automobile market (Bakker et al., 2012; Parra et al., 2014; Moon et al., 2021; Rubio and Llopis-Albert, 2019, 2021). This, together with the digital transformation, will mark the future of the automotive industry (Llopis-Albert et al., 2021a, b; Zeng et al., 2022). The main advantages of HFCVs over EVs are that they have a similar range, without the need for refueling, to that of conventional internal combustion engine vehicles (ICEV), and the refueling time is much lower than the recharging time of batteries (Baykara, 2018). In addition, hydrogen presents a high energy conversion efficiency (Dabbous and Tarhini, 2021), carbon-free emissions (Romero-Castro et al., 2022), diverse storage alternatives, easy transportation over long distances (e.g., by means of hydrocarbon blending), the possibility of conversion into different fuel options (for instance, ammonia, methanol, ethanol, dimethyl ether), high heating value compared with other conventional fuels, and it can be produced from renewable sources with a lower environmental impact (Mathews et al., 2014). Nevertheless, HFCVs present the disadvantages of higher vehicle costs, a currently inadequate infrastructure with an extremely limited number of hydrogen pumps for refueling, a reduced catalog of existing vehicles to choose from, and scant consumer preference in

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acquiring this type of vehicle (Moriarty and Honnery, 2019; Trapp et al., 2022).

The growing demand for hydrogen not only in automotive applications but also in the traditional refining and ammonia industry, in the production of synthetic fuels, and in the steel industry will require the production of huge amounts of cheap and continuous renewable energy (León and Aoyama, 2022; Wu and Hu, 2015). Hence, a significant increase is expected to cover the needs of a vehicle fleet running entirely on this energy source. Having enough hydrogen to fuel a country's vehicle fleet is a key element of the process and the evolution towards the commitment to decarbonize the economy (Boons et al., 2013).

According to EU reports, there are targets to be met by 2030 and 2050 (EU, 2021). Based on these objectives, this methodology aims to determine how to fulfill the new energy needs of the automotive industry (Jun et al., 2022), considering the environmental and sustainability guidelines set by the EU itself based on the Paris Agreement (Rubio et al., 2020; Rubio and Llopis-Albert, 2021; Ciasullo et al., 2020; Chopra et al., 2022).

In this regard, the methodology developed has been successfully applied to the transportation sector in Spain for analyzing the role of hydrogen in achieving the decarbonization targets, as established in the EU regulations.

The rest of the paper is structured as follows: Section 2 carries out a comparison between the use of hydrogen and fuel vehicles; Section 3 deals with the fuel consumption of some hydrogen and fuel cell vehicles; Section 4 analyzes the amount of energy generated by 1 kg of hydrogen; Section 5 tackles automotive hydrogen production; Section 6 presents the equivalence of consumption between hydrocarbons and hydrogen; Section 7 shows the energy consumption in kWh per year of the vehicle fleet in Spain; Section 8 presents the hydrogen needs for the automotive industry; Section 9 calculates the energy produced by different energy sources; Section 10 obtains the CO_2 produced in coal-fired and gas-fired power stations; Section 11 is devoted to the production costs for each energy source; Section 12 poses an optimization problem considering an energy mix; and Section 13 presents the conclusions.

2. Hydrogen vs gasoline in vehicles

The two properties that make hydrogen a possible energy alternative are: a) its high combustion power and b) the ability to obtain electrical energy directly from hydrogen with the help of a fuel cell without the need for a thermal engine, thus avoiding the theoretical maximum Carnot efficiency.

The following calculations allow us to quantify the differences in mechanical energy per kilogram between a gasoline-powered heat engine and a fuel cell-powered electric motor. The thermodynamic parameters used in those calculations have been extracted from internationally recognized organizations, such as NIST (2021) and Engineering ToolBox (2021).

A gasoline engine ($LHV = 44.5\ MJ/kg$), for which an average efficiency of $\eta = 0.35$ will be taken, would be able to produce a total mechanical energy of

$E_{gasol} = 15.57\ MJ/kg$ per kilogram of gasoline, where LHV stands for lower heating value and HHV for higher heating value.

A vehicle powered with hydrogen (water vapor, with $HHV = 120\ MJ/kg$) by an electric motor with an average efficiency of $\eta_m = 0.9$, powered by a fuel cell of average efficiency $\eta_b = 0.7$ (overall system efficiency $\eta_T = \eta_m \bullet \eta_b = 0.63$), would produce an energy of $E_{H2} = 75.6\ MJ/kg$ per kilogram of hydrogen.

Comparing these results, we obtain an energy ratio of:

$$R_E = \frac{E_{H2}}{E_{gasol}} = 5.03$$

This result applied to two vehicles with the same mechanical performance and a similar range implies that the hydrogen vehicle would consume 5.03 times less fuel, in terms of mass, than another vehicle with a gasoline engine.

However, one of the known drawbacks of hydrogen is its low density ($\rho_{H2} = 0.0899\ kg/m^3$), so in terms of volume, hydrogen loses interest compared to other fuels.

Comparing a hydrogen-powered vehicle and a gasoline-powered vehicle, for the same range, under normal conditions ($T = 0\ ^\circ C, p = 1\ atm$,) and using the previous results, the following results regarding volumes are obtained:

$$V_{gasol} = \frac{5.037\ kg}{680\ kg/m^3} = 0.0074\ m^3$$

$$V_{H2} = \frac{1\ kg}{0.0899\ kg/m^3} = 11.12\ m^3$$

Therefore, the volume ratio would be

$$R_V = \frac{V_{H2}}{V_{gasol}} = 1,502.7$$

This indicates that, for the same range, despite the high calorific value of hydrogen and the possibility of more efficient energy use, a tank 1500 times larger than the gasoline equivalent would be needed, which makes high-pressure storage for mobile applications absolutely necessary.

However, operating at a pressure of 700 bar, the density is $\rho_{H2} = 62.93\ kg/m^3$, so 1 kg of hydrogen would occupy a volume of:

$$V_{H2} = \frac{1\ kg}{62.93\ kg/m^3} = 0.016\ m^3$$

Therefore, at 700 bar, the new volume ratio is:

$$R_{V'} = \frac{V_{H2}}{V_{gasol}} = 2.16$$

Assuming a gasoline vehicle equipped with an average fuel tank of 50 l, the equivalent hydrogen car would require a tank of 108 l, which, although large, is beginning to be feasible.

3. Fuel consumption of some hydrogen and fuel cell vehicles

As an example, the fuel consumption of some hydrogen and fuel cell vehicles is provided:

Toyota Mirai: the consumption of this vehicle is 19.49 kWh/100 km.

Mercedes B-Class F-cell: consumption is equivalent to 18 kWh/100 km.

Volkswagen ID.4 (204 horsepower, hp): consumption of 18–18.3 kWh/100 km (1 kg H_2/100 km).

Honda Clarity Fuel Cell (178 hp): 3.46 l/100 km (0.22 kg/100 km).

Hyundai Nexo: fuel consumption of 1 kg H_2 per 100 km.

4. Fuel cell and electric power generated by 1 kg of hydrogen

The electrical energy W produced per mole of hydrogen can be calculated from the equation $W = n \bullet F \bullet E$,where:

n is the number of moles of electrons (e^-) per mole of hydrogen involved in the reaction.

F is Faraday's constant: $F = 96,485 \frac{C}{mol\ of\ e^-}$

E is the potential of the charged cell: $E = 0.7\ V$

Therefore,

$$W = n \bullet F \bullet E = 2\frac{mol\ of\ e^-}{mol\ of\ H_2} \bullet 96,485\frac{C}{mol\ of\ e^-} \bullet 0.8\ V$$
$$= 154,376\ \frac{C \bullet V}{mol\ of\ H_2} = 154,376\ \frac{J}{mol\ of\ H_2}$$

Since 1 kg of hydrogen equals 500 mol, the fuel cell energy for 1 kg of hydrogen is:

$$W_{1kgH2} = 154,376\ \frac{J}{mol\ of\ H_2} \bullet 500 \frac{mol}{kg} = 77.188\ MJ \Big/ kg$$

The energy consumed by the Toyota Mirai (154 hp) per 100 km is *70.16 MJ*, so it can travel 110 km on 1 kg of H_2, assuming 100 % fuel cell efficiency.

5. Automotive hydrogen production

Hydrogen does not exist in its pure state in nature. It must be produced from other compounds using different processes. Only two techniques are used industrially: reforming and electrolysis. Reforming is the most common method. It consists of reacting a hydrocarbon, usually natural gas, although it is also possible to do so with coal, using water vapor at high pressure and temperature. However, this method is not completely clean since about 10 kg of $CO_2$are produced for each kg of hydrogen produced.

Electrolysis consists of decomposing water using an electric current. It is a very minor method since only 1 % of the world's hydrogen is produced in this way. However, it is a clean process, generating 8 kg of oxygen for every 1 kg of hydrogen produced, although it requires a lot of energy. If the energy source used is clean - for example, solar photovoltaic or wind power - CO_2 emissions are reduced to practically zero.

5.1. Electrolyzer

An electrolyzer is a device that allows hydrogen to be produced by the chemical process of electrolysis to separate the hydrogen and oxygen molecules of which water is composed using electricity. Hydrogen produced in this sustainable way, i.e., without emitting carbon dioxide into the atmosphere, can form the basis of a decarbonized economy (Méndez-Picazo et al., 2021).

5.2. Electrolyzer power consumption

According to Faraday, the energy required to separate water into hydrogen and oxygen is $W = n \bullet F \bullet E$.

The reversible potential of the reaction is $E = 1.23\ V$, but a potential between 1.6 and 1.8 V (e.g., 1.7 V) must be applied to overcome the resistances. As each electrolyzed water molecule produces two electrons:

$$W = n \bullet F \bullet V = 2 \frac{mol\ of\ e^-}{mol\ of\ H_2} \bullet 96,485 \frac{C}{mol\ of\ e^-} \bullet 1.7\ V$$
$$= 328,049 \frac{C \bullet V}{mol\ of\ H_2} = 45.46 \frac{kWh}{kg\ H_2}$$

Considering the efficiency of the electrolyzer ($\eta = 0.8$), its consumption is:

$$E_{Electrolyz} = \frac{W}{\eta} = \frac{45.76 \frac{kWh}{kg\ H_2}}{0.8} = 56.825 \frac{kWh}{kg\ H_2}$$

5.3. Energy to compress the gas

Hydrogen must be supplied under pressure for the reasons given in Section 2. Raising the pressure of gaseous H_2 to 700 atm (70 MPa) implies a significant energy consumption that must be considered:

$$E_{com} = \frac{\gamma}{\gamma - 1} p_0 \bullet V_0 \bullet \left[\left(\frac{p_1}{p_0} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right]$$

where:

E is the energy required to compress the gas (J/kg).

P_0 is the initial pressure in Pa

P_1 is the final pressure in Pa

V_0 the initial specific volume (m^3/kg)

$\gamma = 1.41$ (adiabatic coefficient of hydrogen at 20 °C)

Considering that the hydrogen produced by the electrolyzer comes out at atmospheric pressure ($P_0 = 1$ atm ≈ 105 Pa), the energy required to compress it to 700 atm is:

$$E_{com} = \frac{1.41}{1.41 - 1} 10^5 Pa \bullet 12.225 \frac{m^3}{kg} \bullet \left[\left(\frac{70 \bullet 10^6}{10^5} \right)^{\frac{1.41-1}{1.41}} - 1 \right]$$
$$= 24 \bullet 10^6 J \Big/ kg$$

Expressed in kWh per kg of hydrogen compressed at 700 atm:

$$E_{com} = 24 \bullet 10^6 \frac{J}{kg} \bullet \frac{1\ kW}{1,000\ W} \bullet \frac{1\ h}{3,600\ s} = 6.7\ kWh \Big/ kgH_{2(at\ 70\ MPa)}$$

Expressed in Wh/m^3:

$$E_{com} = 6.7 \bullet \frac{kWh}{kgH_{2(at\ 70\ MPa)}} \bullet \frac{1\ kg}{1,000\ g} \bullet 2 \frac{g}{mol} \bullet \frac{1}{24.45} \frac{mol}{l} \bullet \frac{1,000\ l}{m^3}$$
$$= 548 \bullet \frac{Wh}{m^3}$$

If the electrolyzing process delivers 2.73 Nm^3/h, the compressor power must be:

$$P_{compressor} = 548 \bullet \frac{Wh}{m^3} \bullet 2.7 \bullet \frac{Nm^3}{h} = 1.5\ kW$$

However, many electrolyzers already supply hydrogen directly at the pressure desired by the user, so the previously calculated power must be modulated according to the type of electrolyzer.

Hydrogen is usually supplied at two reference pressures depending on the country of production: 35 MPa and 70 MPa. In a vehicle making short trips (urban circuit), it would be sufficient to use hydrogen at 35 MPa.

6. Equivalence of consumption between hydrocarbons and hydrogen

In order to analyze the effort required to transform an economy based on the generation of energy from fossil fuels (non-renewable and polluting) into a decarbonized economy based on renewable energies, it is important to determine the energy that can be obtained in each case. For this, it is essential to know the calorific value of the different fuels and their equivalences.

The enthalpy of combustion per unit mass of hydrogen is as follows: HHV = 142.5 MJ/kg and LHV = 120 MJ/kg (more important in practice).

On the other hand, 1 kg of hydrogen is equivalent to 2.69 kg of gasoline, 2.82 kg of diesel, and 2.4 kg of natural gas, as shown in Tables 1 and 2 (EU, 2021):

7. Energy consumption per year of the vehicle fleet in Spain

Different analyses are carried out:

Analysis 1: considering the energy consumption (kWh) of a mid-range passenger car.

It can be concluded that the energy required per 100 km travelled is $E_N = 15.60\ kWh$, where it is assumed that the vehicle travels at an

Table 1
Calorific values for different compounds.

Calorific value	LHV (MJ/kg)	HHV (MJ/kg)
Methane	50.0	55.5
Propane	45.6	50.3
Gasoline	44.5	47.3
Diesel	42.5	44.8
Hydrogen	120.0	142.5

Table 2

Calorific values for natural gases.

Calorific value HHV	kWh/l	kWh/kg
Natural gas (0 °C)	0.0117	15.75
Compressed natural gas (CNG)	2.5	15.75
Liquefied natural gas (LNG)	6.79	15.75
LPG (Liquefied petroleum gas)	7.73	13.80
Diesel	10.26	12.44
Gasoline	9.23	13.14

average speed of 80 km/h in normal wind and temperature conditions. Let us assume that this vehicle has a mass of 1850 kg.

The energy required to move this vehicle is related to the kinetic energy needed to reach that speed and then maintain it, considering the energy losses due mainly to aerodynamic forces and resistant forces acting on the vehicle. It is also necessary to consider the losses due to mechanical transmission and the losses in the internal combustion engine because its performance is not 1:

- Translational kinetic energy:

o

$$E_{CT} = \frac{1}{2} \bullet m \bullet v^2 = 0.5 \bullet 1,850 \bullet \left(80 \bullet \frac{1,000}{3,600}\right)^2 \bullet \frac{kg \bullet m^2}{s^2} = 246,913.57\ N \bullet m\ (J) = 0.247\ MJ$$

The kinetic energy of rotation of the wheels can be neglected, therefore, the kinetic energy is:

o

$$E_C = E_{CT}$$

-Aerodynamic energy:

o

$$E_a = \left(\frac{1}{2} \bullet C \bullet S \bullet \rho \bullet v^2\right) \bullet d = 0.5 \bullet 0.29 \bullet 2.5 \bullet 1.225 \bullet \left(80 \bullet \frac{1,000}{3,600}\right)^2 \bullet 100 \bullet 1,000 \bullet \frac{kg \bullet m^2}{s^2} = 28,734,567.86\ J = 28.73\ MJ$$

-Frictional energy in the contact area of the tires:

o

$$E_r = f_r \bullet W \bullet d = 0.015 \bullet 1,850 \bullet 9.81 \bullet 100 \bullet 1,000 = 50,000,000\ J = 27.22\ MJ$$

Total energy: $E_T = E_C + E_a + E_r = 56.197\ MJ$

If the vehicle runs on gasoline, considering that 1 l of gasoline contributes 9.23 kWh/l and taking into account an engine efficiency of $\mu = 0.25$, 2.3 kWh/l equivalent to 6.78 l of gasoline is needed.

If the vehicle runs on diesel, considering that 1 l of diesel contributes 10.26 kWh/l and taking into account an engine efficiency of $\mu = 0.25$, 2.56 kWh/l and 6.08 l of diesel would be needed.

If the vehicle runs on LPG, considering that 1 l of LPG contributes 6.79 kWh/l and taking into account an engine efficiency of μ = 0.25, 1.69 kWh/l and 9.23 l of LNG would be needed.

If the above vehicle runs on hydrogen, considering that 1 kg of hydrogen contributes 141.6 MJ/kg = 39.33 kWh/kg and taking into account an electric motor and fuel cell efficiency of μ = 0.75, 29.49 kWh/kg and 0.52 kg of hydrogen would be needed.

To calculate the amount of fuel for any type of trip, one has to proceed in a similar way. For a WLTP (Worldwide Light-duty vehicle Test Procedure, on the European car fleet CO_2 emissions) type approved trip, the energy consumption must be discretized by sections.

The above calculations can be summarized in Table 3, where average consumption values are given according to the fuel used:

Analysis 2: calculation of the annual amount of fuel needed to move the vehicle fleet in Spain.

For this calculation, we analyze types of vehicles, average trips, average lifetimes, and average fuel consumption, which are provided in Table 4 (DGT, 2021).

Average values can also be taken; considering the average consumption, density, and average travel for each type of vehicle, the data provided in Table 5 are obtained.

Table 6 shows the annual fuel consumption according to the energy source and the production in *kWh* needed to supply the corresponding fleet of vehicles.

According to this analysis, the total amount of kWh (Q_2) that would need to be replaced by hydrogen is:

$$Q_2\ (MWh) = 199.79 \bullet 10^{11}\ \text{MWh}$$

Analysis 3: calculation of total annual fuel quantity

The consumption of automotive fuels in Spain for 2019, the latest year for which these data are available, was as follows (Table 7):

a) Gasoline consumption reached 5385 kT.
b) Diesel consumption reached 31,566 kT.
c) LPG consumption was 86,016 T.

8. Hydrogen needs for the automotive sector

The equivalent amount of hydrogen needed to move the vehicle fleet described in the previous section for analysis 3 can be calculated using the following equation:

$$M_{H_2}(kg) = \frac{5,385,452 \bullet 10^3 \bullet \text{X} + 31,566,516 \bullet 10^3 \bullet \text{Y} + 86,016 \bullet \text{Z}}{W}$$

where:

$$X = 12.39 \bullet \frac{kWh}{kg}$$

$$Y = 12.14 \bullet \frac{kWh}{kg}$$

$$Z = 13.80 \bullet \frac{kWh}{kg}$$

$$W = 39.34 \bullet \frac{kWh}{kg}$$

Operating, the kg of hydrogen needed are:

Table 3

Average consumption values.

100 km	Quantity	Density	Mass
Hydrogen	5.52 m^3	0.0893 kg/m^3	0.52 kg
Gasoline	6.78 l	0.750 kg/l	5.08 kg
Diesel	6.08 l	0.850 kg/l	5.16 kg
LPG	9.23 l	0.560 kg/l	5.16 kg

Table 4
Vehicle fleet data for Spain in 2020.

Vehicle	Units	km/ year	Average consumption/ 100 km	Total consumption
Trucks	2,514,750 (<3000=2,213,661 >3000 = 301,089)	< 3000 kg = 14,467 > 3000 = 47,543	25 l 40 l	$9.095 \cdot 10^{11}$ l $5.725 \cdot 10^{11}$ l
Buses	63,387	52,951	28 l	$9.397 \cdot 10^{10}$ l
Vans	2,516,177	14,467	11 l	$4.004 \cdot 10^{11}$ l
Cars	24,716,898 (Gasoline=10,992,736 Diesel = 13,724,162)	12,266	Gasoline = 7.6 l Diesel = 5.6 l	$1.024 \cdot 10^{12}$ l $9.427 \cdot 10^{11}$ l
Motorcycles	3,735,920	2903	4.4 l	4771·1010 l
Tractors	235,511	2100	110 l	5440·1010 l

Table 5
Average annual consumption for different energy sources.

	Consumption (l)	Density	Consumption (kg)
Hydrogen	16,200 kg/year	0.0893 kg/m^3	16,200 kg/year
Gasoline	75,000 l/ year	0.750 kg/l	56,250 kg/year
Diesel	82,500 l/ year	0.850 kg/l	70,125 kg/year
LPG	132,000 l/year	0.560 kg/l	73,920 kg/year

Table 6
Annual fuel consumption by vehicle type.

	Vehicle fleet	Annual consumption in kg	Annual consumption in kWh
Gasoline	15 million	$8.43 \cdot 10^{11}$ kg/year	$104.45 \cdot 10^{11}$ kWh
Diesel	10 million	$7.0125 \cdot 10^{11}$ kg/year	$85.14 \cdot 10^{11}$ kWh
LPG	1 million	$7.3920 \cdot 10^{10}$ kg/ year	$102.01 \cdot 10^{10}$ kWh

Table 7
Consumption in tons for Spain in 2019. Data obtained from DGT (2021).

Year	Gasoline (T)	Diesel (T)	LPG (T)
2019	5385,452	31,566,516	86,016

$$M_{H_2}(kg) = 1,706,204,836 \text{ kg} = 1,706.2 \bullet 10^6 \text{ kg} = 1,706,204.836 \text{ T}$$

Considering that the consumption of an electrolyzer is:

$$W = 45.46 \frac{kWh}{kg\ H_2}$$

to produce the $M_{H_2}(kg)$ of hydrogen, the quantity R(kWh) is needed:

$$R\ (kWh) = 1,706,204,836 \text{ kg} \Big/ 45.46 \frac{\text{kWh}}{\text{kg}} = 7.756 \bullet 10^{10} \text{ kWh}$$

In addition, to compress the gas to 700 atm, an auxiliary energy of S (kWh) is needed:

$$S\ (kWh) = 1,706,204,836 \text{ kg} \bullet 6.7 \text{ kWh/kg} = 1.14315 \bullet 10^{10} \text{ kWh}$$

In total, it would be necessary to produce Q_3 (MWh):

$$Q_3\ (MWh) = \text{R(kWh)} + \text{S(kWh)} = 8.899 \bullet 10^7 \text{ MWh}$$

9. Calculation of the energy produced in a wind, solar photovoltaic, and hydraulic power plant

9.1. Wind plant

A wind turbine measuring 138 m high and 126 m in diameter between blades can generate 6 MW per year.

$$P_{wt} = 6\ MW$$

9.2. Solar photovoltaic

A typical solar panel can provide between 250 W and 300 W of power and up to 500 W. Let us look at a typical panel of about 500 W, which means that power is going to be generated for every hour of sunshine. For a sunny spring day in a warm area, the power generated would be:

$$P_{500W\ day} = 500 \text{ W} \bullet 5 \frac{h}{day} = 2500 \frac{Wh}{day} = 2.5 \frac{kWh}{day}$$

Assuming an average of 5 h of sunshine a day for 300 days, the average annual power would be:

$$P_{500W\ yearly} = 2.5 \frac{kWh}{day} \bullet 300 \frac{day}{year} = 0.75 \frac{MWh}{year}$$

9.3. Hydraulic

The power output of a hydroelectric power plant is generally measured in megawatts (MW) and is calculated using the following formula:

$$P_h = \rho \bullet g \bullet \eta_t \bullet \eta_g \bullet \eta_m \bullet Q \bullet H$$

where:

- P_e: power in (kW)
- ρ: fluid density in (kg/m^3)
- g: acceleration of gravity in (m/s^2)
- η_t: hydraulic turbine performance (between 0.75 and 0.94)
- η_g: electric generator performance (between 0.92 and 0.97)
- η_m: mechanical performance of the turbine-alternator coupling (0.95–0.99)
- Q: turbine flow in m^3/s
- H: available head difference in the dam between upstream and downstream, in (m).

Assuming a hydropower plant discharging a flow rate of $Q = 50 \bullet 10^2 \frac{m^3}{s}$ from a height of $H = 200\ m$, the power produced is:

$$P = 997 \frac{kg}{m^3} \bullet 9.81 \frac{m}{s^2} \bullet 0.75 \bullet 0.92 \bullet 0.95 \bullet 50 \frac{m^3}{s} \bullet 200\ m = 6,411.163\ kW$$

The energy produced per year can be estimated as follows:

$$E = P \bullet t = 3,077.35\ MWh$$

10. Calculation of CO_2 produced in a coal-fired and gas-fired power station

In the optimization process discussed below, one of the constraints to be considered is the amount of CO_2 produced during the generation of

Table 8
Energy values for coal and compressed natural gas

Product	kcal/kg	MJ/kg
Anthracite	8194	32.72
Compressed Natural Gas (CNG)	11,990	56.25

electricity. We follow several steps to calculate this amount. First, let us consider the energy values for coal and compressed natural gas from Table 8.

Subsequently, we present an analysis of the amount of CO_2 per kWh produced with these substances.

10.1. Stoichiometric equation carbon (anthracite) combustion

The stoichiometric equation for coal (anthracite) combustion is:

C	$+ O_2$	➔	CO_2	+ 32.72 MJ/kg
12 g	32 g		44 g	
1 kg			3.67 kg	

When using other types of coal (e.g., lignite), the process of calculating the energy obtained during combustion and the amount of CO_2 generated is similar.

The energy obtained from the combustion of anthracite is approximately 32.7 MJ/kg, which is equivalent to 9.09 kWh/kg. Considering the efficiency of a thermal power plant with anthracite of value $\eta = 0.35$, the energy obtained from anthracite combustion is $E = 3.18\ kWh/kg$.

Furthermore, in terms of CO_2 produced:

$$3.18 \bullet \frac{kWh}{kg\ C} \bullet \frac{1\ kg\ C}{3.66\ kg\ CO_2} = 0.868 \bullet \frac{kWh}{kg\ CO_2}$$

This relationship implies that 1 kWh produces 1.152 kg of CO_2.

This relationship allows us to determine the amount of CO_2 produced in terms of the kWh generated by the power plant. It will make it possible to introduce a penalty term for the production of CO_2in the optimization problem.

10.2. Stoichiometric equation natural gas combustion

The use of CNG (consisting mainly of methane, between 90 and 95 %) will be considered. When using LPG (propane and butane mixture), the calculations necessary to determine the amount of energy produced and CO_2 emissions are similar.

The stoichiometric natural gas combustion equation is:

CH_4	$+ \mathbf{2}\ O_2$	➔	CO_2	$+ \mathbf{2}\ H_2O$	+ 56.25 MJ/kg
16 g	64 g		44 g		
1 kg			2.75 kg		

The energy obtained from the combustion of natural gas is 15,625 kWh/kg (equivalent to 56.25 MJ/kg). Considering the efficiency of a gas-thermal power plant $\eta = 0.35$, the energy obtained from coal is $E = 5468$ kWh/kg.

Furthermore, in terms of CO_2 produced:

$$5,468 \bullet \frac{kWh}{kg\ CH_4} \bullet \frac{1\ kg\ CH_4}{2.75\ kg\ CO_2} = 2,053 \bullet \frac{kWh}{kg\ CO_2}$$

This ratio implies that 1 kWh produces 0.487 kg of CO_2.

This relationship allows us to determine the amount of CO_2 produced in terms of the kWh generated by the power plant. It will make it possible to introduce a penalty term for the production of CO_2in the optimization problem.

11. Energy production (kWh) costs by technology

Tables 9 to 13 present the estimated costs per MWh produced depending on the energy source used. These data will be used in the optimization problem.

Table 9
Production costs.

Renewables		Non-renewables	
Energy source	Cost €/MWh	Energy source	Cost €/MWh
Wind	81.37	Nuclear	65.87
Solar photovoltaic	81.65	Coal	126.76
Hydro	68.12	Combined cycle	120.34

Table 10
Fuel costs and CO_2 emissions (€/MWh).

Renewables		Non-renewables	
Energy source	Cost €/MWh	Energy source	Cost €/MWh
Wind	0	Nuclear	9.66
Solar photovoltaic	0	Coal	43.28
Hydro	0	Combined cycle	75.07

Table 11
Cost of O&P (€/MWh).

Renewables		Non-renewables	
Energy source	Cost €/MWh	Energy source	Cost €/MWh
Wind	15.3	Nuclear	6.2
Solar photovoltaic	8.24	Coal	8.48
Hydro	9.28	Combined cycle	6.67

Table 12
Marginal cost (€/MWh).

Renewables		Non-renewables	
Energy source	Cost €/MWh	Energy source	Cost €/MWh
Wind	15.3	Nuclear	15.87
Solar photovoltaic	8.24	Coal	51.75
Hydro	9.28	Combined cycle	81.73

Table 13
Transmission and losses (€/MWh).

Renewables		Non-renewables	
Energy source	Cost €/MWh	Energy source	Cost €/MWh
Wind	31.377	Nuclear	31.428
Solar photovoltaic	30.741	Coal	34.658
Hydro	30.835	Combined cycle	37.356

12. Optimization of the energy mix

The purpose is to calculate the amount of MW that must be provided by each energy source to generate enough electricity to produce the hydrogen needed by the automotive industry in order to replace conventional vehicles with hydrogen-powered electric vehicles.

For this calculation, an optimization problem is posed in which the objective function is the profits subject to sustainability restrictions, including the penalty for CO_2 production. The result will be the amount of electricity produced by each energy source.

Let B be the function representing the annual profits to be maximized in the optimization problem.

$$Max\ B \tag{1}$$

which can be expressed as in Eq. (2):

$$B = A_o \bullet B_T - C_T \tag{2}$$

where:

A_o is the opportunity cost of investing money in the production of electricity.

B_T is the gross total profit of selling product m manufactured by the company.

C_T are the expenses associated with the production of greenhouse gases.

A_o can be expressed as follows:

$$A_o = \frac{1}{(1+r)^T} \tag{3}$$

In Eq. (3), r is the annual interest, and T represents the number of years the company is productive. In this paper, we consider $r = 0.03$ and $T = 20$ years. The total gross profit is:

$$B_T = \sum_{m=1}^{n} B_m \tag{4}$$

where B_m is the gross profit of producing electricity from source or technology m. The number of energy sources (technologies used for producing electricity) is n. B_m can be expressed as follows:

$$B_m = \sum_{m=1}^{n} b_m \bullet Q_m \tag{5}$$

where

$b_m = P_m - C_m$ is the unit gross profit of producing electricity from source or technology m. It is obtained as the difference between the unit sale price P_m minus the unit cost of its production C_m. We consider $P_m =$ € $205/MWh$.

C_m takes into account the following terms: C_1 is the cost of the corresponding fuel and the CO_2 production, C_2 considers the operation and maintenance cost, C_3 takes into account the marginal cost, and C_4 is the cost due to transmissions and losses. The value of these terms is presented in Tables 9 to 13.

$$C_m = C_1 + C_2 + C_3 + C_4$$

Q_m is the number of MWh per year produced from source m.

The term C_T is the cost associated with CO_2 production and with nuclear waste management. It can be modeled as follows:

$$C_T = \sum_{m=1}^{n} k_m \bullet Q_m \tag{6}$$

k_m indicates the pollution rate due to each energy source. For example, wind, solar, and hydro energy are considered clean energies and, therefore, this coefficient is zero for these energies.

However, energy from coal, combined cycle (CC), and nuclear power plants does produce pollutants that must be considered, although of a different nature (Payo et al., 2017). Nuclear power plants do not emit greenhouse gases, but they do produce radioactive waste that presents safety problems and is difficult to manage. This term appears in the restrictions section.

Finally, replacing expressions (2) to (6) in (1), the profit can be expressed as follows:

$$B = \frac{1}{(1+r)^T} \bullet \sum_{m=1}^{n} (P_m - (C_1 + C_2 + C_3 + C_4)) \bullet Q_m \tag{7}$$

The constraints considered are:

The amount of electricity produced by wind energy Q_1 must be greater than a threshold value: $Q_1 > U_1$.

The amount of electricity produced by solar photovoltaic Q_2 must be greater than a threshold value: $Q_2 > U_2$.

a) The amount of electricity produced by hydropower Q_3 must be greater than a threshold value: $Q_3 > U_3$
b) The amount of electricity produced by nuclear power Q_4 must be greater than a threshold value: $Q_4 > U_4$

The amount of electricity produced by the rest Q_R (coal Q_5, combined cycle Q_6, etc.) must be less than a threshold value: $Q_R < U_5$.

c) The amount of electricity produced by nuclear power Q_4 must be greater than the amount of electricity produced by the rest Q_R (coal, combined cycle, etc.).

The amount of CO_2 is less than a certain threshold. It is known that the amount of CO_2 produced by 1 kg of coal is 3.66 kg, while 1 g of CNG produces 2.75 g of CO_2.

In a gas power plant (CNG), for each kg of CO_2, 2.053 kWh of energy is produced, considering an efficiency of $\eta = 35$ % for such a plant. This is equivalent to saying that 1 kWh produces 0.487 kg of CO_2.

In a coal power plant, for each kg of CO_2, 0.868 kWh of energy is produced, considering an efficiency of $\eta = 35$ % for that plant.

It is equivalent to say that 1 kWh produces 1.152 kg of CO_2.

In the constraints section, the following term appears: $C_T = \sum_{m=1}^{n} k_m \bullet Q_m$, where k_m indicates the pollution rate due to each energy source and Q_m is the number of MWh per year produced from that source.

d) Maximum energy produced according to needs.
e) Maximum budget for producing energy.

The threshold values used in the optimization process have been chosen considering the electricity production of the year 2020 and according to the energy source considered.

The optimization problem has been solved by a Nonlinear Programming procedure using the Generalized Reduced Gradient (GRG) method. This nonlinear programming algorithm starts from a feasible solution known as the starting point. The algorithm then attempts to move from this point in one direction through the feasible region such that the value of the objective function improves. Two features of the solutions obtained with this algorithm should be noted:

- The algorithm may end in a local optimum that may not be the global optimum of the problem.
- The local optimum at which the algorithm ends depends on the starting point.

The solution of the optimization problem provides the results shown in Table 14. They are presented in terms of Q_m, i.e., the number of GWh per year produced from source m:

These results can be compared with the national electricity production for the year 2020, which is depicted in Table 15.

It is noted that a major transformation effort is needed to decarbonize the automotive sector and, particularly, for the transition from internal combustion engine vehicles to hydrogen-powered electric vehicles.

With the production data from Section 9, one could calculate the units of the different technologies (wind, photovoltaic, and hydro) to be used. This calculation is illustrated in Table 16.

After a transitional period to close coal and gas power plants, hydrogen production will come from wind, solar photovoltaic, hydro, and nuclear power plants.

Table 17 shows the new MWh production considering those conditions.

In a third stage, nuclear energy should also be avoided because it produces radioactive waste that is problematic and difficult to manage.

Table 14
GWh per year produced from source *m*.

Renewable source		Non-renewable source	
Energy source	Production (GWh)	Energy source	Production (GWh)
Wind	45,139.695	Nuclear	16,842.730
Solar photovoltaic	4216.375	Coal	1497.040
Hydraulic	8465.312	Combined cycle	12,834.750

Table 15
Domestic electricity production for the year 2020.

Renewable source		Non-renewable source	
Energy source	Production (GWh)	Energy source	Production (GWh)
Wind	54,899	Nuclear	55,757
Solar photovoltaic	15,289	Coal	5022
Hydraulic	30,614	Combined cycle	44,023

Table 16
Production of renewable energy sources.

Renewable energy source	Production (GWh)/year	MWh per unit/year	Units
Wind	45,139.695	6	7,523,282.5
Solar photov.	4216.375	0.912	4,623,218.20

Table 17
Electricity production from renewable and nuclear sources.

Renewable + nuclear	Production (GWh)/year	MWh per unit/year	Units
Wind	57,344.608	6	9,557,434.66
Solar photovolt.	6342.861	0.912	6,954,891.44
Hydraulic	8465.312		
Nuclear	16,842.730		

13. Conclusions

The fight against climate change is an objective of modern societies, and it implies moving towards a fully decarbonized and emission-free economy. The 2015 Paris Agreement set the framework for the new energy policy. The United Nations 2030 Agenda for Sustainable Development was also presented. The Sustainable Development Goals (SDGs) were developed to protect the planet by 2030 and set their achievement by 2050. These agreements lay the foundations for sustainable global development with low greenhouse gas emissions. One of the most important pillars for achieving these objectives is the European Green Pact, which focuses on the energy transition and the green economy (Lee et al., 2009). The transition to this model involves structural changes related to energy sources.

In the short term, the closure of coal power plants and, in the medium and long term, the closure of gas and combined cycle power plants are part of this process. In the same direction, it is necessary to promote the use of hydrogen as an energy source. Hydrogen is set to become the fuel for the energy transition on the road to decarbonization and for the fulfillment of the SDGs.

Most hydrogen is currently extracted from natural gas through a process that emits polluting gases and requires high electricity consumption. Green hydrogen, however, is generated by electrolysis of water. The process must be carried out using electricity from renewable sources. It must be taken into account that no carbon dioxide is emitted during its combustion or during its production process.

A major consumer of green hydrogen is the automotive sector. If a decarbonized economy is to be achieved, it is necessary to replace internal combustion engine vehicles with electric vehicles. Some of these vehicles will generate electricity from hydrogen.

In this paper, a study has been carried out that involves an optimization process that calculates the amount of hydrogen that must be produced in Spain to proceed with this substitution so that by 2030, conventional vehicles will be dispensed with as GHG emitting sources. As a result, the amount of electricity needed to produce hydrogen through the electrolysis process must be calculated, taking into account renewable energy sources (wind, solar photovoltaic, and hydraulic energy).

The main energy sources currently in use (wind, solar photovoltaic, hydro, nuclear, coal, and gas) have been considered in the optimization process, together with their participation and role in hydrogen production. The ultimate goal is to dispense with coal, gas, and nuclear energy in electricity production. At that point, the desired objectives will have been achieved.

In addition, two stages have been considered. In the first stage, which lasts three years, the different energy sources, including the most polluting ones (coal and gas), are considered. In the second stage, only those that do not produce greenhouse gases (wind, solar photovoltaic, hydro, and nuclear) are considered. And in the long term (third stage), the objective is to dispense with nuclear energy because, although it does not produce GHGs, it generates waste that presents safety problems and is difficult to manage.

The optimization process shows that the main source of energy is wind power, followed by solar photovoltaic, hydroelectric, and finally nuclear energy.

With respect to hydropower, assuming that no new plants are built, it must produce at its maximum capacity in order to take advantage of all the current potential.

The great challenge posed by the increase in electricity production from wind and solar photovoltaic energy can also be appreciated.

The results obtained shed light on the enormous amount of work needed to meet the target of renewable hydrogen and electric power for the automotive industry. It also shows that there are different degrees of electricity production depending on the type of source available. The results can be used for the different actors as a Decision Support System (DSS) to better identify the threats, challenges, and opportunities of the energy transformation of the automobile industry and for an in-depth analysis of the severe economic slowdown of the automotive industry due to the COVID-19 pandemic. They can also aid in the efficient implementation of environmental policies regarding the optimal allocation of energy sources in hydrogen production for the sustainable deployment of electric vehicles.

As further research, the conclusions obtained in this case study should be contrasted with the results of the worldwide automotive industry. Therefore, regional and cross-country comparisons should be performed.

CRediT authorship contribution statement

F. Rubio and C. Llopis-Albert: Conceptualization, Methodology, Software, Data curation, Writing- Original draft preparation, Investigation.

A. Besa: Visualization, Supervision and Software, Validation.

F. Rubio, C. Llopis-Albert, A. Besa: Writing- Reviewing and Editing.

Data availability

Data will be made available on request.

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