**Introduction**

Paris Agreement [1], is the climate mitigation flagship international environmental treaty. It foresees major reduction of anthropogenic carbon emissions. To achieve its objectives, major transformation of the existing system is expected, including the extensive use of zero-carbon emission facilities for energy production as well as alternatives to fossil fuels. A viable solution remains the use of hydrogen. As a mean of storing energy, hydrogen is able to a certain degree, to present specific advantages of continuing the use of existing networks, facilities, and infrastructure [2]. It can be also produced on a variety of procedures and methods, including renewables [3] and biomass [4]. Thus, it contributes to Paris Agreement requirements without the need of substantial infrastructure updates, facilitating the transition.

Hydrogen and methane can also be produced using power-to-gas technology from zero or near to zero emission power sources, such as renewables, nuclear, or biomass [5], nonetheless, it has to be mentioned that it competes to other technologies as well [6]. It has been long time since researchers have developed scenarios for hydrogen
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penetration to energy mix [7], but since technology has been rapidly advancing new opportunities for hydrogen have arisen [8]. Hydrogen has extended potential to compete to electric vehicles in offering sustainable transportation solutions [9]. The importance of hydrogen to transport sector has been explained by van der Zwaan et al. [10] and Anandarajah et al. [11]. Rössler et al. [12] connect hydrogen transport, electric vehicles, and the requirements for climate change mitigation. Dodds et al. [13] provide an approach of hydrogen for heating and Morfeldt et al. [14] explain how hydrogen can contribute to steel production. However, a holistic approach that covers total hydrogen production under carbon emissions constraints is still to be proposed.

In this study, a procedure based on widely accepted assumptions of the research and policy making community, is applied to predict its contribution to the future energy mix. This contribution is transparently connected to the efficiency of the technology per se. It is assumed that hydrogen technology advances its efficiency in different rates across time. Based on the above, this study intensifies the contribution of hydrogen as fuel in meeting the future emission scenarios, as they were described under the expected Represented Concentration Pathways [15] using prudently, Integrated Assessment Models [16].

Hydrogen has been on the interest of the Integrated Assessment Models research community. A comprehensive review on the subject is developed by Hanley et al. [17], from which appears the complexity of the issue. However, it is important to understand hydrogen contribution to global energetic system based on carbon emission policy considerations. A generic description that analyses hydrogen contribution pathways to energetic system on integrated assessment models is provided by Bolat and Thiel [18]. Nevertheless, a connection of hydrogen production to policy decisions is not quantified.

Debate among scientists and policy makers portrays complex and abstract processes, such as climate change mitigation, in a manner which is described as an evolving procedure in time, a transition, namely as a pathway [19]. As such, representative concentration pathways (RCP) [15] is one of the prominent ways to quantitatively depict climate change and its mitigation. Specifically, four RCP describe the radiative forcing values up to the end of the century that are connected to greenhouse gases at the atmosphere of the time. Specifically, RCP 8.5 represents the “business as usual” case, observing an increasing radiative forcing to 8.6 W/m² at 2100 that corresponds to ~1370 ppm CO₂ eq [15]. RCP 6.0 expresses a stabilization at 2100 radiative force to 6 W/m² or ~850 ppm CO₂ eq. Similarly, RCP 4.5 corresponds to 4.5 W/m² or ~650 ppm CO₂ eq and RCP 2.6 to a peaked radiative force of 3 W/m² or ~490 ppm CO₂ eq that decreases to 2.6 W/m² at 2100. From the above, we simulate RCP 2.6, 4.5, and 6.0.

RCP 2.6 represents the scenario which foresees the lower carbon emissions compared to the four available [28]. As a matter of fact, to achieve this goal a wide selection of measures has to be applied. This includes the installation of zero emission power sources to the electricity system but also it requires substantial measures toward energy efficiency and the de-carbonization of transport. Several technologies are currently available toward this direction, including renewables, nuclear, carbon capture, and storage and the use of hydrogen as a fuel for transport. A sustainable future essentially requires minimum or insignificant use of fossil fuels and negative carbon emissions much before the end of the century. According to the researchers RCP 2.6 nears Paris Agreement expectations; however, it still remains a target that needs better adjustment [29] to express safely such a statement. Paris Agreement would probably require additional measures compared to RCP2.6 in order to achieve its carbon emissions global goals.

Continuing this analysis, RCP 4.5 is as it is so called, a pathway toward stabilization of the radiating forcing [30]. It foresees mild carbon emissions reduction to the degree that negative carbon emissions are not required even if they need to be reduced almost in half compared to the actual. RCP 6.0 remains the most pessimistic of the simulated scenarios [31] and unacceptable in terms of emissions to achieve Paris Agreement mitigation goals. Even so, an RCP6.0 scenario is provided in this analysis.

The present study applies Global Change Assessment Model (GCAM) [21, 22], which is able to translate RCPs directly to, among others, the expected energy production. This is being accomplished using Hector [23], an open source software, part of GCAM. A paramount aspect of this analysis is the expected hydrogen contribution as a mean of clean energy transferring and storing. GCAM is placed predominantly in this aspect since it considers input data from the hydrogen program of the Department of Energy [24] as they are described to the report of National Renewable Energy Laboratory “H2A Production Model” [25].

Input Data and Simulation Procedure

Intergovernmental Panel on Climate Change [26], published its Fifth Report [27] on which it defines the four representative concentration pathways 2.6, 4.5, 6.0, and 8.5. These express the radiative forcing levels at the end of the century that are connected to greenhouse gases at the atmosphere of the time. Specifically, RCP 8.5 represents the “business as usual” case, observing an increasing radiative forcing to 8.6 W/m² at 2100 that corresponds to ~1370 ppm CO₂ eq [15]. RCP 6.0 expresses a stabilization at 2100 radiative force to 6 W/m² or ~850 ppm CO₂ eq. Similarly, RCP 4.5 corresponds to 4.5 W/m² or ~650 ppm CO₂ eq and RCP 2.6 to a peaked radiative force of 3 W/m² or ~490 ppm CO₂ eq that decreases to 2.6 W/m² at 2100. From the above, we simulate RCP 2.6, 4.5, and 6.0.

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RCP 8.5 is a pessimistic approach to our research question. According to our estimations, had this pathway been adopted, hydrogen contribution would have been slim. Having mentioned the above, it has been decided RCP 8.5 not to be simulated in our approach.

Global Change Assessment Model Hector [23] is the tool of preference to conduct the RCP simulations of this study. Input data for anthropogenic carbon emissions were collected from the RCP database [32]. In this database, data for RCP 2.6 are published on [33], for RCP 4.5 on [34–36] and for RCP 6 on [37, 38]. Additionally, analytical data and a graphical depiction of the emissions across the simulated input data are provided to the Supporting Information of this manuscript’s spreadsheets. We observe that our simulation results are directly connected to the expected emissions pattern depicted in these data. This is especially apparent to RCP4.5 simulations that demonstrate at 2080 a local decrease in the production, probably connected to the corresponding expectation for not reducing emissions in this period. This situation creates also minor simulation convergence issues that undermine, to a certain degree, the accuracy of our results.

The contribution of this analysis is based on the expectation that hydrogen production technologies will advance in a manner, which is 5 years steeper than predicted from GCAM developers. Having this said, we assume that hydrogen production from electrolysis increases gradually according to the attached spreadsheet data (RCP_input_graphs.xlsx). We have chosen for electrolysis, because this is the technology applied for the production of hydrogen from renewable sources. The default scenario includes the GCAM data provided in the source code. These values are applied to hydrogen production from solar, wind, and from the electricity grid, whereas hydrogen is produced from electrolysis. Spreadsheet data depict electrolysis efficiency in central and forecourt production. Central production efficiency is on average superior. This is because of the capability of larger systems to demonstrate better operational characteristics. However, forecourt production efficiency also increases in time leading to significant improvements. On the other hand, central production faces transportation to the consumption losses that are not applicable to forecourt production, which is adjacent to consumption. These 16 efficiency scenarios are also supported by a respective decrease in the production cost. Other than that, no other changes to GCAM source code have been implemented. Based on the above, if electrolysis efficiency improves, this will be translated in time to the results provided to the next chapter.

For the scenarios #1 to #16 the efficiency of electrolysis is being increased. It is assumed a five-year advance for each scenario. Specifically, the value of the following simulation time step is transferred to previous one. In this study, we conduct a simulation for each of the scenarios at each of the RCP concerned. GCAM foresees that hydrogen will start to be produced in a wider scale after 2020. However, it has to be mentioned the increased production of hydrogen requires the installation of supportive facilities, such as distribution networks if production is central. But this is not part of the present analysis.

Results

The source code and simulation results are provided to the datasets uploaded to Harvard Dataverse [39] and are available in [40]. The uploaded data include our source code modifications of the file hydrogen.xml, which is located in the GCAM folder input>gcam-data-system>xml>energy-xml. RCPs are simulated based on their expected emissions as this is described to Hector submodule. The rest of the data are the default provided by GCAM. The aforementioned 16 scenarios are applied for simulation to all three RCPs under investigation. Figures for input and output data are provided in the attached spreadsheets (files: RCP_input_graphs.xlsx, RCP_26_scenarios_output_graphs.xlsx, RCP_45_scenarios_output_graphs.xlsx and RCP_60_scenarios_output_graphs.xlsx).

Results for RCP2.6

The first group of simulations presented here is connected to RCP2.6. This is the most optimistic group of scenarios, as far as anthropogenic carbon emissions are concerned that has been here simulated. For illustration purposes, the manuscript provides in figure the results for scenario #16 (Fig. 1). However, additional information is available in the attached datasets and spreadsheets. As a matter of fact, these scenarios also created greater need for hydrogen production. RCP2.6 demonstrates a stable decrease in anthropogenic carbon emissions after 2020, that is the entry year for hydrogen production. This creates a pattern of production steadily increasing in time as it appears to Figure 1. As expected, higher hydrogen production per volume will mostly appear to the developed regions of the world, where energy requirements are higher.

Scenario #1 demonstrates a substantial increase in hydrogen production compared to the default RCP26 scenario. Before 2040 the increase is below 1% compared to the respective values of the default scenario but immediately afterward expands up to 30% for 2090. The total energy production for all periods for hydrogen as fuel at scenario #1 is 250 EJ, when for the default scenario is expected to be 195 EJ. It is according to our expectations, scenario #1 to demonstrate substantial differences

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compared to the default, due to expanded values for hydrogen production efficiency. These changes are not observed between scenarios #1 to #16. The increase appears to be maintained even after the increase in the efficiency, showing that production efficiency increase keeps hydrogen production momentum in time. Having this said, it is important if hydrogen efficiency improvement happens at the earliest possible.

For the second scenario, we observe minor changes compared to scenario #1 (file: RCP_26_scenarios_output_graphs.xlsx). In this case, except from the simulation time period of 2090, there is production increase on the level of PJ for energy production from hydrogen as fuel. This value remains large as such but since it represents global production in five (5) years per period it remains marginal for the accuracy of our calculations. Nevertheless, this minor expansion expresses the importance of improving efficiency for hydrogen production. For the rest, we observe the same behavior in terms of production patterns. Each geographic region produces hydrogen analogically to the previous scenario, with the larger countries or geographic regions in terms of population and wealth to exhibit most of the contribution.

Scenario #3 demonstrates minor increase to all time periods compared to scenario #2. The total energy production for all simulated periods at scenario #3 is expected to be 252.46EJ, while for scenario #2 the value is 252.42EJ. The observed increase in 40PJ corresponds to 1.1x10^4 GHh or more than the annual electric energy production capability of a 1.1GW nuclear power plant. This value remains relatively low but it represents our calculation results for the given improvement of production efficiency. In reality, this can be affected from various factors but it is able to showcase in kind the results of improving technology.
Similarly, for scenario #4 there is minor increase in all time periods compared to scenario #3. The total energy production for all simulated periods at scenario #4 is expected to be 252.51EJ. We observe that this value is almost similar to the previous increase. Therefore, it is an indication of production improvement due to efficiency improvement, however it shall not be considered as a definite value since in practice additional factors may affect this value.

Scenario #5 demonstrates a variety of production changes across simulation time, compared to scenario #4. It has to be mentioned that the 16 scenarios for RCP2.6 was the only simulation group of scenarios which demonstrated almost steady increase in production. On the other hand, as it is mentioned below, RCP6.0 group of scenarios demonstrated no improvement based on hydrogen as fuel production efficiency.

Scenario #6 there is also a minor increase to all time periods compared to scenario #5. The total energy production for all simulated periods at scenario #6 is expected to be 252.57EJ, while for scenario #5 the value is 252.51EJ. In this case, the behavior of the simulation results is according to our expectations as far as the increase is concerned. It has to be mentioned that repeating simulations provided to us with consistent results per se, but slightly different. Having this said, it is important to have a wide selection of simulations for the same simulation points in order to further increase confidence. However, such an endeavor is extensively demanding in computational power.

In scenario #7 there is minor increase to all time periods compared to scenario #6. The total energy production for all simulated periods at scenario #7 is expected to be 252.66EJ. Similarly, for each one of the scenarios

Figure 2. RCP4.5, scenario #16 predicted hydrogen as fuel total production per Global Change Assessment Model geographical region.
#8 to #15, there is a minor increase in all time periods, in respect to the previous scenario, and the total energy production for all simulated periods is expected to be respectively 252.82EJ, 253.13EJ, 253.34EJ, 253.64EJ, 254.06EJ, 254.6EJ, 255.37EJ, and 256.26EJ.

As a general observation, RCP2.6 was the only Representative Concentration Pathway that was simulated under our scenarios and has shown the most stable and higher increase in production across almost all cases.

**Results for RCP4.5**

For RCP4.5, hydrogen production is mostly increasing across time except from 2080 to 2085 and after 2090 (Fig. 2). Results for all the scenarios are available on: RCP_45_scenarios_output_graphs.xlsx and to the connected datasets.

The period 2080–2085 demonstrates a steep production decline of ~10%. To our opinion, this predicted behavior is connected to the respective RCP4.5 emissions. The will of the decision makers to stabilize for a few years the requirements for anthropogenic emissions decrease, leads to immediate consequences to hydrogen production that affect the situation up to the end of the century. According to predictions, hydrogen production recovers after 2085 but soon afterward declines substantially, creating only a local maximum production at 2090. The society would be better served, if this foreseen steep decline could be avoided, maybe restricting in practice hydrogen production after 2085, trying to keep the momentum to the end of the century.

Scenario #1 for RCP4.5 shows consistent increase in hydrogen production across time, which starts to be evident after 2045. The higher increase in percentage,
compared to the default scenario, is observed at 2090 for 26% and the lower at 2020–2030, where production remains almost identical. For the rest of the simulation periods from 2075 to 2095, it is above 10%. At 2100, the increase remains on the level of 2045 at around 2%.

The increase trend is dependent on the expectations of emissions reduction. RCP45 requires that after a certain period of time, no increase in emissions is expected. This is the point where hydrogen as fuel efficiency improvement leads to substantial increase in hydrogen as fuel. Up to then, the increase in anthropogenic emissions reduces the need for hydrogen as fuel to the degree that technology improvement, according to our calculations, does not affect production.

Scenarios #2 and #3 do not demonstrate significant change of hydrogen production, probably because of our simulation accuracy limitations.

On the other hand, scenario #4 for RCP4.5 shows similarities with scenario #1 except from the production at the latest circles of the simulation. At 2090, we observe a reduction compared to scenario #1 but 2095 and 2100 demonstrate significant increase to the level of 25% and 50% accordingly. Our read to these results is that while the software seeks to find a solution to the problem, proposes massive increase at the very last time. According to our opinion, it is more of a value of this increase happens steadily in time, starting probably from the early simulations, even as soon as 2020. In this case, we had to observe a mild increase in a few percentage units per five-year simulation interval.

Scenarios #4 up to the end demonstrate that the expected hydrogen production has similar behavior. As a matter of fact, scenario #16 which is the most optimistic scenario in our RCP4.5 analysis shows that hydrogen production efficiency increase is expected to create a further increase in almost one percent per simulation circle up to 2085. Then it is also observed a substantial increase after 2090 that is lower compared to scenario #4. We believe that this discrepancy is due to simulation stability issues, but also it represents the expected reality many years ahead, were prediction based on current data becomes more complicated. The next RCP we investigate is RCP6.0.

All the results are available to the attached datasets but only scenario #16 is presented below (Fig. 3).

Scenario #8 demonstrated similar pattern to the default except from a minor increase in hydrogen production. This increase is maximized for 2090 and 2095 to the level of 2% but it remains low to zero or below 1% for the most of the rest simulation circles. The increase in production efficiency, based on our simulations, does not show any significant increase in hydrogen production per se. That said, it is particularly interesting that hydrogen production mostly seems to be driven by the restrictions imposed due to emission. RCP6.0, compared to our previous work, demonstrates comparatively the least constraints on emissions, and based on this, hydrogen production is foreseen as low, even after substantially increasing production efficiency.

Scenario #16 for RCP6.0 demonstrates similar behavior to the previous scenarios. As a matter of fact, it appears to show minor on the level of 1% or no increase in foreseen hydrogen production.

From the results presented above, it is clear that RCP2.6 demonstrates higher expected hydrogen production compared to RCP4.5. RCP6.0 remains even lower. This is an expected trend however due this analysis the differences are clearer. Hydrogen production on the forecourt and centrally is directly analogous to anthropogenic emission restrictions and to the increase in electrolysis efficiency. Electrolysis is connected to hydrogen production from renewable energy sources. Based on this observation, by definition an increase in efficiency and consequently the reduction of the hydrogen cost from renewables, would increase its production across time, however to our real restrictions of anthropogenic emissions is a factor which affects more this trend. GCAM, along to our understanding connects directly hydrogen production to carbon emission targets, describing hydrogen technology as a major tool in this direction.

RCP6.0 is the most pessimistic scenario as far as climate change mitigation is concerned. In this case, not a significant increase in hydrogen production is observed, thus, any further consideration on lower climate mitigation actions would not be necessary to the requirements of this manuscript.

Results for RCP6.0

RCP6.0 is the least optimistic scenario, as far as climate change mitigation is concerned, which is simulated in our research. Similarly to the previously mentioned cases, an increase in hydrogen production is observed across time, that steadily sustained up to the end of the simulation circle. Our simulations have shown minor increase in production across the proposed scenarios for all RCPs.

Discussion

Representative concentration pathways-based simulations provided the expected hydrogen total production across time in 16 hydrogen production efficiency scenarios. RCP6.0 demonstrated minor increase in hydrogen production based on the increase in the efficiency. This was also observed for RCP4.5 but to a lesser degree. Additionally, the production pattern remained similar being steadily

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increasing for RCP2.6 and 6.0, when for RCP4.5 is increasing up to 2080 and then creates a valley and increases more rapidly again. Our simulations also have shown to a certain degree replicability, nevertheless results after every simulation of the same type, RCP and scenario, were similar but not exactly the same. To our reading this is caused by the simulation procedure GCAM uses to perform policy limitation scenarios such as RCP modeling. Having mentioned the above, we have chosen here to produce only a selection of results. The presentation of more information could not be considered as necessary since we observed that basic patterns of behavior remain consistent and the increases in the cases we describe could be small to the simulation accuracy we apply. However, all simulation results and source code are available online for further consultation.

Our figures depict the situation in 32 geographical regions or countries, as by default applies to GCAM. These are United States of America (USA), Africa (Eastern, Northern, Southern and Western), Australia and New Zealand, Brazil, Canada, Central America and Caribbean, Central Asia, China, European Union (EU) 12, EU 15, Eastern Europe, non-EU, European Free Trade Association, India, Indonesia, Japan, Mexico, Middle East, Pakistan, Russia, South Africa, South America (Northern and Southern), South Asia, South Korea, Southeast Asia, Taiwan, Argentina, and Colombia. From the above, the developed countries demonstrate higher capability of producing hydrogen. Paradoxically, Western Africa even if on average demonstrates lower gross domestic product, according to GCAM is expected to be the simulated region with the higher contribution to hydrogen production. Then follows USA, EU 15, Eastern Africa, Middle East, Southeast, and South Asia. China has on average low hydrogen production even if it is an economy rapidly expanding. To our understanding, higher hydrogen production could be connected to hydrogen production from hydrocarbons, to which Western Africa and Middle East are rich but this assumption does not adequately depict generation of hydrogen as fuel from renewable energy sources. Additionally, to the above, we support the opinion that additional analysis to the level of countries for example EU countries, could be further useful in supporting decision making for the appropriate policy for hydrogen as fuel. As anthropogenic carbon emissions are expected to be restricted in order to satisfy stricter RCPs, all geographical regions increase production analogically.

In comparison to bibliography, our simulation data are consistent to previous works. Hanley et al. [17] provide a comparative analysis of future hydrogen production based on the default scenarios for different integrated assessment models. As far as GCAM is concerned we observe that our results are similar, for the default scenario and then are changing based on the policy constraints of our analysis.

**Conclusions and Future Work**

As general remarks, geographic regions across the world behave with the same consistency. This is a strong indication of the globalized manner in which all the human affairs are being contacted. Having this said, political decisions against or in favor of stricter intervention toward carbon emission of a specific region can be de facto overruled by the rest of the world and affect it. This is also evident on integrated assessment models such as GCAM. It has to be mentioned that the accuracy we receive from our simulations, the assumptions of GCAM and the long-time span to provide results could be considered as an informed guess of hydrogen contribution to global energy situation. Based on this our work also shows consistency to the expected situation based on the RCP simulated and hydrogen production efficiency.

To our reading of the results, hydrogen production is directly connected to the expected anthropogenic carbon emissions and to a lesser degree on the capability of the researcher to achieve higher efficiency for electrolysis. This is an expected outcome; however, we were able through our scenarios and simulations to demonstrate the importance of each policy decision. If policy makers embrace RCP2.6 or stricter then hydrogen production would be substantially affecting the society, which is expected to perform more of its daily activities using hydrogen. In practice this can be hydrogen for transportation, use of hydrogen in public gas networks but also more active use on industrial processes. It was not the target of this work to point out the importance of phasing out fossil fuels, but on the other hand hydrogen would be a viable solution to achieve the environmental goals based, to a certain degree, on the existing facilities and equipment.

The full simulation database and our results are available online. This provides the capability to perform further analysis based on the simulated results or through the use of the same source code. Further investigation of the results could lead to additional knowledge on the consequences that hydrogen as fuel production efficiency creates to global energy balance. Having mentioned the above, we observed that it is important if additional simulation datasets are available for the scenarios we propose. In this way, we would able to draw more accurate conclusions on future hydrogen penetration as such and its contribution to the global effort for the climate change mitigation and the reduction of anthropogenic carbon emissions. Additionally, more optimistic case to RCP2.6 would be useful to be investigated. Henceforth, our future work would include a wide selection of additional
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Conflict of Interest

None declared.

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