Data Article

Life cycle inventory data for power production from sugarcane press-mud

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tables

**A B S T R A C T**

This data article is associated with the research article “Technical and environmental analysis on the power production from residual biomass using hydrogen as energy vector”. This paper shows the procedure to calculate the Life Cycle Inventory (LCI) of the foreground system to perform the Life Cycle Assessment (LCA) of the power production from sugarcane press-mud. Said process encompasses four main stages: i) bioethanol production; ii) bioethanol purification; iii) syngas production and purification; and iv) power production. Additionally, other processes such as biomethane production and manufacturing of catalyst were included. Foreground data related to bioethanol production was gathered from experimental procedures at lab-scale. While foreground data, concerning the other processes such as bioethanol purification, syngas production and purification, power production, and biomethane production, was built by using material and energy flows obtained from Aspen Plus\textsuperscript{\textregistered}. Lastly, LCI of the catalyst manufacturing was built based on literature review and the approach stated by Ecoinvent. All the inventories are meaningful to carry out future environmental assessments involving sustainable energy systems based on bioethanol, biomethane, or hydrogen.

**Dataset link:** Dataset for the production of power from sugarcane press-mud (Original data)

**Keywords:** Bioethanol, Biomethane, Catalyst, Fuel cells, Hydrogen, Life Cycle Assessment
Specifications Table

| Subject | Renewable Energy, Sustainability, and the Environment |
|-----------------|-----------------------------------------------------|
| Specific subject area | Life Cycle Assessment |
| Type of data | Table |
| Figure |
| How data were acquired | Data of bioethanol production were acquired by experimental procedure at lab-scale and subsequent material and energy balances. |
| | Data of power production from bioethanol and biomethane were taken from Aspen based on material and energy balances. |
| | Data of catalyst manufacturing were taken from scientific literature, databases, material, and energy balances. |
| | Transportation distances were taken by means of Google-maps. |
| Data format | Raw and processed |
| Parameters for data collection | Samples of sugarcane press-mud were processed to produce bioethanol at a lab-scale. Material and energy balances were performed based on that experimental data. Bioethanol composition at lab-scale was used as the main input in an Aspen flowsheet to estimate the Material and energy balances of power production. Key data to gather primary data was retrieved from scientific papers and databases. |
| Description of data collection | Primary data concerning bioethanol production were obtained from experimental work at lab-scale conditions. Other data were obtained from Aspen simulations, databases, scientific reports, academic theses, and patents. |
| Data source location | Institution: Universidad de La Sabana |
| City/Town/Region: Chia, Cundinamarca |
| Country: Colombia |
| Data accessibility | Raw data |
| Repository name: Mendeley Data |
| Data identification number: doi: 10.17632/5nhfjhh778.2 |
| Direct URL to the data: http://dx.doi.org/10.17632/5nhfjhh778.2 |
| Processed data |
| With the article |
| Related research article | N. Sanchez, R. Ruiz, A. Rödl, M. Cobo, Technical and environmental analysis on the power production from residual biomass using hydrogen as energy vector, Renewable Energy 175 (2021) 825-839. |

Value of the Data

- The data shown in this contribution allow to strengthen the Life Cycle Assessment depicts in the main article.
- The data shown in this document could be used by anyone who wants to assess the environmental performance of energy systems based on bioethanol, hydrogen, and power from fuel cells.
- The data could be employed to model and simulate similar processes.

1. Data Description

This article shows the life cycle inventory (LCI) of the foreground system needed to perform a life cycle assessment (LCA) of power production from sugarcane press-mud. These data give transparency to the main results shown in the reference article [1]. LCI was gathered from experimental data at lab-scale, simulation from Aspen Plus V9 (Aspentech, Bedford, USA), Ecoinvent database V3.4, scientific and academic reports, and websites. **Fig. 1** shows the foreground
system for producing power from sugarcane press-mud, while Table 1 shows the data sources employed to build the complete LCI. Mostly of the data information were retrieved from Aspen Plus and the main simulation flowsheets are depicted in the main manuscript [1]. Tables 2 and 3 describe the operating conditions of main processes highlighting that three scenarios were addressed under three different separation processes units: i) flash distillation (scenario 1); ii) mash column (scenario 2); and iii) mash column followed by a rectification unit (scenario 3). Figs. 2–4 validate the simulation results by comparing them with both experimental (i.e., \( \text{H}_2 \) composition) and commercial (i.e., polarization curves of fuel cell) data. Table 4 shows both the energy consumption and the cooling water demand of main energy blocks, such as pumps, compressors, heat exchangers, reactors, and condensers. Figs. 5 and 6 depict the Aspen flowsheets to produce biomethane and power in a Rankine cycle, respectively. Table 5 describes the operating conditions to produce biomethane from the solid fraction of sugarcane press-mud. Tables 6 and 7 show the power distribution in the 32 departments of Colombia. Fig. 7 portrays the block flow diagram to synthesize \( \text{RhPt/\text{CeO}_2-\text{SiO}_2} \) and \( \text{AuCuO/\text{CeO}_2} \) under laboratory conditions. Whilst Fig. 8 illustrates the block flow diagram to manufacture the main precursors to produce the above catalysts at industrial level. Table 8 describes the Ecoinvent assumptions to build the LCI of chemicals that are not included within Ecoinvent databases. Tables 9–26 summarize the LCI of the foreground systems detailed in Fig. 1.

Aside from the data shown in this document, the raw data to calculate the inventory data for both the power production from sugarcane press-mud and the synthesis of catalysts are shown in the repository in Mendeley [15]. On the one hand, the dataset associated with the power production from sugarcane press-mud included: (i) mass and energy balances from Aspen Plus

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**Table 1**

Data source of the processes required to produce power from sugarcane press-mud.

| Process                  | Data source                                      | Reference |
|--------------------------|--------------------------------------------------|-----------|
| Bioethanol production    | Lab-scale experiments                            | [2,3]     |
| Bioethanol purification  | Scientific papers, Aspen plus simulation data    | [4]       |
| \( \text{H}_2 \) production | Aspen plus simulation, lab-scale data          | [2,5]     |
| \( \text{H}_2 \) purification | Scientific papers, lab-scale data                | [6]       |
| Biomethane production    | Aspen plus simulation data, scientific papers    | [7]       |
| Colombian power grid     | Colombian Databases, Ecoinvent                   | [8]       |
| Catalyst manufacturing   | Scientific papers, lab-scale data, Ecoinvent assumptions | [9–14] |

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**Fig. 1.** Foreground system to produce power from sugarcane press-mud.
Table 2
Aspen subroutines description for bioethanol purification processes.

| Aspen subroutine | Scenario 1 (Flash distillation) | Scenario 2 (Mash column) | Scenario 3 (Mash column + rectification) |
|------------------|---------------------------------|--------------------------|----------------------------------------|
| P-101            | $P_{out} = 1$ atm
Efficiency: 75% | $P_{out} = 1$ atm
Efficiency: 75% | $P_{out} = 1$ atm
Efficiency: 75% |
| E-100            | $T_{out} = 93$ °C
$\Delta P = 0$ atm | $\Delta P = 0$ atm
$\Delta T_{min} = 10$ °C | $\Delta P = 0$ atm
$\Delta T_{min} = 10$ °C |
| T-101            | Duty: 0 MJ/h
$\Delta P = 0$ atm | Condenser: none
Reboiler: none
Stages: 24
Feed tray: 1 (on-stage)
Column pressure: 0.81 atm
$\Delta P = 0.015$ atm/tray | Increases the pressure to the column pressure
Efficiency: 75%
Condenser: Total
Reflux ratio: 4.3
Stages: 58
Feed tray: 58 (on-stage)
Column pressure: 0.81 atm
$\Delta P = 0.015$ atm/tray |
| K-100            | N/A                             | N/A                      | Increases the steam-to-ethanol ratio to 3 |
| T-REC            | N/A                             | N/A                      | Evaporates water to steam |
| M-100            | N/A                             | N/A                      | Increases the pressure of the water to 1.2 atm |
| E111             | N/A                             | N/A                      | |
| P-102            | N/A                             | N/A                      | |

Fig. 2. Effect of the molar reflux ratio in the rectification column on the sugarcane press-mud consumption and ethanol recovery.

and (ii) life cycle inventory and life cycle impact assessment of power production from sugarcane press-mud. On the other hand, the data associated with the synthesis of catalysts includes: (i) mass and energy balances to synthesize all precursors and catalysts at laboratory scale and (ii) life cycle inventory of the catalysts precursors and catalysts.
Table 3
Description of main subroutines to produce power from raw bioethanol.

| Aspen subroutine | Description | Conditions | Assumptions |
|------------------|-------------|------------|-------------|
| R-101            | Steam reforming of bioethanol modelled with a Gibbs reactor | $T = 700$ °C  
$P = 1$ atm | ● The steam reforming reactor was modelled as Gibbs reactor.  
● A calculator block was employed to calculate $H_2$ yield ($Y_{H_2}$) based on the impurities concentration ($x_i$) and the following equation:  
$$Y_{H_2} = -15.269x_i + 5.402$$ [2]  
● CO, CO$_2$, CH$_4$, C$_3$H$_6$, C$_4$H$_8$, acetaldehyde, acetone, higher alcohols were including within the Gibbs analysis.  
● RhPt/CeO$_2$-SiO$_2$ was used as catalyst.  
● The amount of catalyst was calculated based on laboratory conditions. |
| R-102            | CO removal from the syn-gas stream | $T = 260$ °C  
$P = 1$ atm | ● The CO removal reactor was modelled as Gibbs reactor.  
● The temperature was set to 260 °C based on previous works.  
● A calculator block was employed to calculate the $H_2$ mole flow rate.  
● The $O_2/CO$ ratio was adjusted to 0.9 using a Fortran statement.  
● Au-CuO/CeO$_2$ was used as catalyst.  
● The amount of catalyst was calculated similar to R-101. |
| Pressure swing adsorption (PSA) | $H_2$ purification | $T = 35$ °C  
$P = 15$ bar  
$H_2$ recovery = 80%  
$H_2$ purity = 99.99 vol.% | ● A double layer adsorbent formed by activated carbon and zeolite was used to clean the gas from the CO removal reactor.  
● The amount of adsorbent employed was assumed to be 0.85 g per kg of fuel based on a conceptual project developed in Germany to produce $H_2$ from biogas [6].  
● A carbon-zeolite ratio of 8:2 was assumed to be used in the PSA stage according to literature. |
| Furnace          | Burn the gases from the PSA unit to produce energy to heat up the reformer | Adiabatic | ● The furnace was modelled with a Gibbs reactor.  
● CO$_2$, NO$_2$, NO, N$_2$, CO, CH$_4$, $H_2$ were considered as output products.  
● Biogas, obtained from anaerobic digestion of mud, was employed as additional fuel to heat up some stream processes. |
| K-system         | Compress the clean gas to PSA conditions | Polyprotic efficiency = 83% | ● Compression system was built according to heuristics rules.  
● 4 compressors were included to increase the pressure from 1 to 15 atm.  
● Intermediate cooling was used.  
● The outlet temperature for the cooling system was selected according to the dew temperature of the gas. |
Table 4
Heat and water-cooling demand of subroutines required to produce power from sugarcane press-mud under different scenarios of separation processes. Functional unit = 1 kWh of power.

| Subroutine | Stage process                      | Heat demand (MJ/h) | Water cooling demand (kg/h) |
|------------|------------------------------------|--------------------|----------------------------|
|            |                                    | Scenario 1 | Scenario 2 | Scenario 3 | Scenario 1 | Scenario 2 | Scenario 3 |
| P-101      | Bioethanol purification             | 0.0044     | 0.0022     | 0.00018    | NA         | NA         | NA         |
| P-102      | Bioethanol purification             | NA         | 5.85E-5    | 4.67E-5    | NA         | NA         | NA         |
| K-100      | Bioethanol purification             | NA         | NA         | 0.13       | NA         | NA         | NA         |
| E-100      | Bioethanol purification             | NA         | 1.82       | 1.46       | NA         | NA         | NA         |
| E-111      | Bioethanol purification             | 41.79      | 2.96       | 2.36       | NA         | NA         | NA         |
| Condenser  | Bioethanol purification             | NA         | NA         | 1.82       | NA         | NA         | 87.25      |
| E-101      | Syngas production                  | 3.91       | 4.00       | 1.82       | NA         | NA         | NA         |
| E-113      | Syngas production                  | 11.08      | 8.11       | 2.61       | NA         | NA         | NA         |
| Q-R101     | Syngas production                  | 2.55       | 2.84       | 2.15       | NA         | NA         | NA         |
| E-102      | Syngas production                  | 4.99       | 2.82       | 2.06       | 239.05     | 135.29     | 98.77      |
| Q-R102     | Syngas production                  | 11.08      | 2.82       | 2.61       | NA         | NA         | NA         |
| E-104      | Syngas purification                | 2.11       | 1.25       | 0.86       | 101.2      | 59.84      | 41.27      |
| E-105      | Syngas purification                | 5.67       | 2.99       | 1.49       | 271.4      | 143.5      | 71.57      |
| E-106      | Syngas purification                | 0.49       | 0.31       | 0.24       | 23.67      | 14.93      | 11.62      |
| E-107      | Syngas purification                | 0.85       | 0.53       | 0.41       | 40.55      | 25.52      | 19.79      |
| E-108      | Syngas purification                | 0.29       | 0.18       | 0.14       | 14.00      | 8.83       | 6.85       |
| K-101      | Syngas purification                | 2.16       | 1.29       | 0.91       | NA         | NA         | NA         |
| K-102      | Syngas purification                | 0.74       | 0.47       | 0.37       | NA         | NA         | NA         |
| K-103      | Syngas purification                | 0.46       | 0.29       | 0.23       | NA         | NA         | NA         |
| K-104      | Syngas purification                | 0.33       | 0.21       | 0.16       | NA         | NA         | NA         |
| E-109      | Power production                   | 0.04       | 0.04       | 0.04       | NA         | NA         | NA         |

NA: No applied
Table 5
Subroutines employed to simulate the biomethane production from the residual waste and the Rankine Cycle.

| Subroutine | Purpose |
|------------|---------|
| M-101      | Adjusts the solid content to 10 wt.% |
| E-101      | Heats up the mixture to 35 °C which is the anaerobic digestion temperature |
| S-101      | Separates the water fraction from the biomass and separate the unreacted biomass fraction |
| R-101      | RYIELD converts the non-conventional solid into C, H₂, O₂, N₂, water, and ash |
| R-102      | ROIBBS calculates the biogas composition based on the minimization of the Gibbs Free Energy. CO₂, NH₃, CH₄, and water were considered as the main reaction products according to Eq. (1) |
| S-102      | Separates the gas and liquid phase at the anaerobic digestion conditions, i.e., T = 35 °C, and atmospheric pressure |
| X-101      | Simulates the leakage of the biogas during the anaerobic digestion |
| M-102      | Mixes the biogas with the unrecovered gas from the absorption process |
| K-system   | Increases the pressure to 10 bar which is the operating pressure of the high-pressure scrub system |
| T-101      | Simulates the absorption tower (P = 10 bar, T = 20 °C, N = 7, L/V = 137) |
| T-102      | Simulates the stripping tower (P=atmospheric, T = 20 °C, N = 10, L/V = 133) |
| S-103      | Separates CH₄ and CO₂ from water |
| V-101      | Reliefs the pressure from 10 bar to atmospheric pressure |
| P-101      | Increases the water pressure to 10 bar. Efficiency = 85% |
| K-101      | Decreases the pressure from 10 to 0.82 bar |
| Boiler     | Produces steam in the Rankine cycle |
| P-103      | Increases the water pressure to 10 bar in the Rankine cycle. Efficiency = 85% |
| E-105      | Condenses the water in the Rankin cycle |
| K-103      | Decreases the pressure from 10 to 0.04 bar. Efficiency = 85% isentropic |

P = pressure, T = temperature, N = number of equilibrium stages, L/V = liquid-to-vapor molar ratio

2. Experimental Design, Materials and Methods

The detailed process to produce power from sugarcane press-mud is described in the related research paper [1]. Fig. 1 shows the main foreground systems. Detailed information about data acquisition, for each of the main units, is explained below.

2.1. Raw bioethanol production

Raw bioethanol production from sugarcane press-mud encompasses 3 main stages: i) pretreatment; ii) fermentation; and iii) inoculum preparation. Material and energy flows for said processes were calculated based on experimental work. The mass was measured in each stage by using an analytical balance. Moreover, the energy flows were calculated based on the thermodynamic properties and the chemical composition. Chemical composition of liquid samples was quantified by gas chromatography, whereas the sugarcane press-mud composition was quantified by SGS (Société Générale de Surveillance), a certified laboratory [2]. Thermodynamic properties were retrieved from Aspen Plus V9 (Aspentech, Bedford, USA).

For the subsequent stages: bioethanol purification, syngas production and purification, and power production in a low temperature proton exchange membrane fuel cell (LT-PEMFC), Aspen plus V9 (Aspentech, Bedford, USA) was used and the non-random two liquid – Redlich-Kwong (NRTL-RK) thermodynamic package was employed.

2.2. Bioethanol purification

Bioethanol purification is the second stage, as shown in Fig. 1. Material and energy flows were retrieved from Aspen Plus V9. The design specification tool along with calculator subrou-
### Table 6
Electricity generation in Colombia (MW).

| Department        | Cogeneration (Bagasse) | Wind | Hydropower | Solar | ACPM | Biogas | Carbon | Oil | Gas | Jet | Total  |
|-------------------|------------------------|------|------------|-------|------|--------|--------|-----|-----|-----|--------|
| Antioquia         | 4733                   | 353  | 9          |       |      |        | 1      | 1   | 5   | 5096 |        |
| Arauca            |                        |      | 5          | 8     | 912  | 1000   |        |     | 5   | 5    |        |
| Atlántico         |                        | 8    | 184        | 434   |      |        |        |     |     |     | 626    |
| Bolivar           |                        | 1020 | 343        |       |      |        |        |     |     |     | 1363   |
| Boyacá            |                        | 606  |            |       |      |        |        |     |     |     | 650    |
| Caldas            |                        |      | 168        |       |      |        |        |     |     |     | 168    |
| Casanare          |                        |      |            | 168   |      |        |        |     |     |     | 168    |
| Cauca             | 30                     | 353  |            |       |      |        |        |     |     |     | 383    |
| Córdoba           | 338                    |      |            |       |      |        |        |     |     |     | 775    |
| Cundinamarca      | 2191                   | 4    |            |       |      |        |        |     |     |     | 2422   |
| Huila             | 951                    |      |            |       |      |        |        |     |     |     | 951    |
| La Guajira        | 18                     |      |            | 286   |      |        |        |     |     |     | 304    |
| Magdalena         |                        |      |            | 610   |      |        |        |     |     |     | 610    |
| Meta              | 20                     | 2    |            |       |      |        |        |     |     |     | 61     |
| Nariño            | 23                     |      |            | 40    |      |        |        |     |     |     | 61     |
| Norte de Santander|                        |      |            |       |      |        |        |     |     |     | 23     |
| Putumayo          | 0                      |      |            | 333   |      |        |        |     |     |     | 333    |
| Quindío           | 4                      |      |            | 1     |      |        |        |     |     |     | 1      |
| Risaralda         | 17                     | 28   |            |       |      |        |        |     |     |     | 45     |
| Santander         | 838                    |      |            | 446   |      |        |        |     |     |     | 1284   |
| Tolima            | 204                    |      |            | 4     |      |        |        |     |     |     | 208    |
| Valle del Cauca   | 73                     | 643  | 10         | 454   | 27   |        |        |     |     |     | 1206   |
| **Total**         | **139.6**              | **18.42** | **11933.71** | **17.98** | **807** | **3.95** | **1660.3** | **272** | **2621.89** | **44** | **17518.85** |
### Table 7
Power grid distribution by department in Colombia (%).

| Department          | Cogeneration (Bagasse) | Wind | Hydropower | Solar | ACPM | Biogas | Carbon | Oil | Gas | Jet | Total |
|---------------------|------------------------|------|------------|-------|------|--------|--------|-----|-----|-----|-------|
| Antioquia           | 0.0                    | 0.0  | 92.9       | 0.0   | 6.9  | 0.2    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Arauca              | 0.0                    | 0.0  | 0.0        | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Atlántico           | 0.0                    | 0.0  | 0.0        | 0.0   | 0.0  | 0.0    | 0.0    | 8.8 | 91.2| 0.0 | 100   |
| Bolívar             | 0.0                    | 0.0  | 1.3        | 0.0   | 0.0  | 0.0    | 25.2   | 0.0 | 0.0 | 0.0 | 100   |
| Boyacá              | 0.0                    | 0.0  | 74.8       | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Caldas              | 0.0                    | 0.0  | 93.2       | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Casanare            | 0.0                    | 0.0  | 0.0        | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Cauca               | 7.8                    | 0.0  | 92.2       | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Córdoba             | 0.0                    | 0.0  | 43.6       | 0.0   | 0.0  | 0.0    | 56.4   | 0.0 | 0.0 | 0.0 | 100   |
| Cundinamarca        | 0.0                    | 0.0  | 90.4       | 0.0   | 0.0  | 0.2    | 9.3    | 0.0 | 0.0 | 0.0 | 100   |
| Huila               | 0.0                    | 0.0  | 100.0      | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| La Guajira          | 0.0                    | 6.1  | 0.0        | 0.0   | 0.0  | 93.9   | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Magdalena           | 0.0                    | 0.0  | 0.0        | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Meta                | 32.5                   | 0.0  | 2.6        | 0.0   | 0.0  | 0.0    | 64.9   | 0.0 | 0.0 | 0.0 | 100   |
| Nariño              | 0.0                    | 0.0  | 100.0      | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Norte de Santander  | 0.0                    | 0.0  | 0.0        | 0.0   | 0.0  | 100.0  | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Putumayo            | 0.0                    | 0.0  | 32.0       | 0.0   | 0.0  | 0.0    | 0.0    | 68.0| 0.0 | 0.0 | 100   |
| Quindío             | 0.0                    | 0.0  | 100.0      | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Risaralda           | 37.4                   | 0.0  | 62.6       | 0.0   | 0.0  | 0.0    | 0.0    | 0.0 | 0.0 | 0.0 | 100   |
| Santander           | 0.0                    | 0.0  | 65.3       | 0.0   | 0.0  | 0.0    | 0.0    | 34.7| 0.0 | 0.0 | 100   |
| Tolima              | 0.0                    | 0.0  | 98.2       | 0.0   | 0.0  | 0.0    | 0.0    | 1.8 | 98.2| 0.0 | 100   |
| Valle del Cauca     | 6.0                    | 0.0  | 53.3       | 0.8   | 37.6 | 0.0    | 2.2    | 0.0 | 0.0 | 0.0 | 100   |

Total general: 0.797 0.105 68.119 0.103 4.606 0.023 9.477 1.553 14.966 0.251 100
Table 8
Assumptions required to build a dataset for chemicals manufacturing based on Ecoinvent framework [9].

| Item                          | Description                                                                 |
|-------------------------------|-----------------------------------------------------------------------------|
| Mass requirements             | • Input materials were calculated based on stoichiometric reactions.        |
|                               | • Reaction equations can be obtained from technical books like the Ullmann’s  |
|                               |   Encyclopedia [11,12].                                                     |
| Energy consumption            | • Energy and heat consumption were based on the information of several      |
|                               |   chemical companies in Germany.                                           |
|                               | • Heat consumption was assumed to be 1.9840 MJ kg⁻¹ chemical.              |
|                               | • Electricity consumption was assumed to be 1.2160 MJ kg⁻¹ chemical.       |
|                               | • For exothermic reactions, heat was assumed to be 0 MJ kg⁻¹.              |
| Water consumption             | • Water consumption was based on the information of several chemical       |
|                               |   companies in Germany.                                                    |
|                               | • Cooling water was assumed to be 24 kg kg⁻¹ chemical.                     |
|                               | • Process water was assumed to be 6 kg kg⁻¹ chemical.                      |
| Emission to air/to water      | • Emission to air was assumed to be 0.2% of the input material.            |
| Solid waste                   | • Water emission was calculated by mass balance.                           |
| Transportation                | • Solid wastes were excluded from this approach.                           |
|                               | • Standard distances were employed.                                        |
|                               | • For most materials, 100 km with lorry and 200 – 600 km by train were    |
| Infrastructure                | • “Chemical plant, organics” in Ecoinvent is used as an approximation.     |
|                               | • 4 × 10⁻¹⁰ units kg⁻¹ chemical was assumed. This number represents 50,000  |
|                               |   ton per year and a plant lifetime of 50 years.                           |

Table 9
Life cycle inventory for producing 1 kg of hydrolysate from sugarcane press-mud.

| Stream name            | Kind of stream | Unit | Value | Ecoinvent V3.4                                                                 |
|------------------------|----------------|------|-------|-------------------------------------------------------------------------------|
| Sugarcane press-mud¹   | Input          | kg   | 2.432 | Created by the user                                                           |
| Electricity²           | Input          | MJ   | 1.306 | Market for electricity, low voltage | electricity, low voltage| APOS, S - CO                      |
| Water process          | Input          | kg   | 0.1583| Water, unspecified natural origin, CO                                          |
| Cooling water          | Input          | kg   | 11.1214| Water, cooling, unspecified natural origin, CO                                 |
| Transport              | Input          | kg/km| 72.96 | Transport, freight, lorry 3.5 – 7.5 metric ton, EURO 4 | transport, freight, lorry 3.5 – 7.5 metric ton, EURO 4 | APOS, S - RoW                      |
| Steam                  | Emission to air| kg   | 0.0567| Water vapour, Emission to air/unspecified                                      |
| Mud³                   | Output         | kg   | 1.5336| Created by the user                                                           |

1 Sugarcane press-mud is the product studied for its further conversion to power
2 Power grid electricity was build based on information retrieved from Colombian data
3 Agroindustrial by-product obtained experimentally at the defined conditions

tines were used to define the operating conditions that warrant a steam-to-ethanol molar ratio (S/E) of 3. Three main scenarios were assessed, and the Aspen flowsheets are shown in the reference article. Besides, Fig. 2 shows the effect of molar reflux ratio on the sugarcane press-mud consumption and ethanol recovery in the rectification unit.

2.3. Syngas production and purification

Syngas production was carried out in a Gibbs reactor system which models the Ethanol Steam Reforming (ESR) by using RhPt/CeO₂–SiO₂, as catalyst at 700 °C. Table 3 shows the description of main subroutines employed to simulate the syngas production and purification. Since impurities
Table 10
Life cycle inventory for producing 1 kg of raw bioethanol from sugarcane press-mud hydrolysate.

| Stream name              | Kind of stream | Unit | Value   | Ecoinvent V3.4                        |
|--------------------------|----------------|------|---------|---------------------------------------|
| Hydrolysate              | Input          | kg   | 1.0864  | Data from Table 9                     |
| Energy for fermentation¹ | Input          | MJ   | 0.7958  | Market for electricity, low voltage | |
|                          |                |      |         | electricity, low voltage | [electricity, low voltage] | APOS, S - GLO |
| Cooling water            | Input          | kg   | 11.627  | Water, cooling, unspecified natural origin, CO |
| Peptone                  | Input          | kg   | 0.0113  | Chemical production, organic | [chemical organic] | APOS, S - GLO |
| Yeast extract            | Input          | kg   | 0.0158  | Market for fodder yeast [fodder yeast] | APOS, S - GLO |
| Ammonium sulfate         | Input          | kg   | 0.0011  | Market for ammonium sulfate, as N | ammonium sulfate, as N | APOS, S - GLO |
| MgSO₄.7H₂O               | Input          | kg   | 0.0009  | Market for magnesium sulfate | magnesium sulfate | APOS, S - GLO |
| Ca₃(PO₄)₂                | Input          | kg   | 0.0004  | Chemical production, inorganic | [Chemical, inorganic] | APOS, S -GLO |
| Freight ship transport   | Input          | kg*km| 218.9246| Transport, freight, sea, transoceanic ship | transport, freight, sea, transoceanic ship | APOS, S -GLO |
| Freight road transport   | Input          | kg*km| 26.55   | Transport, freight, lorry 7.5 - 16 metric ton | EURO 4 | transport, freight, lorry 7.5 - 16 metric ton | EURO4| APOS, S RoW |
| Freight road transport   | Input          | kg*km| 1.76172 | Transport, freight, lorry 7.5 - 16 metric ton | EURO 6 | transport, freight, lorry 7.5 - 16 metric ton | EURO6| APOS, S RER |
| Inoculum                 | Input          | kg   | 0.105   | Data from Table 11                    |
| Steam                    | Emission to air| kg   | 0.0346  | Water vapour, Emission to air/unspecified |
| CO₂                      | Emission to air| kg   | 0.2011  | Carbon dioxide, non-fossil, Emission to Air/unspecified |

¹ Power grid electricity was build based on information retrieved from Colombian data

have an important effect on H₂ production, a linear model developed experimentally was used to forecast the H₂ production. Fig. 3 shows the validation between experimental work and simulation data. Material data of output streams were directly gathered from the simulation to define the water and air emissions to the ecosphere. Table 4 shows the energy demand and cooling requirements of each subroutine employed to produce power from raw bioethanol. These data were used to calculate LCI associated with heat, power, and cooling water requirements.

Syngas purification was performed in a CO-removal reactor at 260 °C over a Au-CuO/CeO₂ catalyst. RGIBBS subroutine was employed to model this operation. Both CO and H₂ conversion models, retrieved from experimental data at lab-scale [5], were used to forecast the clean gas composition. To produce pure H₂, a pressure swing adsorption (PSA) unit was employed. PSA unit was modelled by using a separator and defining both H₂ purity and recovery. Prior PSA, a train compressor system was employed to adjust the operating pressure of PSA (i.e., 15 atm). Moreover, intermediary cooling systems and separators were employed to remove the water present in the syngas stream.
Table 11
Life cycle inventory for producing 1 kg of yeast inoculum in YPD medium.

| Stream               | Kind of stream | Unit | Value    | Ecoinvent 3.4                          |
|----------------------|----------------|------|----------|----------------------------------------|
| Peptone              | Input          | kg   | 0.0191   | Chemical production, organic | chemical, organic] APOS, S -GLO |
| Yeast extract        | Input          | kg   | 0.00955  | Market for fodder yeast [fodder yeast] APOS, S - GLO |
| Lyophilized yeast    | Input          | kg   | 0.00061  | Glucose production | glucose | APOS, S -RoW |
| Glucose              | Input          | kg   | 0.0191   | Table 12                             |
| Electrical energy¹   | Input          | MJ   | 0.57321  | Market for electricity, low voltage | electricity, low voltage| APOS, S - Co |
| Water cooling        | Input          | kg   | 5.64496  | Water, cooling, unspecified natural origin, Co |
| Water process        | Input          | kg   | 0.95224  | Water, unspecified natural origin, Co |
| Freight ship         | Input          | kg⋅km | 386.95328 | Transport, freight, sea, transoceanic ship | transport, freight, sea, transoceanic ship | APOS, S -GLO |
| Freight road         | Input          | kg⋅km | 43.524   | Transport, freight, lorry 7.5 - 16 metric ton, EURO 4 [transport, freight, lorry 7.5 - 16 metric ton, EURO04] APOS, S RoW |
| Freight road         | Input          | kg⋅km | 0.13664  | Transport, freight, lorry 7.5 - 16 metric ton, EURO 6 [transport, freight, lorry 7.5 - 16 metric ton, EURO06] APOS, S RER |
| Carbon dioxide       | Emission to air| kg   | 0.00934  | Carbon dioxide, Emission to air, unspecified |

¹ Power grid electricity was build based on information retrieved from Colombian data

Table 12
Life cycle inventory for producing 1 kg of lyophilized yeast [3].

| Stream                  | Kind of stream | Unit | Value   | Ecoinvent 3.4                          |
|-------------------------|----------------|------|---------|----------------------------------------|
| Molasses, from sugar beet| Input          | kg   | 3.90    | Market for molasses, from sugar beet [molasses, from sugar beet] APOS, S – GLO |
| Ammonia                 | Input          | kg   | 0.08    | Market for ammonia, liquid | ammonia liquid] APOS, S – RER |
| P₂O₅                    | Input          | kg   | 0.03    | Market for phosphate fertilizer, as P205 | phosphate fertilizer, as P205] APOS, S – GLO |
| Steam                   | Input          | MJ   | 13.0    | Market for heat, from steam, in chemical industry | heat, from steam, in chemical industry] APOS, S – RER |
| Electricity             | Input          | MJ   | 3.10    | Market for electricity, low voltage | electricity, low voltage] APOS, S – FR |

2.4. Fuel cell simulation

The electrochemical behavior of LT-PEMFC was modelled in Aspen Plus V9 along with FORTRAN statements based on the model recommended in the literature [16]. Moreover, the anode was modelled using a SEPARTOR (SEP), while the cathode was modelled using an adiabatic RGIBBS. The SEP splits the H₂ fraction that is used in the LT-PEMFC and the RGIBBS simulates
the chemical reaction between \( \text{H}_2 \) and oxygen to yield water and heat as main products. RGIBBS was considered adiabatic. The design specification tool was used to calculate the cooling air needed to keep the fuel cell temperature at 70 °C. Heat was not considered as by-product. Fig. 4 shows the validation of the simulation according to the polarization curves between a commercial Ballard Mark V LT-PEMFC and Aspen results.
Table 14
Life cycle inventory for producing 1 kg of clean syngas.

| Stream name | Kind of stream | Unit | Scenario 1 | Scenario 2 | Scenario 3 | Ecoinvent 3.4 |
|-------------|----------------|------|------------|------------|------------|---------------|
| Bioethanol (S/E=3) | Input | kg | 0.2831 | 0.2750 | 0.2902 | Table 13 |
| RhPt/CoO2-SiO2 | Input | kg | 4.13E-06 | 4.04E-06 | 4.27E-06 | Table 25 |
| AuCuO/CoO2 | Input | kg | 4.13E-06 | 4.04E-06 | 4.27E-06 | Table 26 |
| Carrier (N2) | Input | kg | 0.63098 | 0.6141 | 0.6494 | Market for nitrogen, liquid [nitrogen, liquid] APOS, S - RoW |
| Quartz | Input | kg | 1.03E-5 | 1.01E-5 | 1.07E-5 | Market for glass tube, borosilicate [glass tube, borosilicate] APOS, S - GLO |
| Oxygen | Input | kg | 0.0859 | 0.1109 | 0.0634 | Market for oxygen, liquid [oxygen, liquid] APOS, S - RoW |
| Cooling water | Input | kg | 28.4154 | 28.040 | 31.0694 | Water, cooling, unspecified natural origin, CO |
| Energy Transport | Input | MJ | 0.3036 | 0.5890 | 1.2506 | Table 16 |
| Energy Transport | Input | kg*km | 0.0037 | 0.0036 | 0.0038 | Transport, freight, light commercial vehicle [transport, freight, light commercial vehicle] APOS, S - RoW |

Fig. 4. a) Validation of a Ballard Mark V fuel cell. Continuous line: Aspen model; ◦ Experimental data. Fuel cell parameters: T = 343 K, P = 1 atm, P_H2 = 1 atm; P_O2 = 1 atm; A = 50.6 cm²; and n = 1. b) Fuel cell performance at the operating conditions of the power production plant. T = 348 K, P = 0.81 atm.

2.5. Aspen simulation to produce biomethane from residual biomass

Fig. 5 shows the simulation to produce biomethane from the solid fraction of sugarcane press-mud. Herein, a theoretical estimation of the biogas production by anaerobic digestion was used according to the Boyle’s formula (Eq. 1) and the following assumptions: (i) constant temperature and perfect mixing; (ii) ideal bacterial condition; (iii) biomass is modelled from ultimate analysis; (iv) products reaction include only CH4, CO2, NH3, and H2S; and (v) no accumulation of ashes [7]. The non-random two liquids (NRTL) thermodynamic model was used along with Henry law. Biogas upgrade to biomethane was done by high pressure water scrubbing. Proximate and ultimate analysis were included in the simulation. The solid fraction was created as a non-conventional solid. HCOALGEN and DCOALIGT were used to estimate the enthalpy
Table 15
Life cycle inventory for producing 1 kg of H₂ (99.99 vol.%).

| Stream name         | Kind of stream | Unit    | Scenario 1 | Scenario 2 | Scenario 3 | Ecoinvent 3.4 |
|---------------------|----------------|---------|------------|------------|------------|---------------|
| Clean syngas        | Input          | kg      | 116.389    | 66.208     | 43.993     |               |
| Zeolite             | Input          | kg      | 1.70E-4    | 1.70E-4    | 1.70E-4    |               |
| Activated carbon    | Input          | kg      | 6.8E-4     | 6.8E-4     | 6.8E-4     |               |
| Cooling water       | Input          | kg      | 6236.78    | 3466.65    | 2090.99    |               |
| Electrical power    | Input          | MJ      | 51.1308    | 31.099     | 23.036     |               |
| Freight ship transport | Input      | kg*km   | 2.527      | 2.527      | 2.527      |               |
| Freight road transport | Input      | kg*km   | 0.7637     | 0.764      | 0.764      |               |
| Exhaust gas         | Output        | kg      | 97.029     | 56.570     | 40.415     |               |
| Water               | Emission to water | kg   | 17.7408    | 8.322      | 2.475      |               |
| Carbon monoxide     | Emission to water | kg   | 5.78E-4    | 0.0004     | 5.35E-05   |               |
| Carbon dioxide      | Emission to water | kg   | 0.3241     | 0.1962     | 0.0610     |               |
| Methane             | Emission to water | kg   | 0.0261     | NR         | NR         |               |
| Nitrogen            | Emission to water | kg   | 0.0237     | 0.0115     | 0.0032     |               |
| Water               | Emission to air | kg     | 0.0054     | 0.0022     | 7.30E-4    |               |
| Carbon monoxide     | Emission to air | kg     | 0.0019     | 0.0010     | 1.73E-04   |               |
| Carbon dioxide      | Emission to air | kg     | 0.1172     | 0.0605     | 0.022      |               |
| Methane             | Emission to air | kg     | 0.0150     | NR         | NR         |               |
| Nitrogen            | Emission to air | kg     | 0.1051     | 0.0434     | 0.014      |               |

and density of the biomass, respectively. FORTRAN statements were used along with simulation to adjust input and outputs of the flowsheet according to the requirements. Table 5 shows the description of the subroutines described in Fig. 5.

\[ \text{C}_4\text{H}_8\text{O}_\text{CaN}_\text{Se} + \text{AH}_2\text{O} \rightarrow \text{BCO}_2 + \text{CCH}_4 + \text{DNH}_3 + \text{EH}_2\text{S} \]
Table 16
Power from burner for producing 1 MJ of energy.

| Stream name       | Kind of stream | Unit | Scenario 1 | Scenario 2 | Scenario 3 | Ecoinvent 3.4 |
|-------------------|----------------|------|------------|------------|------------|---------------|
| Exhaust anode     | Input          | kg   | 0.00033    | 0.0025     | 0.0023     | Table 17     |
| Exhaust gas       | Input          | kg   | 0.1582     | 0.7103     | 0.4608     | Table 15     |
| Air               | Input          | kg   | 0.3428     | 0.1425     | 0.3512     | Resource/in Air |
| Biomethane        | Input          | kg   | 0.0190     | 0.0079     | 0.0195     | Table 18     |
| Steam             | Emission to air| kg   | 0.0551     | 0.0684     | 0.0861     | Water vapour, emission to air, unspecified |
| Carbon dioxide    | Emission to air| kg   | 0.0612     | 0.0997     | 0.1109     | Carbon dioxide, non-fossil, emission to air, unspecified |
| Nitrogen          | Emission to air| kg   | 0.1051     | 0.6191     | 0.5949     | Nitrogen, emission to air, unspecified |
| Oxygen            | Emission to air| kg   | 2.51E-7    | 4.71E-14   | 5.57E-13   | Oxygen, in air, Emission to air, unspecified |
| Carbon monoxide   | Emission to air| kg   | 2.15E-2    | 7.60E-2    | 4.17E-2    | Carbon monoxide, non-fossil, emission to air, unspecified |
| Ammonia           | Emission to air| kg   | 2.10E-8    | 9.62E-7    | 3.89E-7    | Ammonia, emission to air, unspecified |
| Nitrogen dioxide  | Emission to air| kg   | 1.65E-11   | 1.32E-18   | 1.65E-17   | Nitrogen dioxide, emission to air, unspecified |
| Dinitrogen monoxide| Emission to air| kg   | 2.57E-10   | 1.53E-14   | 6.03E-14   | Dinitrogen monoxide, emission to air, unspecified |
| Nitrogen monoxide | Emission to air| kg   | 3.93E-6    | 2.10E-10   | 8.44E-10   | Nitrogen monoxide, emission to air, unspecified |
| Methane           | Emission to air| kg   | 8.88E-14   | 6.19E-9    | 3.68E-10   | Methane, emission to air, unspecified |
| LPG               | Avoided product| kg   | 0.3166     | 0.1542     | 0.0732     | Market for liquefied petroleum gas [liquefied petroleum gas] APOS, S, RoW |

Fig. 5. Aspen flowsheet for the simulation of biomethane using sugarcane press-mud. E: Heat exchanger; S: Separator; M: Mixer; X: Component splitter; T: Absorption/Stripping towers; P: pumps; K: Compressor system.
Table 17
Life cycle inventor for producing 1 kWh in a low-temperature proton exchange membrane fuel cell.

| Stream                              | Kind of stream | Unit | Value  | Ecoinvent 3.4       |
|-------------------------------------|----------------|------|--------|---------------------|
| Hydrogen (99.99 vol.%)              | Input          | kg   | 0.073  | Table 15           |
| Air fuel cell                       | Input          | kg   | 123.24 | Resource/in Air     |
| Electricity                         | Input          | MJ   | 0.042  | Market for electricity, low voltage | APOS, S – CO |
| Fuel cell stack                     | Input          | unit | 1.56E-5| Market for fuel cell, stack polymer electrolyte, 2 kW electrical, future | APOS, S – GLO |
| Oceanic transport                   | Input          | kg*km| 8.666  | Transport, freight, sea, transoceanic ship | APOS, S – GLO |
| Freight transport                   | Input          | kg*km| 1.202  | Transport, freight, lorry 3.5 – 7.5 metric ton, EURO4 | APOS, S – RoW |
| Exhaust anode                       | Output         | kg   | 0.014  | Avoided product     |
| Water                               | Emission to air| kg   | 2.234  | Water vapour, emission to air, unspecified |
| Nitrogen                            | Emission to air| kg   | 93.571 | Nitrogen, emission to air, unspecified |
| Oxygen                              | Emission to air| kg   | 28.059 | Oxygen, in air, Emission to air, unspecified |

Fig. 6 shows the aspen flowsheet diagram to produce combined heat and power in a Rankine cycle. Heat and power were used to supply the energy demand of the biomethane production process described in Fig. 5.

Fig. 6. Aspen flowsheet to produce power and heat from biomethane by using a Rankine cycle.
Table 18
Life cycle inventory for producing 1 kg of biomethane from mud.

| Stream     | Kind of stream  | Unit | Value     | Ecoinvent 3.4 |
|------------|-----------------|------|-----------|---------------|
| Mud        | Input           | kg   | 13.6863   | Table 9       |
| Water      | Input           | kg   | 218.938   |               |
| Air        | Input           | m³   | 0.3668    |               |
| Energy     | Input           | MJ   | 4.1234    |               |
| Cooling water | Input     | kg   | 234.53    |               |
| Carbon dioxide | Emission to air | kg   | 1.7255    |               |
| Methane    | Emission to air | kg   | 0.0562    |               |
| Ammonia    | Emission to air | kg   | 0.0047    |               |
| Water      | Emission to air | kg   | 0.0849    |               |
| Oxygen     | Emission to air | kg   | 0.7565    |               |
| Nitrogen   | Emission to air | kg   | 2.4948    |               |
| Carbon dioxide | Emission to water | kg | 2.03E-13 | Carbon dioxide, emission to water, fresh water |
| Methane    | Emission to water | kg | 1.11E-29 | Methane, emission to water, unspecified |
| Ammonia    | Emission to water | kg | 0.0024 | Ammonia, emission to water, unspecified |
| Water      | Emission to water | kg | 9.6253 | Water, emission to water, unspecified |
| Nitrogen   | Emission to water | kg | 0.0001 | Nitrogen, emission to water, unspecified |
| Digestate  | Output          | kg   | 42.2517   | Avoided product as ammonium nitrate |

2.6. Modelling of Colombia power grid in different regions

Colombia power grid was modelled by modifying the process unit “market for high voltage, APOS, U, CO” from Ecoinvent database V3.4 in the software OpenLCA V1.9. Different power grids could be modelled by using the data present in Table 6 to calculate the power share, as shown in Table 7.

2.7. Modelling LCI of catalysts

Table 8 shows the assumptions made to calculate LCI of catalysts based on the Ecoinvent guidelines [9]. Besides, the use of scientific reports and lab-scale data were used to build the LCI [2,5]. Fig. 7 shows the block flow diagrams to synthesize RhPt/CeO$_2$-SiO$_2$ and Au-CuO/CeO$_2$ catalysts at lab-scale. Fig. 8 shows the block flow diagrams to synthesize main precursors to yield the aforementioned catalysts. All the block flow diagrams were built based on scientific reports. All the precursors were assumed to be manufactured in Germany, except cerium nitrate which was assumed to be synthesized in China. Detailed information of material flow calculation is shown in the up-coming section.
Table 19
Life cycle inventory for producing 1 kWh of power in a Rankine cycle.

| Stream                  | Kind of stream   | Unit | Value  | Ecoinvent 3.4                                                                 |
|-------------------------|------------------|------|--------|-----------------------------------------------------------------------------|
| Biomethane              | Input            | kg   | 0.0683 | Table 18 Market for compressed air, 1000 kPa gauge | compressed air, 1000 kPa gauge APO, S - GLO |
| Air                     | Input            | m^3  | 0.0029 | Water, unspec. natural origin CO                                            |
| Water                   | Input            | kg   | 0.5542 | Water vapour, Emission to air, unspec.                                      |
| Steam                   | Emission to air  | kg   | 0.1357 | Carbon dioxide, from soil or biomass stock                                  |
| Carbon dioxide          | Emission to air  | kg   | 0.1718 | Methane, from soil or biomass stock                                         |
| Methane                 | Emission to air  | kg   | 5.45E-20 | Ammonia, emission to air, unspec.                                          |
| Ammonia                 | Emission to air  | kg   | 3.55E-10 | Oxygen in air, emission to air, unspec.                                     |
| Oxygen                  | Emission to air  | kg   | 0.0371 | Oxygen in air, emission to air, unspec.                                     |
| Nitrogen                | Emission to air  | kg   | 0.9199 | Nitrogen, emission to air, unspec.                                          |
| Dinitrogen monoxide     | Emission to air  | kg   | 1.10E-06 | Dinitrogen monoxide, emission to air, unspec.                                |
| Nitrogen monoxide       | Emission to air  | kg   | 0.0050 | Nitrogen monoxide, emission to air, unspec.                                  |
| Nitrogen dioxide        | Emission to air  | kg   | 1.11E-05 | Nitrogen dioxide, emission to air, unspec.                                   |
| Carbon monoxide         | Emission to air  | kg   | 6.92E-04 | Carbon monoxide, emission to air, unspec.                                    |

Fig. 7. System boundaries to produce a) 1 g of RhPt/CeO₂-SiO₂ and b) 1 g of Au-CuO/CeO₂ catalysts.

2.7.1. Synthesis of Rhodium chloride trihydrate (RhCl₃.3H₂O)

Fig. 8a depicts the block flow diagram to synthesize RhCl₃.3H₂O based on literature review, described by Kleinberg [10]. The manufacturing of RhCl₃.3H₂O starts with the mining of rhodium (Rh), a noble metal which is found in the platinum group metal (PGM) ore in small quantities (i.e., 0.01%). After mining, synthesis process is carried out. The process involves four reactions (Eqs. (2) – (5)) and the overall yield is 1.64 kg RhCl₃.3H₂O kg⁻¹ metallic Rh [10]. Stoichiometric relations and assumptions described in Table 8 were used to build the complete LCI to produce RhCl₃.3H₂O.

\[
2\text{Rh} + 6\text{KCl} + 3\text{Cl}_2 \rightarrow 2\text{K}_3\text{RhCl}_6 \tag{2}
\]
\[
\text{K}_3\text{RhCl}_6 + \text{H}_2\text{O} \rightarrow 2\text{K}_2[\text{Rh(H}_2\text{O)}\text{Cl}_5] + \text{KCl} \tag{3}
\]
\[
2\text{K}_2[\text{Rh(H}_2\text{O)}\text{Cl}_5] + 6\text{KOH} \rightarrow \text{Rh}_2\text{O}_3.\text{5H}_2\text{O} + 10\text{KCl} \tag{4}
\]
Table 20
Life cycle inventory for producing 1 kg H₂PtCl₆·H₂O.

| Input                  | kind of flow | Unit | Value       | Ecoinvent V3.4               |
|------------------------|--------------|------|-------------|-----------------------------|
| Pt metallic            | Input        | kg   | 0.3764      | Platinum group metal mine   |
|                        |              |      | operation, | operation, ore with high   |
|                        |              |      |             | palladium | APOS, S - RU     |
| HCl                    | Input        | kg   | 0.1412      | Market for Hydrochloric acid, |
|                        |              |      |             | without water, in 30% solid  |
|                        |              |      |             | state, APOS S-RER            |
| Cl₂                    | Input        | kg   | 0.2747      | Market for chlorine, gaseous,|
|                        |              |      |             | APOS S-RER                   |
| Water cooling, unspecified | Resource   | m³   | 0.024       | Water, cooling, unspecified  |
| Water process, unspecified | Resource  | m³   | 0.00023     | Water, unspecified           |
| Electricity            | Input        | MJ   | 1.216       | Market for electricity, medium |
|                        |              |      | voltage | electricity, medium voltage | |
| Heat                   | Input        | MJ   | 1.984       | Heat and power cogeneration, |
|                        |              |      |             | natural gas, conventional    |
|                        |              |      |             | power plant, 100 MW          |
|                        |              |      |             | electrical | heat, district or        |
|                        |              |      |             | industrial, natural gas | APOS, |
|                        |              |      |             | S - DE                      |
| Freight transport      | Input        | ton·km | 1.2295     | Market for transport, freight,|
|                        |              |      |             | lorry > 32 metric ton, EURO 6|
|                        |              |      |             | [transport, freight, lorry >32|
|                        |              |      |             | metric ton, EURO             |
|                        |              |      |             | 6lory] APOS,S-GLO             |
| Rail train transport   | Input        | ton·km | 0.193      | Market for transport, freight |
|                        |              |      |             | train [Transport freight train]||
|                        |              |      |             | APOS, S - Europe without     |
|                        |              |      |             | Switzerland                  |
| Infrastructure         | Input        | Unit | 4.00E-10    | Market for chemical factory, |
|                        |              |      |             | organics | chemical factory          |
|                        |              |      |             | organics | APOS, S, GLO               |
| HCl                    | Emission to air | kg | 0.00028   | Hydrogen chloride, emission to |
| Water vapour           | Emission to air | kg | 0.2658  | Water vapour, emission to air, |
| Cl₂                    | Emission to air | kg | 0.000549 | Chlorine, emission to air,    |
| Heat                   | Emission to air | MJ | 1.216 | Heat, emission to air,        |

\[
\text{Rh}_2\text{O}_3\cdot\text{H}_2\text{O} + 6\text{HCl} \rightarrow 2\text{RhCl}_3\cdot\text{H}_2\text{O} + 2\text{H}_2\text{O} \tag{5}
\]

2.7.2. Synthesis of acid Hexachloroplatinic hexahydrate (PtH₂Cl₆·6H₂O)

Fig. 8b shows the block flow diagram to synthetize PtH₂Cl₆·6H₂O. Similar as Rh, the process starts from the mining and extraction of platinum (Pt) in the PGMs. Therefore, similar transport distances were assumed. Synthesis process was done according to the Ullman’s Encyclopaedia where metallic Pt is dissolved in a 7M solution HCl and Cl₂, as shown in Eq. (6). Conversion of both HCl and Cl₂ was assumed to be 100% [11]. Production of the hydrated salt was done through an evaporation-crystallization system.

\[
\text{Pt} + 2\text{HCl} + 2\text{Cl}_2 \rightarrow \text{PtH}_2\text{Cl}_6 \tag{6}
\]

2.7.3. Synthesis of copper nitrate trihydrate (Cu(NO₃)₂·3H₂O)

Fig. 8c displays the manufacturing process to produce Cu(NO₃)₂·3H₂O. The process starts from the mining and extraction of metallic copper (Cu). After mining, Cu is mixed with nitric
Table 21
Life cycle inventory for producing 1 kg of RhCl$_3$.3H$_2$O.

| Input                                | kind of flow    | Unit | Value     | Ecoinvent V3.4                                                                 |
|---------------------------------------|-----------------|------|-----------|--------------------------------------------------------------------------------|
| Rh metallic                           | Input           | kg   | 0.6098    | Market for rhodium, APOS S-GLO                                                   |
| Cl$_2$                                | Input           | kg   | 0.4489    | Market for chlorine, gaseous [chlorine, gaseous] APOS, S - RER                   |
| KCl                                   | Input           | kg   | 1.6798    | Potassium chloride production [potassium chloride as K2O] APOS, S - RER          |
| KOH                                   | Input           | kg   | 0.6726    | Potassium hydroxide production [potassium hydroxide] APOS, S - RER              |
| HCl                                   | Input           | kg   | 0.4199    | Market for Hydrochloric acid, without water, in 30% solid state, APOS S-RER     |
| Water cooling, unspecified            | Resource        | m$^3$| 0.0240    | Water, cooling, unspecified natural origin, DE                                   |
| Water process, unspecified            | Resource        | m$^3$| 0.0360    | Water, unspecified natural origin, DE                                           |
| Freight transport                     | Input           | ton$^\times$km | 4.2160 | Market for transport, freight, lorry > 32 metric ton, EURO 6 [transport, freight, lorry > 32 metric ton, EURO 6] APOS,S-GLO |
| Rail train transport                  | Input           | ton$^\times$km | 1.7650 | Market for transport, freight train [Transport freight train] APOS, S - Europe without Switzerland |
| Electricity                           | Input           | MJ   | 1.2160    | Market for electricity, medium voltage | electricity, medium voltage| APOS, S, DE |
| Heat                                  | Input           | MJ   | 1.9840    | Heat and power cogeneration, natural gas, conventional power plant, 100 MW electrical [heat, district or industrial, natural gas] APOS, S - DE |
| Infrastructure                        | Input           | Unit | 4E-10     | Market for chemical factory, organics | chemical factory organics | APOS, S, GLO |
| Chlorine                              | Emission to air | kg   | 0.0009    | Chlorine, emission to air, unspecified                                          |
| Steam                                 | Emission to air | kg   | 0.7534    | Water vapour, emission to air, unspecified                                       |
| HCl                                   | Emission to air | kg   | 0.0042    | Hydrogen chloride, emission to air, unspecified                                  |
| Heat                                  | Emission to air | MJ   | 1.2160    | Heat, waste, emission to air, unspecified                                       |
| Cl ions                               | Emission to water | kg | 0.5179  | Chlorine, emission to water, unspecified                                      |
| Rh ions                               | Emission to air | kg   | 0.0206    | Rhodium, emission to air, unspecified                                           |
| Water                                 | Emission to water | m$^3$ | 0.0364 | Wastewater, m$^3$, emission to water, unspecified                                |
| K ions                                | Emission to water | kg | 1.1408 | Potassium, emission to water, unspecified                                     |
Table 22
Life cycle inventory for producing 1 kg of Ce(NO₃)₃·6H₂O.

| Input                | kind of flow | Unit  | Value  | Ecoinvent V3.4                                                                 |
|----------------------|--------------|-------|--------|--------------------------------------------------------------------------------|
| Bastnäsite           | Input        | kg    | 0.6120 | Rare earth production, 70% REO, from bastnäsite | APOS, S-CN                       |
| HNO₃                 | Input        | kg    | 1.1203 | Nitric acid production, product in 50% solution state | APOS, S - RoW                  |
| TBP                  | Input        | kg    | 0.0075 | Market for chemical, organic | APOS, S - GLO                     |
| H₂SO₄                | Input        | kg    | 0.3164 | Sulfuric acid production | APOS, S                          |
| NaCl                 | Input        | kg    | 0.8840 | Market for sodium chloride, powder | APOS, S - GLO                 |
| NaOH                 | Input        | kg    | 0.1177 | Market for sodium hydroxide, without water, in 50% solution state | APOS, S - GLO                  |
| HCl                  | Input        | kg    | 0.0840 | Market for Hydrochloric acid, without water, in 30% solid state | APOS S-RoW                   |
| Process water        | Input        | m³    | 0.0004 | Water, unspecified natural origin, CN                         |
| Cooling water        | Input        | m³    | 0.0240 | Water, cooling, unspecified natural origin, CN                 |
| Heat                 | Input        | MJ    | 0.0008 | heat and power cogeneration, hard coal | heat, district or industrial, other than natural gas | APOS, S - RoW                  |
| Electricity          | Input        | MJ    | 0.0078 | Market group for electricity, medium voltage | electricity, medium voltage | APOS, S-CN                      |
| Steam                | Input        | MJ    | 0.2106 | Market for steam, in chemical industry | heat from steam, in chemical industry | APOS, S - RoW                  |
| Freight transport    | Input        | ton·km| 0.3142 | Market for transport, freight, lorry > 32 metric ton, EURO 5 | APOS, S-GLO                     |
| Rail train transport | Input        | ton·km| 0.6284 | Market for transport, freight train | transport freight train | APOS, S-CN                      |
| Infrastructure       | Input        | Unit  | 4E-10  | Market for chemical factory, organics | chemical factory organics | APOS, S, GLO                     |
| Sodium               | Emission to water | kg  | 0.4103 | Sodium, emission to water, unspecified                         |
| Sulfate              | Emission to water | kg  | 0.2152 | Sulfate, emission to water, unspecified                       |
| Fluorine             | Emission to water | kg  | 0.0320 | Fluorine, emission to water, unspecified                      |
| Chlorine             | Emission to water | kg  | 0.5021 | Chlorine, emission to water, unspecified                      |
| Water                | Emission to water | m³  | 0.0001 | Wastewater, m³, emission to water, unspecified               |
Table 23
Life cycle inventory for producing 1 kg of HAuCl₄·3H₂O.

| Input            | kind of flow | Unit | Value   | Ecoinvent V3.4 |
|------------------|--------------|------|---------|----------------|
| Gold             | Input        | kg   | 0.540   | Gold production [gold] APOS, S - RoW |
| HNO₃             | Input        | kg   | 13.57   | Nitric acid production, product in 50% solution state [nitric acid, without water, in 50% solution] APOS, S -RER |
| HCl              | Input        | kg   | 68.07   | Market for Hydrochloric acid, without water, in 30% solid state, APOS S-RER |
| Water cooling    | Input        | m³   | 0.0240  | Water, cooling, unspecified natural origin, DE |
| Water process    | Input        | m³   | 0.0150  | Water, unspecified natural origin, DE |
| Electricity      | Input        | MJ   | 1.2160  | Market for electricity, medium voltage [electricity, medium voltage] APOS, S, DE |
| Freight transport| Input        | Ton·km | 3.0762 | Market for transport, freight, lorry > 32 metric ton, EURO 6 [transport, freight, lorry >32 metric ton, EURO 6]APOS,S-GLO |
| Rail train transport | Input | Ton·km | 21.755 | Market for transport, freight train [Transport freight train] APOS, S - Europe without Switzerland |
| Infrastructure   | Input        | Unit | 4E-10   | Market for chemical factory, organics | chemical factory organics | APOS, S, GLO APOS, S-RER |
| Hydrogen chloride| Emission to air | kg | 0.3660  | Hydrogen chloride, emission to air, unspecified |
| Nitrogen dioxide | Emission to air | kg | 0.3772  | Nitrogen dioxide, emission to air, unspecified |
| Nitrogen monoxide | Emission to air | kg | 5.9048  | Nitrogen monoxide, emission to air, unspecified |
| Chlorine         | Emission to air | kg | 17.567  | Chlorine, emission to air, unspecified |
| Heat             | Emission to air | MJ | 1.2160  | Heat, waste, emission to air, unspecified |
| Gold ions        | Emission to water | kg | 0.0385  | Gold, emission to water, unspecified |
| Water            | Emission to water | m³ | 0.0105  | Wastewater, m³, emission to water, unspecified |
| Chlorine ions    | Emission to water | kg | 0.0139  | Chlorine, emission to water, unspecified |

acid (HNO₃) according to the Ullman’s encyclopedia [12]. The reaction between Cu and HNO₃ is shown in Eq. (7). The effluent from the reaction step is evaporated and concentrated to obtain crystals of Cu(NO₃)₂·3H₂O. To determine the amount of crystal, solubility of the hydrated copper salt was considered as 77.4 g Cu(NO₃)₂·3H₂O per 100 g water.

\[
4Cu + 12HNO₃ \rightarrow 4Cu(NO₃)₂ + 6H₂O + 2NO + 2NO₂ \tag{7}
\]

2.7.4. Synthesis of Acid chloroauric trihydrate (HAuCl₄·3H₂O)

Fig. 8d shows the block flow diagram to produce HAuCl₄·3H₂O, which starts with the mining and extraction of gold (Au) from the ore. The process to convert Au into HAuCl₄·3H₂O was described by Gross [14]. Firstly, Au is diluted in aqua regia (75% HCl, 25% HNO₃) to produce HAuCl₄ according to Eq. (8). However, a side reaction takes place between HCl and HNO₃ (Eq. (9)). The reaction between Au and aqua regia is highly exothermic. Therefore, heat was assumed to be 0
Table 24
Life cycle inventory for producing 1 kg of Cu(NO\textsubscript{3})\textsubscript{2}.3H\textsubscript{2}O.

| Input                  | kind of flow | Unit | Value  | Ecoinvent V3.4                                                                 |
|------------------------|--------------|------|--------|--------------------------------------------------------------------------------|
| Cu metallic            | Input        | kg   | 0.2930 | Copper production, primary | copper | APOS, S, RER                                                                 |
| HNO\textsubscript{3}   | Input        | kg   | 0.8654 | Nitric acid production, product in 50% solution state | nitric acid, without water, in 50% solution | APOS, S - RER |
| Electricity            | Input        | MJ   | 1.2160 | Market for electricity, medium voltage | electricity, medium voltage | APOS, S, DE |
| Heat                   | Input        | MJ   | 1.9840 | Heat and power cogeneration, natural gas, conventional power plant, 100 MW electrical | heat, district or industrial, natural gas | APOS, S - DE |
| Freight transport      | Input        | Ton\textsuperscript{−}km | 0.5460 | Market for transport, freight, lorry > 32 metric ton, EURO 6 | transport, freight, lorry >32 metric ton, EURO 6 | APOS,S-GLO |
| Rail train transport   | Input        | Ton\textsuperscript{−}km | 0.5192 | Market for transport, freight train | Transport freight train | APOS, S - Europe without Switzerland |
| Cooling water          | Input        | m\textsuperscript{3} | 0.0240 | Water, cooling, unspecified | natural origin, DE |
| Process water          | Input        | m\textsuperscript{3} | 0.0009 | Water, unspecified natural origin, DE |
| Infrastructure         | Input        | Unit | 4E-10  | Market for chemical factory, organics | chemical factory organics | APOS, S, GLO |
| Nitrogen monoxide      | Emission to air | kg | 0.0652 | Nitrogen monoxide, emission to air, unspecified |
| Nitrogen dioxide       | Emission to air | kg | 0.1000 | Nitrogen dioxide, emission to air, unspecified |
| Heat                   | Emission to air | MJ | 1.2160 | Heat, waste, emission to air, unspecified |
| Steam                  | Emission to air | kg | 0.2231 | Water vapour, emission to air, unspecified |
| Copper ions            | Emission to water | kg | 0.0286 | Copper, emission to water, unspecified |
| Nitrates               | Emission to water | kg | 0.0561 | Nitrates, emission to water, unspecified |
| Water                  | Emission to water | kg | 6.80E-5 | Water, emission to water, unspecified |

and no energy source is required. Besides, water consumption was estimated according to the methodology process showed by Gross [14].

\[
Au + 3HNO_3 + 4HCl \rightarrow HAuCl_4 + 3NO_2 + 3H_2O \tag{8}
\]

\[
3HCl + HNO_3 \rightarrow Cl_2 + 2H_2O + NOCl \tag{9}
\]

2.7.5. Synthesis of cerium nitrate hexahydrate \((\text{Ce(NO}_3)_3.6\text{H}_2\text{O})\) \n
\(\text{Ce(NO}_3)_3.6\text{H}_2\text{O}\) is the precursor to produce the catalyst support in both cases. Cerium is a rare earth element and is mainly found on Bastnäsite ores (50%) in China. Hence, energy consumption was based on the Chinese power grid available in Ecoinvent V3.4.

\[
\text{Re(OH)}_3 + 3\text{HNO}_3 \rightarrow \text{Re(NO}_3)_3 + 3\text{H}_2\text{O} \tag{10}
\]
### Table 25
Life cycle inventory for producing 1 g RhPt/CeO$_2$-SiO$_2$.

| Input                                                        | kind of flow | Unit | Value   | Ecoinvent V3.4          |
|--------------------------------------------------------------|--------------|------|---------|-------------------------|
| Ce(NO$_3$)$_3$.6H$_2$O                                       | Input        | g    | 2.3431  | Table 22                |
| RhCl$_3$.3H$_2$O                                             | Input        | g    | 0.0102  | Table 20                |
| PtH$_2$Cl$_6$.6H$_2$O                                        | Input        | g    | 0.0106  | Table 21                |
| SiO$_2$                                                      | Input        | g    | 0.0633  | Silica sand production [silica sand] APOS, S-DE |
| Water tap deionized                                         | Input        | g    | 5.9341  | Market for water, deionized, from tap water, at [water deionized, from tap water, at user] APOS, S - RoW |
| Rail train transport                                        | Input        | kg$^*$km | 0.0496  | Market for transport, freight train [Transport freight train] APOS, S - Europe without Switzerland |
| Rail train transport                                        | Input        | kg$^*$km | 6.1765  | Market for transport, freight train [Transport freight train] APOSS-CN |
| Oceanic transport                                           | Input        | kg$^*$km | 71.6836 | Market for transport, freight, sea, transoceanic ship [transport, freight, sea, transoceanic ship] APOS, S - GLO |
| Freight transport                                           | Input        | kg$^*$km | 1.2727  | Market for transport, freight, lorry, 3.5-7.5 metric ton, EURO 3 [Transport freight train] | APOS, S - GLO |
| Light commercial transport                                  | Input        | Kg$^*$km | 0.0585  | Market for transport, freight, light commercial vehicle [transport, freight commercial vehicle] APOS, S - GLO |
| Hydrogen                                                    | Input        | g    | 0.1120  | Market for hydrogen, liquid [hydrogen, liquid] APOS, S - RoW |
| Argon                                                       | Input        | g    | 14.108  | Market for Argon, liquid [argon, liquid] APOS, S - GLO |
| Electricity                                                 | Input        | g    | 1.3613  | Market for electricity, low voltage [electricity, low voltage] APOS, S - CO |
| NOx                                                         | Emission to air | g | 0.8315  | Nitrogen oxides, emission to air, unspecified |
| Chlorine                                                    | Emission to air | g | 0.0085  | Chlorine, emission to air, unspecified |

#### 2.8. Transport

Transport distances among the locations on the different stages of the life cycle were calculated by using Google maps. Oceanic distances were calculated by using free calculators in web sites, such as sea-distances.org. When transport distances were unknown, 100 km and 200 km by lorry and railway, respectively, were assumed according to the standard distances set by Hischier et al. [9]

#### 3. Life Cycle Inventories

Tables 9–26 show the LCI for all the stages involved in the production of power from sugarcane press-mud. LCI were used to calculate the environmental impacts, as shown in the main manuscript.
| Input                                      | kind of flow     | Unit | Value | Ecoinvent V3.4                                                                 |
|-------------------------------------------|------------------|------|-------|--------------------------------------------------------------------------------|
| Ce(NO$_3$)$_3$·6H$_2$O                     | Input            | g    | 2.4725| Table 22                                                                        |
| Cu(NO$_3$)$_2$·3H$_2$O                     | Input            | g    | 0.0303| Table 23                                                                        |
| HAuCl$_4$·3H$_2$O                         | Input            | g    | 0.2000| Table 24                                                                        |
| Sodium hydroxide                          | Input            | g    | 0.8940| Market for sodium hydroxide, without water, in 50% solution state [sodium hydroxide without water, in 50% solution state] APOS, S-GLO |
| Water tap deionized                       | Input            | g    | 595.24| Market for water, deionized, from tap water, at user [water deionized, from tap water, at user] APOS, S-RoW |
| Rail train transport                      | Input            | Kg'km| 0.0297| Market for transport, freight train [Transport freight train] APOS, S-Europe without Switzerland |
| Rail train transport                      | Input            | Kg'km| 6.5176| Market for transport, freight train [transport freight train] APOS,S-CN |
| Oceanic transport                         | Input            | Kg'km| 75.161| Market for transport, freight, sea, transoceanic ship [transport, freight, sea, transoceanic ship] APOS, S-GLO |
| Freight transport                         | Input            | Kg'km| 1.3022| Market for transport, freight, lorry, 3.5-7.5 metric ton, EURO 3 [transport, freight, lorry 3.5 - 7.5 metric ton, EURO 3] APOS, S-GLO |
| Light commercial transport                | Input            | Kg'km| 0.0608| Market for transport, freight, light commercial vehicle [transport, freight commercial vehicle] APOS, S-RoW |
| Hydrogen                                  | Input            | g    | 0.0985| Market for hydrogen, liquid [hydrogen, liquid] APOS, S-GLO |
| Air                                       | Input            | m$^3$| 0.0001| Market for compressed air, 600 kPa gauge [compressed air, 600 kPa gauge] APOS, S-GLO |
| Argon                                     | Input            | kg   | 44.885| Market for Argon, liquid [argon, liquid] APOS, S-GLO |
| Electricity                               | Input            | kWh  | 4.1711| Market for electricity, low voltage [electricity, low voltage] APOS, S-CO |
| NOx                                       | Emission to air  | g    | 0.8776| Nitrogen oxides, emission to air, unspecified |
| Nitrogen dioxide                          | Emission to air  | g    | 0.0116| Nitrogen dioxide, emission to air, unspecified |
| Oxygen                                    | Emission to air  | g    | 0.0032| Oxygen in air, emission to air, unspecified |
| Steam                                     | Emission to air  | g    | 2.6171| Water vapour, emission to air, unspecified |
| Sodium ions                               | Emission to water| g    | 1.3740| Sodium, emission to water, unspecified |
| Water                                     | Emission to water| m$^3$| 0.5932| Wastewater, m$^3$, emission to water, unspecified |
| Chlorine ions                             | Emission to water| g    | 0.0036| Chlorine, emission to water, unspecified |
Fig. 8. Block flow diagram to produce a) RhCl$_3$.3H$_2$O; b) PtH$_2$Cl$_6$.6H$_2$O; c) Cu(NO$_3$)$_2$.3H$_2$O; d) HAuCl$_4$.3H$_2$O; e) Ce(NO$_3$)$_3$.6H$_2$O. Values in parenthesis are mass allocation factors.

Ethics Statement

Not applicable

CRediT Author Statement

Nestor Sanchez: Conceptualization, Methodology, Validation, Formal analysis, Writing – Original Draft, Visualization; Ruth Ruiz: Writing – Review & Editing, Visualization, Supervision, Formal analysis; Anne Rödl: Writing – Review & Editing, Visualization, Supervision, Forma analysis; Martha Cobo: Resources, Methodology, Writing – Review & Editing, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.
Data Availability

Dataset for the production of power from sugarcane press-mud (Original data) (Mendeley Data).

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