Data for the simulation of different CO₂ utilization processes

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Abstract

The simulation of chemical processes is a useful tool that provides valuable information and data for process analysis. The obtained data from simulations could be used later in optimization, economic, environmental, energetic, exergetic and different kind of analysis. In this work, it is presented the data that serves as basis for the simulation of different chemical process that use CO₂ as a raw material, to produce some value-added chemicals and fuels. The stream of captured CO₂ is taken from a biogas combined cycle power plant, and it is fed to a formic acid production plant, a syngas production plant and a methanol production plant.

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Specifications Table

| Subject                        | Process engineering                                      |
|-------------------------------|----------------------------------------------------------|
| Specific subject area         | Process simulation, chemical engineering                 |
| Type of data                  | Tables, Figures and Text                                 |
| How data were acquired        | Software of process simulation (Aspen Plus™) (continued on next page) |

DOI of original article: 10.1016/j.jenvman.2021.113746

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Table 1. Description of the data

| Subject | Process engineering |
|---------|---------------------|
| Data format | Simulation basis description |
| Parameters for data collection | For all CO₂ utilization processes simulations of the biogas power plant study case, it was consider the same amount of flow of raw carbon dioxide for each process |
| Description of data collection | Common process modules and tools available in Aspen Plus were employed |
| Data source location | Universidad Michoacana de San Nicolás de Hidalgo |
| Data accessibility | Repository name: CCU simulation data. Data identification number: 10aac9 [1] https://github.com/espagio12/CCU-simulation-data.git 10.5281/zenodo.6408798 [1] |
| Related research article | G.G. Esquivel-Patiño and F. Nápoles-Rivera, Environmental and energetic analysis of coupling a Biogas combined cycle power plant with carbon capture, organic Rankine cycles and CO₂ utilization processes, Journal of Environmental Management. 300 (2021) 113746. 10.1016/j.jenvman.2021.113746. |

Value of the Data

- The data gives insights on simulations of steady-state design of various CO₂ utilization processes.
- The data shown in this document could be used by anyone who wants to assess the performance of the CO₂ utilization processes.
- This dataset can be used for validation/verification of further simulation studies.
- The data presented could be used in several further studies of analysis (economic, energetic, exergetic, environmental, optimization, etc.) of the different CO₂ utilization processes.

1. Data

This article contains data related to the research article entitled “Environmental and energetic analysis of coupling a Biogas combined cycle power plant with carbon capture, organic Rankine cycles and CO₂ utilization processes” [2]. The tables contain the necessary data for the realization of the CO₂ utilization processes simulation, first for comparison and verification, are presented the parameters obtain by other articles [3–5], then the parameters used for the simulations of the study cases of the related article are presented. Fig. 1 and Table 1, presents the flowchart and the parameters used in the simulations of each case, for the formic acid production plant (FAPP), Fig. 2 and Table 2 the parameters for the methanol production plant (MPP), Fig. 3 and Table 3 the parameters for the syngas production plant (SynPP) via hydrogenation, and finally Fig. 4 and Table 4 presents the parameters for the syngas production plant (SynPP) via dry reforming of methane (DRM).

2. Experimental Design, Materials and Methods

With the aim of validating the CO₂ utilization processes (CUPs) simulations, the related simulations data were compared with those available in literature. The simulation shown in Fig. 1, corresponds to the process of formic acid production, the parameters used for the simulation were obtained from the article of Barbera et al. [5] and are shown in Table 1. The simulation of Fig. 2 shows the process of methanol production by CO₂ hydrogenation, the parameters used were obtained from Kiss et al., [3] and are shown in Table 2. Fig. 3 shows the flowchart of the production of syngas by CO₂ hydrogenation, which was carried out with the parameters in Table 3,
### Table 1
Main parameters for the FAPP simulation.

| Parameter                                      | Base case  | BGCC case  | Study case |
|------------------------------------------------|------------|------------|------------|
| CO₂ flow (kg/h)                                | 729.526    | 4478.43    | 1492.81    |
| H₂ flow (kg/h)                                 | 40.604     | 249.26     | 83.08      |
| Triethylamine flow (kg/h)                      | 4233.43    | 32817.91   | 8660.95    |
| Methanol flow (kg/h)                           | 205.63     | 1262.82    | 420.94     |
| Water flow (kg/h)                              | 205.63     | 420.9408   | 151.512    |
| Compressors outlet pressure (bar)              | 105        | 105        | 105        |
| Reactor conversion (%)                         | 42.91      | 42.91      | 42.91      |
| Valve V-1 outlet pressure (bar)                | 70         | 70         | 70         |
| Flash operational conditions (bar/°C)          | (100/50.16)| (100/50.16)| (100/50.16)|
| Valves V-2,3 outlet pressure (bar)             | 1          | 1          | 1          |
| Pump P-1 outlet pressure (bar)                 | 105        | 105        | 105        |
| Heater H-1 outlet temperature °C               | 50         | 50         | 50         |
| Heater H-2 outlet temperature °C               | 50         | 50         | 50         |
| Compressor C-3 outlet pressure (bar)           | 105        | 105        | 105        |
| Heater H-3 outlet temperature °C               | 25         | 25         | 25         |
| Separator S-2 operational conditions (bar/°C)  | 1/25       | 1/25       | 1/25       |
| Distillation tower DT-1 operational conditions (stages/r) | (20/11) | (25/11) | (20/11) |
| Distillation tower DT-2 operational conditions (stages/r) | (10/0.7) | (20/0.7) | (12/0.7) |

### Table 2
Main parameters for the MPP simulation.

| Parameter                                      | Base case  | BGCC case  | Study case |
|------------------------------------------------|------------|------------|------------|
| CO₂ flow (kg/h)                                | 17209.15   | 4478.88    | 1492.81    |
| H₂ flow (kg/h)                                 | 2658.87    | 616.26     | 205.72     |
| Reactor operational conditions (bar/°C)        | 50/250     | 50/250     | 50/250     |
| CO₂ compressors C-1 outlet pressure (bar)      | 50         | 50         | 50         |
| H₂ compressors C-2 outlet pressure (bar)       | 45         | 45         | 45         |
| Heater H-1 outlet temperature °C               | 225        | 225        | 225        |
| Heater H-2 outlet temperature °C               | 250        | 250        | 250        |
| Cooler CO-1 outlet temperature °C              | 93.9       | 93.3       | 93.3       |
| Cooler CO-2 outlet temperature °C              | 31         | 31         | 31         |
| Flash S-1 operational conditions (bar/°C)      | (45/30)    | (45/30)    | (45/30)    |
| Stripper T-1 operational conditions (stages/r) | (4/0.659)  | (4/0.659)  | (2/0.659)  |
| Valve V-1 outlet pressure (bar)                | 5          | 5          | 5          |
| Distillation tower DT-1 operational conditions (stages/r) | (30/0.934) | (18/0.934) | (15/0.934) |

### Table 3
Main parameters for the SynPP by CO₂ hydrogenation simulation.

| Parameter                                      | Base case  | BGCC case  |
|------------------------------------------------|------------|------------|
| CO₂ flow (kmol/h)                              | 35.61      | 101.76     |
| H₂ flow (kmol/h)                               | 160.82     | 349.57     |
| Heater H-1 outlet temperature °C               | 530        | 530        |
| H₂ flow to the stripper ST-1 (kmol/h)          | 125.21     | 342.91     |
| Exchanger HE-1 outlet temperature °C           | 361.7      | 361.7      |
| Exchanger HE-2 outlet temperature °C           | 443.7      | 443.7      |
| Exchanger HE-3 outlet temperature °C           | 515        | 515        |
| Reactor operational conditions (bar/°C)        | 1/530      | 1/530      |
| Cooler CO-1 outlet temperature °C              | 25         | 25         |
| Absorber A-1 stages                            | 12         | 15         |
| Stripper stages                                | 2          | 4          |
| W-IN stream flow (kmol/h)                      | 422.21     | 1206.52    |
| Pump P-1 outlet pressure (bar)                 | 7          | 7          |
| Separator S-2 operational conditions (bar/°C)  | 7/31.12    | 7/31.12    |
Table 4
Main parameters for the SynPP by DRM.

| Parameter                                | Value          |
|-------------------------------------------|----------------|
| CO₂ flow (kmol/h)                         | 141.69         |
| CH₄ flow (kmol/h)                         | 142.54         |
| Reactor RX operational conditions (bar/°K)| 1.97/873       |
| Heater H-1 outlet temperature °K          | 873            |
| Cooler CO-1 outlet temperature °C         | 25             |
| Flash S-1 operational conditions (bar/°C) | 1/25           |

obtained from Barbera et al. [5]. Finally, the process of syngas production by dry reforming of methane is shown in Fig. 4, the parameters of Table 4 were used in the simulation and were obtained from the article of Gangadharan et al. [4].

Once the results of the simulations were consistent with the results obtained by the mentioned articles, the flows of the raw materials and some of the operational conditions of the main equipment of all CUPs simulations were adapted to a study case through sensitivity analysis. The study case consists in the use of the CO₂ captured from a biogas combined cycle power plant in the CUPs. For all CUPs it was assumed an equal CO₂ flow of 1492.81 kg/h, value obtained from the carbon capture plant simulation of the related article.
Fig. 2. Simulation of the MPP.

Fig. 3. Simulation of the SynPP by CO₂ hydrogenation.
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.

CRediT Author Statement

Gerardo G. Esquivel-Patiño: Conceptualization, Methodology, Writing – original draft; Fabricio Nápoles-Rivera: Conceptualization, Resources, Funding acquisition, Writing – review & editing.

Acknowledgments

The authors acknowledge the financial support provided by CONACYT and the Scientific Research Council (CIC_UMSNH) for the development of this project, as well as the support from the faculty of Chemical Engineering at the Universidad Michoacana de San Nicolás de Hidalgo.

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