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# ANALYSIS OF TECHNICAL FEASIBILITY OF A PROCESS FOR CO<sub>2</sub> SEQUESTRATION APPLIED TO A STEELMAKING PROCESS

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**Abstract.** *Currently, there is a growing concern about reducing the carbon dioxide emission in the environment. The present work aims the technical analysis of a plant for the carbon dioxide sequestration from the exhaust gases of a steelmaking process to convert it into methanol. This analysis uses the CAPE-OPEN software, which is a freeware for modeling thermochemical processes. The COFE flowsheet environment is used varying the operational parameters to get an optimum point. The results showed that the change in the percentage of carbon monoxide conversion and carbon dioxide - indicated in previous studies - in the reactor is not interesting, and the change in the number of stages of the distillation column is attractive.*

**Keywords:** *Technical analysis, CAPE-OPEN software, steelmaking process, CO<sub>2</sub> sequestration.*

## 1. INTRODUCTION

Energy is an indispensable input for all human activity. The use of energy in balance with socioeconomic development represents one of humanity's greatest challenges. However, it is important to clearly understand the processes involved in energy transformations and their consequences.

Worldwide, carbon emissions from the steelmaking industry accounted for approximately 6.5% of total emissions and 33.3% of industrial emissions (PAULA, 2012). Regarding the sector's greenhouse gases (GHG), more than 80% result from the consumption of energy inputs (CARVALHO et al., 2015). According to the Brazilian national energy balance (EPE, 2017), in 2016, the steelmaking industry represented 17.8% of national energy consumption, which reveals the energy-intensive characteristic of this industry. The production of steel and iron accounted for about 43% of GHG emissions in industrial processes in Brazil in 2012. Carbon dioxide corresponds to more than 90% of the GHGs emitted in the steelmaking industry.

The main types of carbon dioxide conversion are bioconversion, catalytic, electrochemical, enzymatic, and plasma. Catalytic conversion is the most studied and can be obtained through plasma catalysis, thermal catalysis, electrocatalysis and photocatalysis (XING et al., 2020).

The process that convert carbon dioxide into methanol is a thermal catalytic conversion that has great prominence. Defined as an exothermic reaction process of hydrogen and carbon dioxide, it is responsible for the formation of methanol and water using a metal catalyst. The temperature range of this reaction is between 150 and 500°C and the pressure between 0.1 and 10 MPa (CHANG et al., 2003). The market for this process will reach from 4 to 65 billion cubic meters per year until 2030 (GLOBAL, 2016). Although widely developed, the process has some disadvantages such as flaking the catalyst surface, temperature problems, carbon deposition and pore clogging. For these reasons, the appropriate choice of catalyst and operating conditions must be well-defined (GHAIB et al., 2016).

Metal catalysts, such as Ru, Rh and Ni, have high performance but the cost of these are quite high and often cannot meet large-scale industrial production. Due to these difficulties, transition metals, such as Fe, gained prominence in view of the development of carbon dioxide into methanol catalysts (XING et al., 2020).

The process of carbon dioxide into methanol is carried out by compressing and cooling carbon dioxide and hydrogen to the reaction conditions in the reactor (PAVÃO et al., 2016). This synthesis is described mainly by the following equations (GRAAF and WINKELMAN, 2016):





The water-gas shift reaction is (GRAAF and WINKELMAN, 2016):



Among the operational conditions of the exothermic process are high temperature and pressure, which makes it easier for the catalyst to deactivate carbon deposits and replace active metals (GHAIB et al., 2016). Experiments where two isotherms are fixed in reactors in series, the combination of the gas flow and the catalyst is enough to do an equilibrium.

A hydrogenation reaction can occur through the availability of an external source of CO<sub>2</sub> transforming it into CH<sub>3</sub>OH (VAN DER HAM et al., 2012). The reactor outlet is connected to the condenser / separator where methanol and water are separated (LIU et al., 1994). These two substances have molar fractions of the gas components (CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>), which are calculated from the balance of nitrogen (GRAAF and WINKELMAN, 2016).

The present study aims to technically analyze the carbon dioxide conversion into methanol, using a CAPE-OPEN simulator software, applied to a steelmaking process. The system parameters are changed to find the best operational point.

## 2. METHODOLOGY

First, the gas stream of the blast furnace in the steelmaking process was chosen. According to Steelonthenet (2020), the main process that generates carbon dioxide in iron and steelmaking are the production of coke and hot metal in the blast furnace. Table 1 shows the typical carbon dioxide production volumes per tonne of output for each steelmaking process stage.

Table 1. Carbon dioxide generation in selected steelmaking process (STEELONTHENET, 2020)

PROCESS	DIRECT CARBON DIOXIDE EMISSION [ton CO <sub>2</sub> /ton]
Coke plant	0.794
Sinter plant	0.200
Pellet plant	0.057
Blast Furnace	1.219
BOS plant	0.181
Electric arc furnace	0.240

As can be seen in Table 1, the blast furnace process emits an average of 1.219 ton of carbon dioxide per ton of hot metal produced. This paper assumes 1 ton/h of hot metal produced and 1.219 ton/h of carbon dioxide captured. Table 2 shows the chemical composition of blast furnace gas that will be simulated in the software.

Table 2. Chemical composition of the blast furnace gas (COSTA, 2015)

Specie	Molar Fraction	MW [kg/kmol]	Mass Fraction
Carbon monoxide	0.2310	28	0.2096
Carbon dioxide	0.2104	44	0.3000
Hydrogen	0.0206	2	0.0013
Nitrogen	0.5312	28	0.4820
Oxygen	0.0068	32	0.0071

The system reaction package was defined in the COFE software as shown in Figure 1a. For this purpose, the stoichiometric ratio of hydrogen and carbon dioxide/carbon monoxide needed to be supplied. The other gas input data such as pressure, temperature and molar flowrate were defined as shown in Figure 1b. In this figure, a molar flowrate of hydrogen was added in the stoichiometric proportion given by the equations (1) and (2).

The plant studied in this paper is exhibited in Figure 2. It is composed of compressors, heat exchangers, reactor, flash separators, expansion valve, mixers and distillation column.

In the first iteration, the conversion values of the reactor were 64% for carbon monoxide and 17% for carbon dioxide. The distillation column was first defined with 40 stages and a reflux ratio of 1.5. In order to study the effect in the

conversion of carbon monoxide and dioxide, it was varied the number of stages of the distillation column, operating temperature and pressure. The results are showed in section 3.

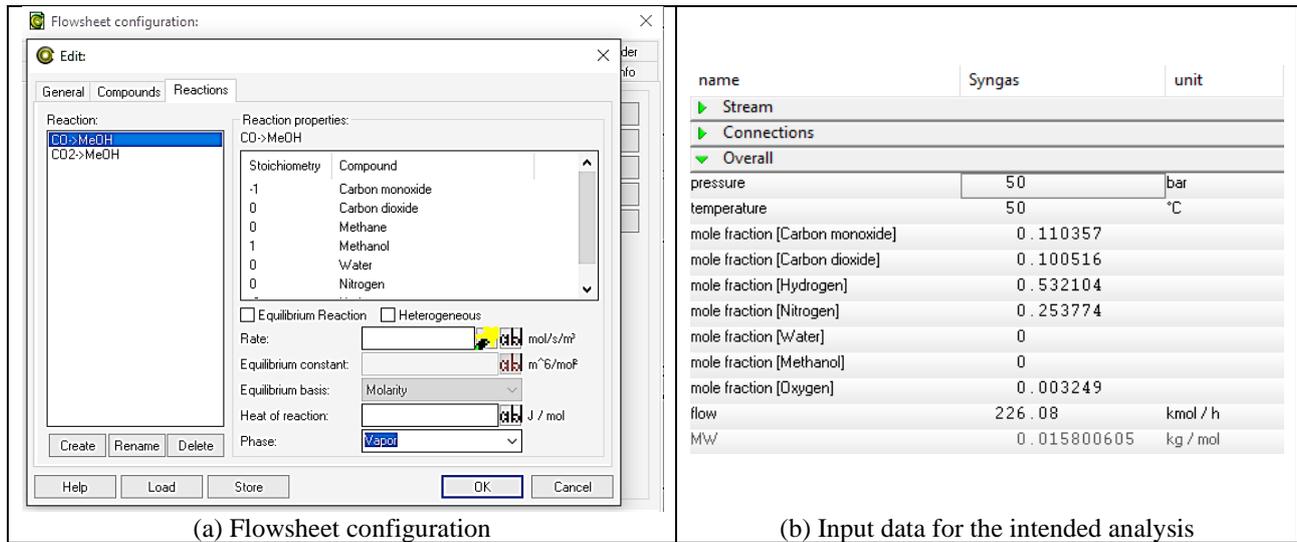


Figure 1. Definition of the (a) gas synthesis reaction package and (b) input data in the COFE software.

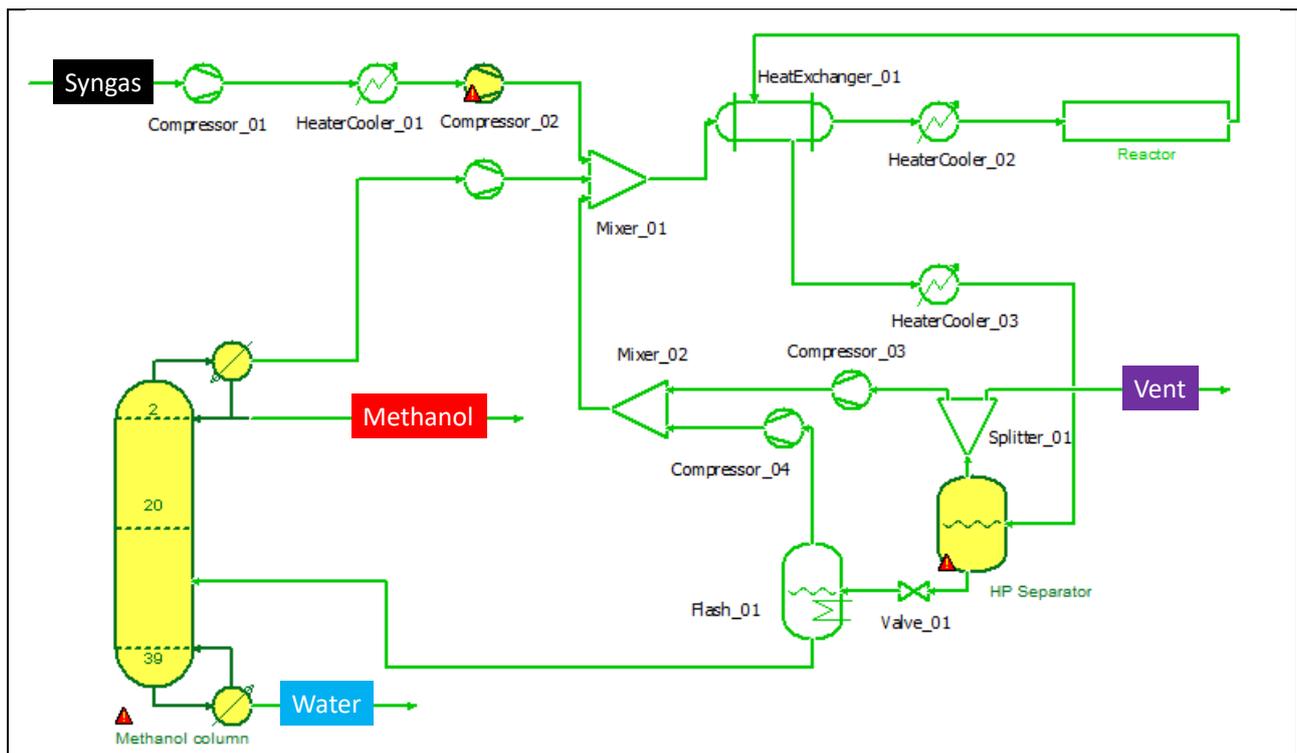


Figure 2. Simulation in the COFE software of the gas synthesis plant.

### 3. RESULTS AND DISCUSSION

#### 3.1 Variation in the percentage of conversion of carbon monoxide and dioxide to methanol in the reactor

The following reaction rates for converting carbon monoxide and carbon dioxide into methanol were simulated in COFE software: (a) 58% of carbon monoxide and 23% of carbon dioxide; (b) 64% of carbon monoxide and 17% of carbon dioxide and (c) 70% of carbon monoxide and 11% of carbon dioxide.

Figures 3, 4 and 5 shows the behavior of the methanol, water and vent stream (Figure 2), respectively, with the mentioned conversion rates.

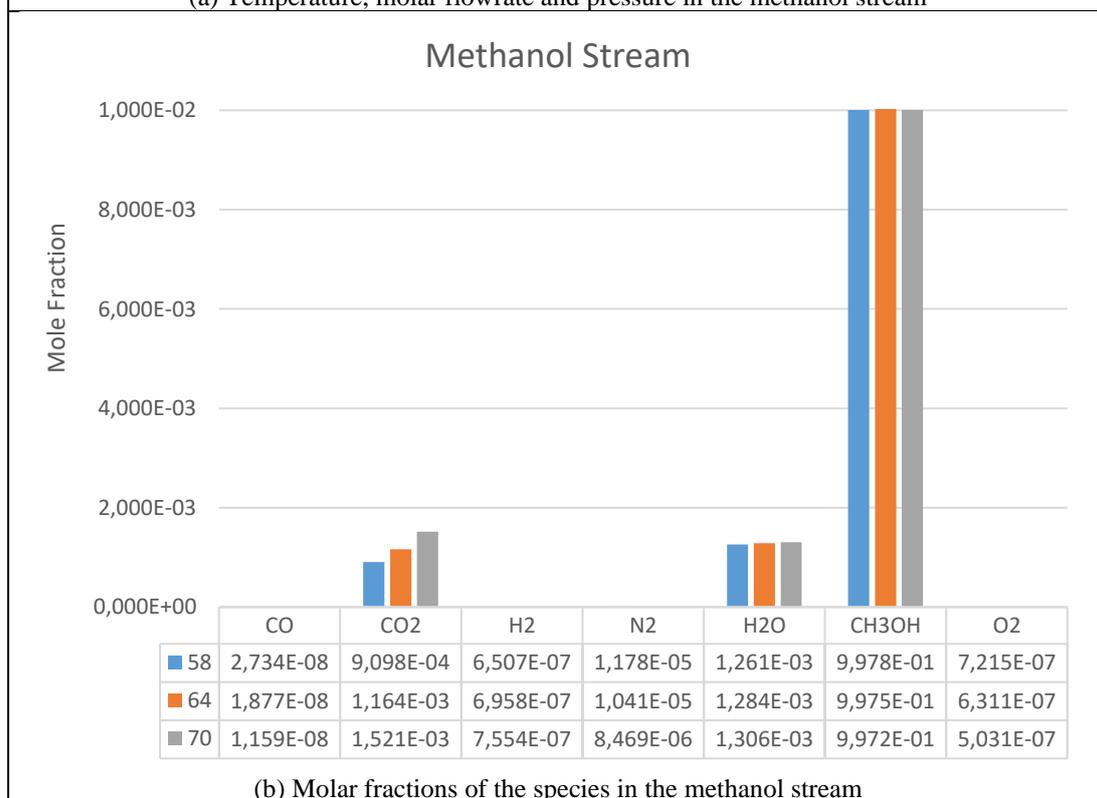
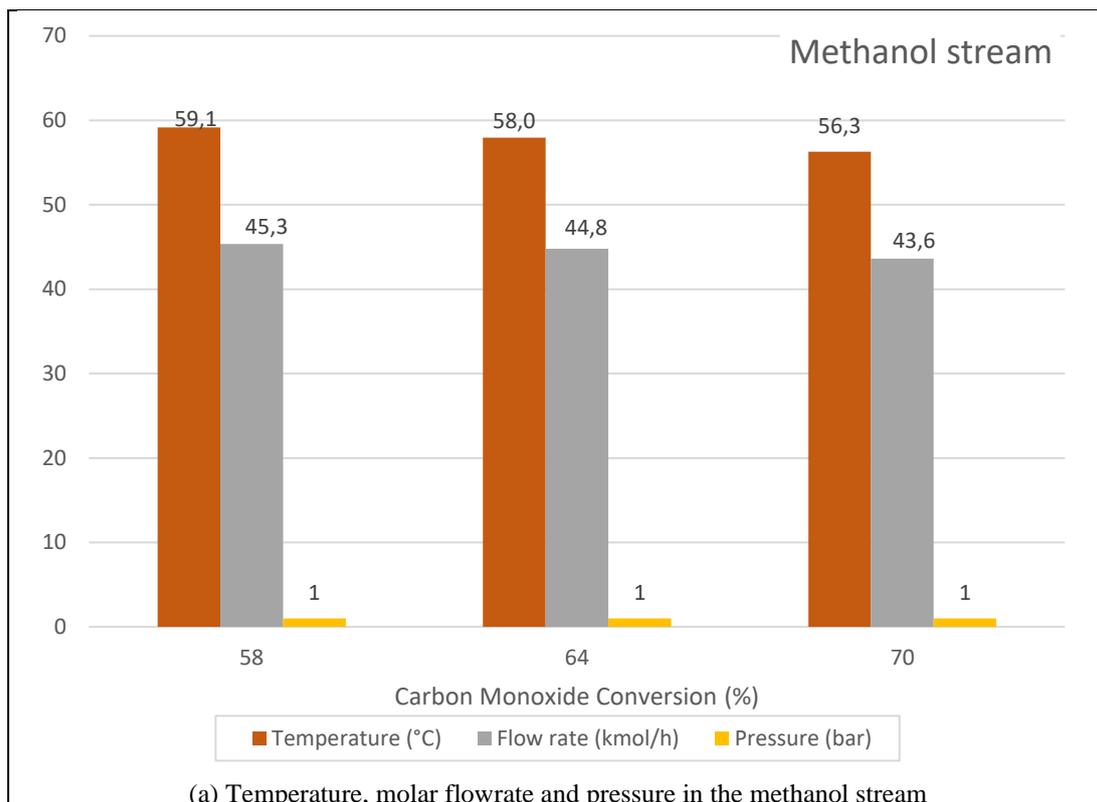


Figure 3. Results of the variation of CO and CO<sub>2</sub> reaction rate in the methanol stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components.

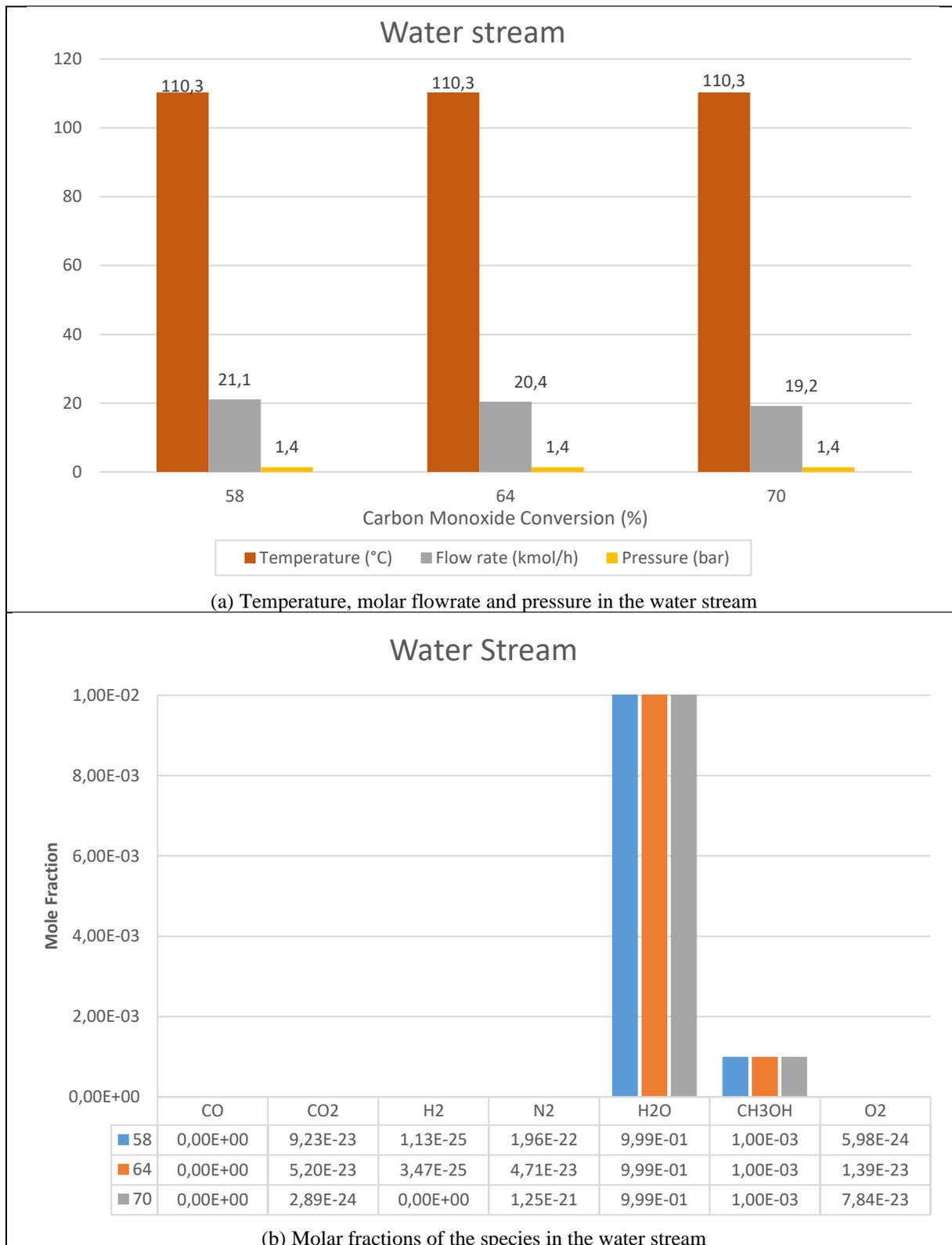


Figure 4. Results of the variation of CO and CO<sub>2</sub> reaction rate in the water stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components.

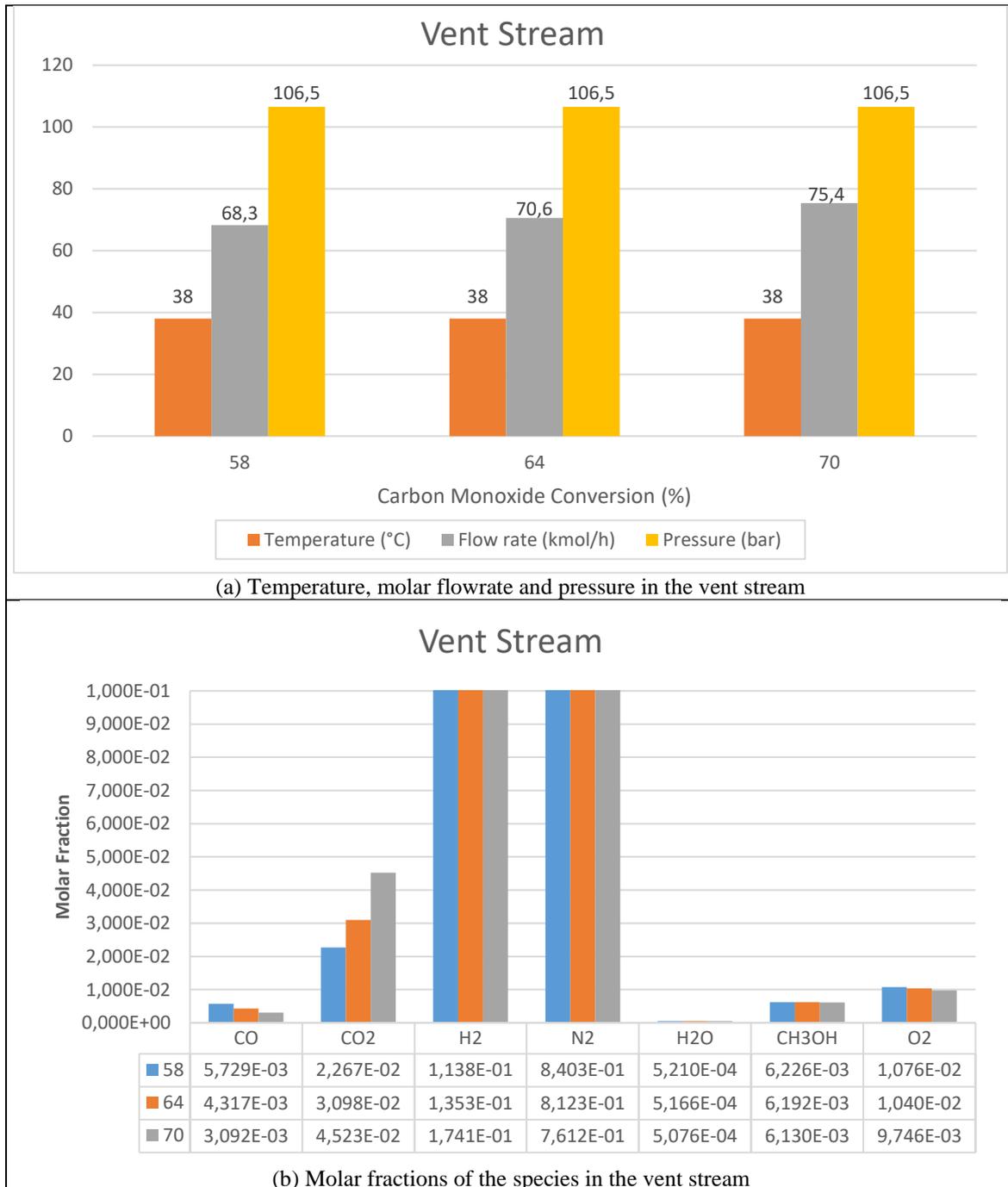


Figure 5. Results of the variation of CO and CO<sub>2</sub> reaction rate in the vent stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components.

In the analysis of the conversion percentages variations in the reactor, the following observations can be made as to the percentage of carbon monoxide conversion decreases and the percentage of carbon dioxide to methanol increases:

- The methanol flow increases, as does the outlet temperature (Figure 3a). The methanol produced has, according to this relationship, a higher molar fraction of carbon monoxide, nitrogen and oxygen, while a reduction in the molar fraction of carbon dioxide, hydrogen and water occurs (Figure 3b).
- The flow of water slows down (Figure 4a). The stream of water has a lower molar fraction of carbon dioxide and higher hydrogen and oxygen (Figure 4b).
- Vent flow decreases, as does the molar fraction of carbon dioxide and hydrogen present in it (Figure 5a). The molar fractions of carbon monoxide, nitrogen, water and methanol increase in this stream (Figure 5b).

### 3.2 Variation in the number of stages of the distillation column

Simulations were performed in the software by varying the number of stages of the distillation column (20, 40, and 60 stages). Figures 6, 7, and 8 represents the behavior of the methanol, water, and vent stream, respectively, with this variation.



Figure 6. Results of the variation of the number of stages in the distillation column in the methanol stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components

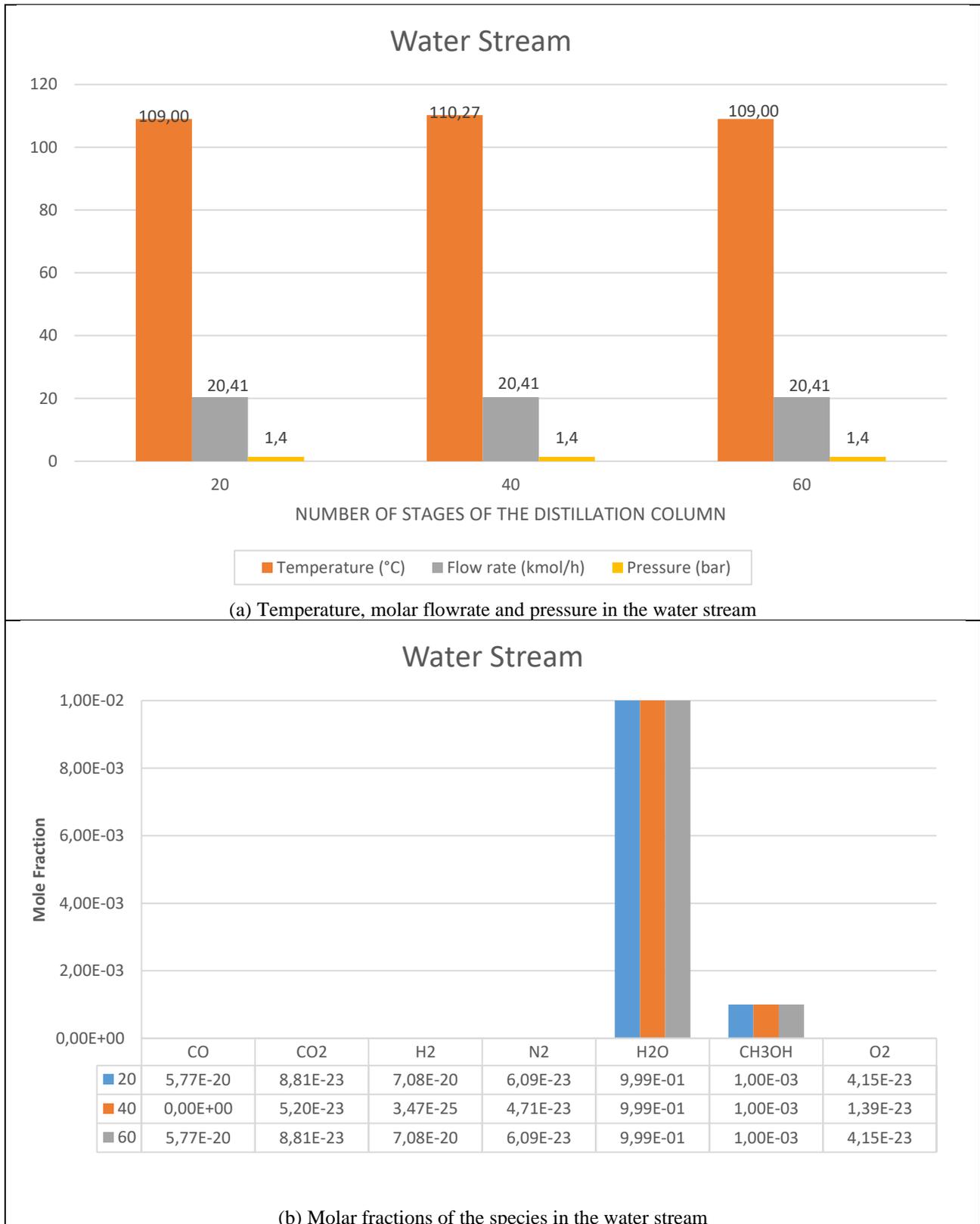


Figure 7. Results of the variation of the number of stages of the distillation column in the water stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components

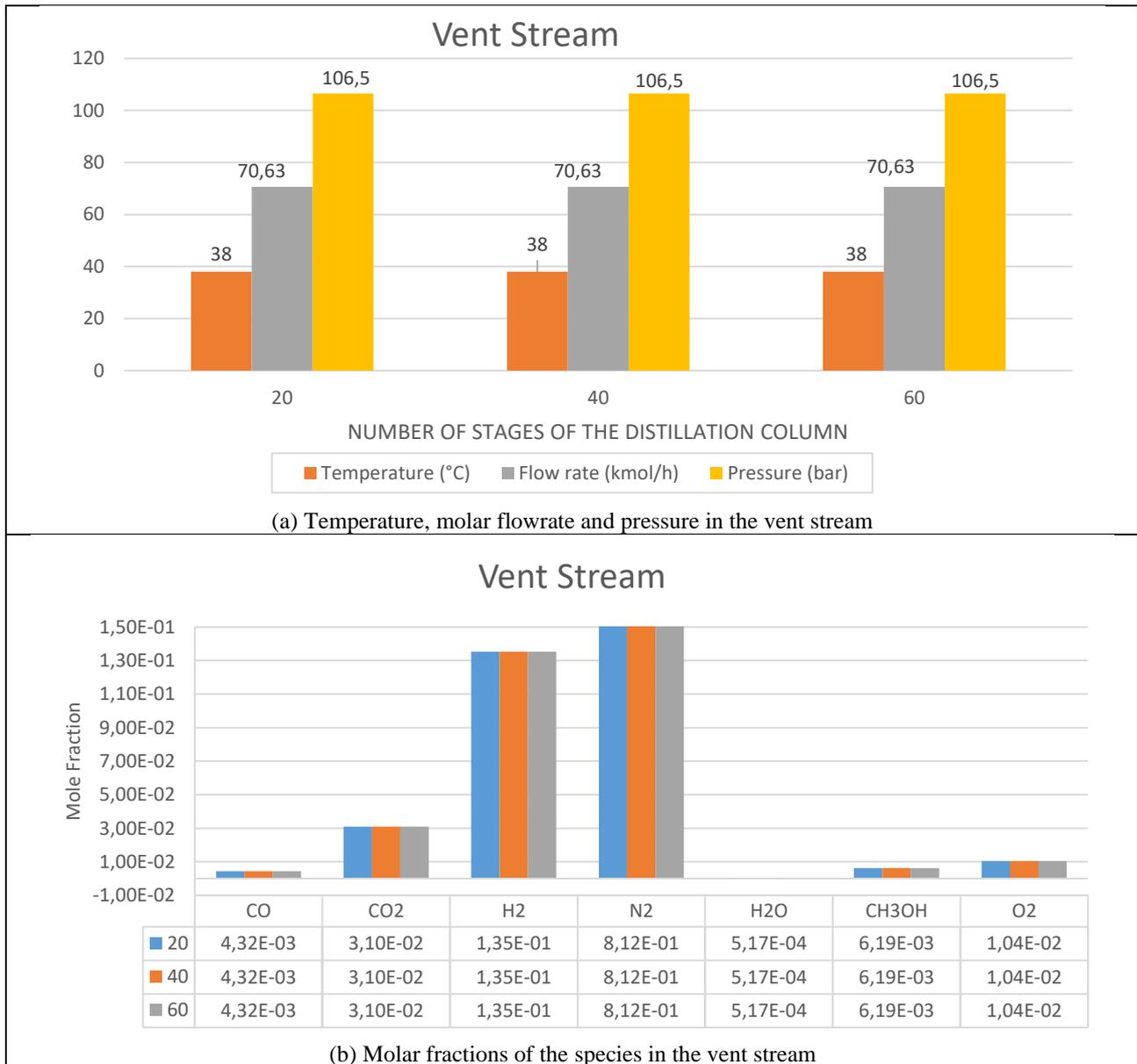


Figure 8. Results of the variation of the number of stages of the distillation column in the vent stream in terms of: (a) temperature, molar flowrate and pressure and (b) molar fractions of the components

Through the analysis of the results in Figures 6 to 8, it is possible to conclude that the water flow is the one that changes the most according to the variation in the number of stages of the distillation column. The temperature and molar fractions of carbon monoxide and carbon dioxide as well as those of hydrogen and nitrogen fluctuate with the increase in stages, but it is necessary to emphasize that they are not significant changes.

#### 4. FINAL REMARKS

In this paper, the simulation of the carbon sequestration process was carried out. The gas stream of the blast furnace in the steelmaking process was chosen. The gas synthesis of carbon monoxide and carbon dioxide into methanol is a great alternative to reduce the emission of carbon dioxide released to the environment. It is a possibility that can be studied and implemented in industries that release greenhouse gases, such as carbon dioxide, due to their production process, like the steelmaking process.

It is notable that the reduction in the percentage of the conversion of carbon monoxide and the increase in the percentage of the conversion of carbon dioxide into methanol in the reactor, as proposed by the previously developed studies in the literature, is not interesting since the molar fractions of other components will be present in the methanol stream. On the other hand, the change in the number of stages of the distillation column is attractive since the change in

molar fractions will be present only in the water stream. In addition, the investment cost of the reactor will decrease with a reduction in the number of stages.

## 5. ACKNOWLEDGEMENTS

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