

Research Article

Numerical Modeling and Performance Evaluation of a New Biogas Purification System

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Abstract

In order to meet the challenges posed by dependence on fossil fuels, it is essential to develop an energy alternative based on renewable sources. Among alternative energy solutions, biogas occupies a prime position. However, before biogas can be used, it must be purified, which involves removing the carbon dioxide (CO₂) and recovering the methane (CH₄), thereby increasing the calorific value of the methane. The most innovative purification solution is cryogenics. Our aim in this work is to use cryogenics to purify biogas by liquefying the carbon dioxide it contains. To achieve this, we have designed and dimensioned the various components of a cryogenic purification unit for biogas production. Using the incremental method based on heat conservation equations, we simulated this purification process on the Aspen plus calculation code. Using the ADMI calculation code, we modeled the model equations to visualize the behavior of the various parameters to be controlled. The temperature, pressure and mass flow profiles affecting the desublimation of carbon dioxide were obtained. Furthermore, the sizing results show that a 450 W compressor and a condenser with a capacity of 2.5 kg are required. The temperature and pressure of the biomethane and carbon dioxide at the condenser outlet are -130 °C and 15 bars. Simulations show curves for variations in temperature, pressure, rate of bio-methane recovery and carbon dioxide evacuation. They show that it is possible to produce biomethane with a purity of 96%, with a very negligible amount of carbon dioxide and a high lower calorific value (LCV) than raw biogas (9.83 kWh/m³ higher than 6 kWh/m³), a significant value in energy terms, showing that this biomethane could be used for a variety of purposes.

Keywords

Biogas, Biomethane, Cryogenic Upgrading, Purification

1. Introduction

The energy crisis of the 1970s, coupled with the predicted depletion of fossil fuels, highlighted the urgent need to find new sources of energy [1, 2]. Several countries have become aware of the fundamental problems of the energy situation and

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have implemented policies aimed at making better use of energy, even resorting to all possible energy sources.

Biogas appears to be one of the most interesting alternatives, as from an environmental point of view, it comes from the valorization of waste from households, the agro-pastoral industry and, in particular, agro-industrial processing [3]. A study based on the impact of multiform waste on pollution shows that odors from waste and car fumes can travel considerable distances and cause ecosystem degradation [4, 5]. Since then, biogas production facilities have sprung up all over the world. The primary objective of biogas production was to generate energy, but the environmental component soon emerged as an important additional reason for improving and popularizing the technology. A number of biogas production and treatment methods have been developed and proposed by various researchers. The general aim is to improve biogas quality, since the carbon dioxide content of the basic mixture considerably reduces its exoegetic power. Biogas purification techniques include amine scrubbing, water scrubbing, pressure swing adsorption (PSA), membrane separation and organic solvent scrubbing [6].

The principle of water purification is simple: biogas is cooled by heat exchangers and then mixed with water. This mixture causes the CO_2 and hydrogen sulfide (H_2S) to dissolve in the water, as their solubility is higher in water than in biogas. The mixture is then sprayed through a tall column [6]. Although this method is common, it is more widely used in Western Europe because of its cold temperature requirements [7, 8]. There have

also been studies into the optimum conditions for carbon dioxide liquefaction using cryogenic techniques [9, 10]. These studies have shown that the overall cost is lower in the case of 15 bars at a temperature of $-50\text{ }^\circ\text{C}$ [11, 12].

Studies have also been carried out on the pressure-temperature relationship, from which it emerges that the evolution temperatures at the biogas outlet are approximate for pressures ranging from 8 to 10 bar [13-15]. However, these studies are limited by the low calorific value and varying temperatures at the biogas outlet.

In this work, we'll be separating and purifying the biogas, using an optimized purification system. We will then run simulations on the Aspen HYSYS calculation code. We will focus on the correlation between influencing factors and key parameters such as pressure, temperature and the percentage of methane obtained at the end of the process.

2. Materials and Methods

2.1. Material

The flow chart proposed for the simulation of cryogenic biogas upgrading, as shown in Figure 1, aimed to achieve the highest methane concentration in the outgoing biogas stream, i.e. all operating conditions were designed to maximize the purity of the biogas produced.

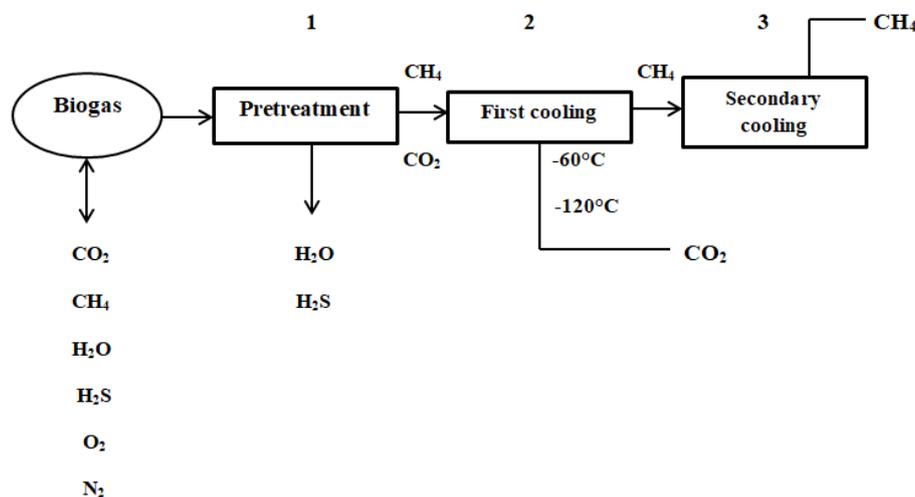


Figure 1. Purification unit process diagram.

The stages are as follows:

- (1) Depollution: The biogas is first treated by activated carbon filtration to eliminate hydrogen sulfide. The biogas is then cooled to $-40\text{ }^\circ\text{C}$. The biogas is then cooled for a similar dehumidification and depollution operation.
- (2) Decarbonation or first cooling: Separation and lique-

faction of carbon dioxide: The cleaned, dry biogas is cooled to a temperature of $-60\text{ }^\circ\text{C}$, so that the carbon dioxide is separated from the biogas.

- (3) Liquefaction or second cooling: The biomethane is then compressed to 15 bars before being liquefied at $-120\text{ }^\circ\text{C}$. The biogas studied for this work is located near the Ngaoundéré university campus. It is obtained by methaniza-

tion and is composed of the following elements:

Table 1. Composition of our biogas.

Elements	Symbol	Percentage (%)
Methane	CH ₄	40-60
Carbon dioxide	CO ₂	40-50
Dihydrogen	H ₂	5-10
Nitrogen	N ₂	1-2
Water value	H ₂ O	0.3

The properties of biogas are linked to its constituent compounds. The properties of some of these compounds are presented as follows:

Table 2. Properties of the biogas components we are studying.

Gas types	Density (kg/m ³)	Ignition temperature (°C)
Methane	0.72	600
Carbon dioxide	1.98	300
Water	1.58	270
Carbon monoxide	1.25	605
Hydrogen	0.09	585

2.2. Methods

In this work, we focus on the following cryogenic purification method:

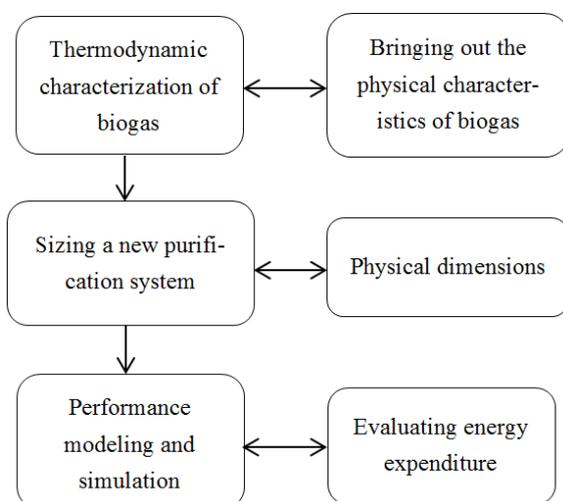


Figure 2. General work methodology.

The Aspen software will enable us to model the physical model and the simulation equations. Once the physical model has been implemented in Aspen, we'll introduce the dimensional information and then move on to the simulation.

2.2.1. Characterization by Sampling

For characterization, one sample per tube is taken. The tube is composed of two adsorbent beds. The first is used to trap target compounds, while the second is used to check that the maximum adsorption capacity of the first bed has not been reached (leak or puncture volume).

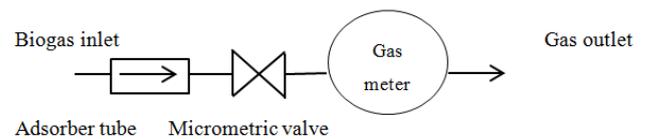


Figure 3. Sampling assembly diagram.

In this diagram, the adsorber tube is connected to the gas inlet and then to a Swagelok 1/8" micrometric valve, which regulates the flow rate of the sample gas. A Ritter gas meter is then added to perform the measurement and check the sample flow rate.

2.2.2. Equation/Mathematical Modeling

The simulation method is based on the CH₄ and CO₂ content equations under Aspen and takes into account a set of input parameters such as: temperature, pressure, flow rate etc.

In our case, for a cryogenic process intended for the purification and separation of biogas (binary mixture (CH₄ /CO₂)). The criteria to be taken into account are:

The rate of CO₂ evacuated (also called "evacuation"). It is given by the following equation:

$$\%CO_2 = \frac{RTY}{Pr+RTYKHPT} CO_2 \quad (1)$$

It focuses on Prandtl which takes into account parameters such as: Biogas inlet temperature and pressure, thermal capacity, biogas viscosity. Methane recovery rate (commonly referred to as "recovery"). It is given by the following equation:

$$Q_C = \frac{RTY}{Pr+RTY(KHPr-CO_2)} Q_M \quad (2)$$

It evaluates the percentage of methane recovery at the biogas outlet and is based on the CO₂ evacuation rate and the compressor power given by the following relationship:

$$W_C = f_{in} (h_{out}-h_{in}) = f_{in} \frac{PinVin}{np(\frac{n-1}{n})} \quad (3)$$

Where:

W_C is the power supplied to the compressor, h : molar enthalpy, f : molar flow rate, P : pressure, n : polytropic index, η_p : polytropic efficiency, V : molar volume and k : is the ratio of constant pressure (CP) calorific capacity to constant volume calorific capacity.

2.2.3. Dimensional Relations

Compressor power is evaluated by the following expression:

$$\Phi_k = \Phi_0 + P \quad (4)$$

Φ_0 : Raw compressor power in watts (or kilowatts).

P : the power required for the compression of the biogas in watts (or kilowatts).

Φ_k : the quantity of heat to be evacuated to the condenser in watts (or kilowatts).

This power is evaluated in order to estimate the compression of the biogas at the outlet of the exchangers [16]. It may help to reduce the energy consumption of the system. The next step will be to assess the exergetic destruction as follows:

$$Ex = (h - h_0) - T_0(s - s_0) \quad (5)$$

This formula is applied to find the consumption of each component present in the unit and by summing the exergies, the final exergy of the system is obtained.

The coefficient of performance (COP) is also evaluated to estimate the yield more accurately. It is given by the expressions (6) and (7).

$$COP = \frac{T_{SFM}}{T_{SC} - T_{SFM}} \quad (6)$$

With:

T_{sf} = the temperature of the cold source (K),

T_{sc} = the temperature of the hot source (K)

$$COP = \frac{Q}{W} \quad (7)$$

Q is the heat output (kW)

W is the work (kW) stored in the compressor

We could also evaluate the exergetic efficiency through formulae (8) and (9)

$$\eta = \frac{W_{min}}{W_{act}} \quad (8)$$

$$\eta = \frac{W_{act} - \sum \Delta ex}{W_{act}} \quad (9)$$

With:

W_{min} the minimum work required by a reversible system.

W_{act} the actual work performed on the system and the sum of the exercise destruction.

The key parameter for the plant is obviously the biogas's net calorific value (NCV).

Since biogas energy comes from methane, the Lower Calorific Value of methane, which is the amount of heat produced by combustion, is 9.94 kWh/m³.

Lower Calorific Value of the biogas will therefore be proportional to the percentage of CH₄ methane present in the biogas after purification [17, 18].

$$\text{Lower Calorific Value (LCV) Biogas} = \text{LCV raw methane} \times \text{Percentage CH}_4 \quad (10)$$

With:

LCV = Lower Calorific Value (kWh/m³)

3. Results and Discussion

The results we present here are derived from the characterization of our biogas, simulation methods and finally aspen modeling.

The thermodynamic properties are divided into three components: hydrogen sulfide, carbon dioxide and methane. They were given using an absorbent tube.

These properties, presented in tabular form, allow us to understand the physico-chemical behavior of our biogas, but they also provide information on the physical state of the biogas.

Table 3. Thermo-physical properties of hydrogen sulfide.

Properties	Values
Molar mass	33.06 g.mol ⁻¹
Temperature	260 °C
Melting point	-82.7 °C
Boiling point at 1.016 bars	-58.3 °C

Table 4. Thermo-physical properties of carbon dioxide.

Properties	Values
Molar mass	44.08 g.mol ⁻¹
Concentration in air	0.4432 Vol %
Melting point	-53.7 °C
Latent heat of melting (1.016 bars at melting point)	69.73 kJ.kg ⁻¹
Boiling point	-60.3 °C

Table 5. Thermo-physical properties of methane.

Properties	Values
Molar mass	15.458 g.mol ⁻¹
Temperature	Ature
Solubility in water (1.016 bars and 0 °C)	0.034 vol/vol
Melting point	-153.7 °C
Latent heat of melting (1.016 bars at melting point)	69.73 kJ.kg ⁻¹
Boiling point	-150.38 °C

These tables show that at ambient temperature and pressure, our biogas is in gaseous form. The properties of biogas vary depending on the nature of the waste and the fermentation conditions [19].

Figure 4 below shows the evolution of liquefied methane energy as a function of flow rate.

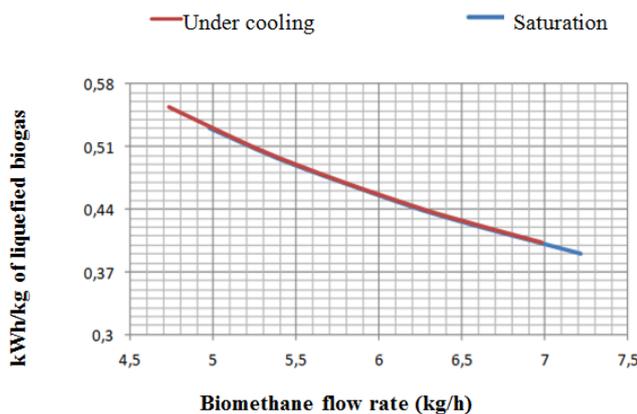


Figure 4. Variation of specific energy consumption as a function of the flow rate of biomethane.

The curve tells us that, for 1 m³ of biogas, we have a calorific value of about 6 kWh. This is the energy equivalent of 0.6 liters of biomethane.

In short, energy consumption decreases when biogas cools [20].

Figure 5 below gives information on the cooling of liquefied methane at different pressure ranges; the relationship between the flow rate of purified methane and the saturation pressure at the outlet of the biogas is discussed.

It emerges from this that, for pressures greater than 10 bars, the flow rate of biogas increases until the liquefied methane is completely cooled. The more the pressure decreases, the more the flow rate increases [21, 22] (for a pressure of 12 bars, there is 6.4 kg/h). Saturation is achieved at a pressure of 11 bars.

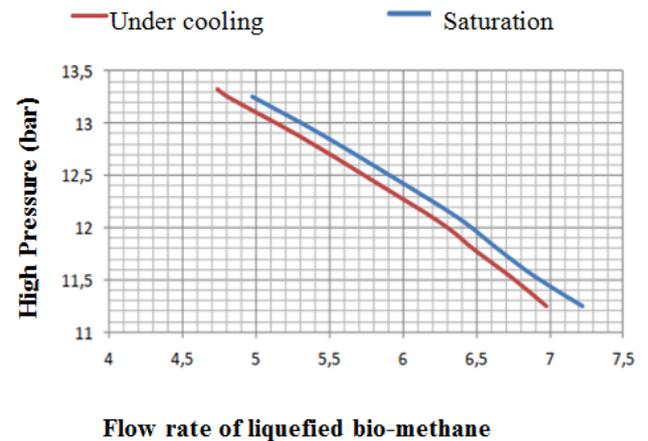


Figure 5. Variation of the biogas cooling pressure as a function of flow rate.

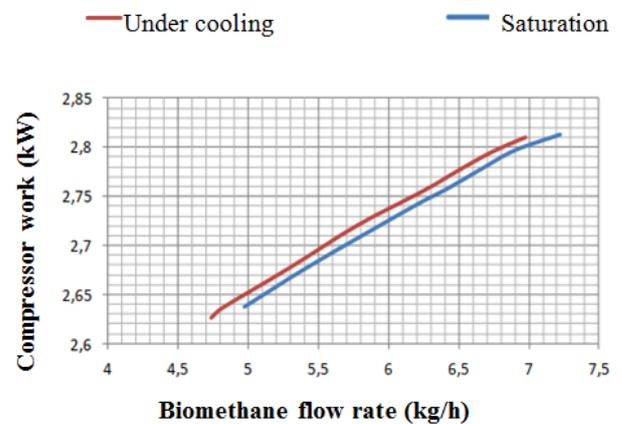


Figure 6. Variation of the work of the compressor as a function of the flow rate of the biomethane.

The saturation and sub-cooling curves indicate that, the more the power of the compressor increases, the more the purification flow rate increases. Saturation is achieved at a power of 2.8 kW.

Once the simulations have been carried out, it is important to highlight the general performance of our biogas purification system.

The table below shows the levels of the various elements present in our biogas after purification.

Table 6. Composition of purified biogas.

Component	Reduction Rate	Remaining Purity level
Methane		98.8
Carbon dioxide	96.1	
Oxygen		0.6
Nitrogen		0.6

Component	Reduction Rate	Remaining Purity level
Water	1.3	
Ammoniac	1.2	
Hydrogen		
Hydrogen sulfide	1.4	

The purification and separation rates show that filtration at the separators was effective (+30% of methane recovered).

It is then important to carry out a comparative study of energy values.

Table 7. Exergy values for the two systems.

Equipment	Energy (kW) Reference	Energy (kW) Improved
Compressor	1.444	1.1
Exchanger-100	2.443	1.8
Exchanger-101	1.720	1.2
Exchanger-102	0.175	0.1
VLV1 Cooler	0.884	0.44
VLV2 Cooler	2.189	1.05
SUM	8.525	5.69

After optimization, a reduction in the destruction of exergy at the compressor (1.444 kW to 1.1 kW) and that of the air cooler (2.189 kW to 1 kW) are observed. The difference between the compressor temperature and the cooling air temperature has decreased. Overall, the exergy

destruction after optimization is quantified at 5.69 kW and the exergetic yield is 21%.

It would also be wise to make a general comparison between our system and the system before the physical performance of our purification system.

Table 8. Comparative performance values of the two systems.

Settings	Reference System	Improved System
System Power	8.25 Kw	1.444
COP	0.7	2.443
Temperature	-90 °C	1.720
Cooling Pressure	12 bars	0.175
LCV	6.96 kWh/m ³	9.83 kWh/m ³
Percentage CH ₄	70%	96%
Percentage CO ₂	30%	Negligible

The other 4% represent the other negligible components such as: H₂, H₂O including the negligible amount of CO₂ (0.9%) etc.

It can be seen that the new system gives more satisfactory results, a reduction of 2.5 kW in the consumption of the system. And that of biogas cooling, an increase in the calorific value (from 6.96 kWh/m³ to 9.83 kWh/m³), an increase in the rate of methane recovery. It should be noted that a well purified biogas is based on a calorific value of less than 8 kWh/m³ and an increase in the percentage of methane by 90%, a coefficient of performance of 1 [23].

The diagrams below allow us to better identify the exergetic proportions of each element of the systems.

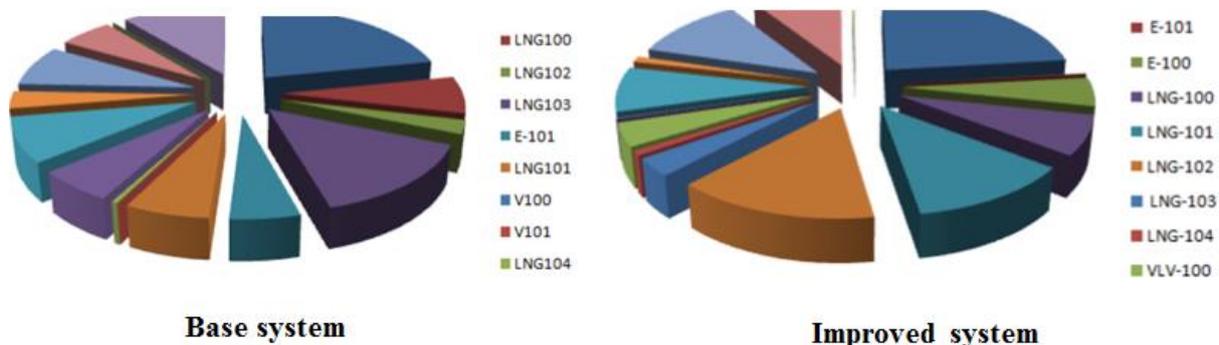


Figure 7. Comparative diagrams of system exergy losses.

It can be seen that the destruction of exergy at the level of the compressor and air cooler E-101 decreased significantly after optimization (by 31% for compressor and 78% for air).

The destruction of exergy decreased by 46% and consequently the electrical power supplied to the process was reduced by 50.3%.

At the air level, the compressor discharge temperature was reduced. As a result, the difference between this temperature and the temperature of the cooling air decreased and thus the exercise destruction decreased.

4. Conclusion

In this paper, the modeling of a cryogenic system has been presented, focusing on phase equilibrium. Some conclusions can be drawn as follows: The results of the simulations show a purity of methane of 96% in liquid phase under a temperature of -130 °C to 15 bars. A purified biogas with a negligible amount of CO₂ (0.9%) present in the final product.

Our system is less energy-intensive, consuming 5.69 kW, which is lower than the previous 8.25 kW system. Our purified biogas has a high calorific value with raw biogas (9.83 kWh/m³ higher than 6 kWh/m³) [24].

It can be said that the cryogenic purification of biogas, although a new purification technique offers a very high purity of methane as this study shows, the figures also show that the greatest end use is electricity production [25].

Abbreviations

CO ₂	Carbon Dioxide
CH ₄	Methane
LCV	Lower Calorific Value
PSA	Pressure Swing Adsorption
H ₂ S	Hydrogen Sulfide
H ₂	Dihydrogen
N ₂	Nitrogen
H ₂ O	Water
CP	Constant Pressure
NCV	Net Calorific Value
O	Oxygen

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Author Contributions

Tchatcha Abanda Ghratien: Formal Analysis, Funding acquisition, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review & editing

Gnepie Takam Nicolas Wilfred: Data curation, Investigation, Software

Edoun Marcel: Conceptualization, Project administration, Resources, Supervision, Validation

Tientcheu Nsiewe Maxwell: Data curation, Formal Analysis, Investigation, Methodology, Resources, Software,

Validation

Kuitche Alexis: Conceptualization, Funding acquisition, Project administration, Supervision, Validation

Data Availability Statement

The data supporting the outcome of this research work has been reported in this manuscript.

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Conflicts of Interest

The authors declare no conflicts of interest.

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