

Universidad de Valladolid



# UNIVERSIDAD DE VALLADOLID

# ESCUELA DE INGENIERIAS INDUSTRIALES

# Grado en Ingeniería Química

Modelado, optimización y análisis tecno-económico de un proceso para producir aire enriquecido en oxígeno por desorción de agua.

Aplicación y diseño para un hospital en África subsahariana

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Politecnico di Milano

Valladolid, julio de 2017.

## TFG REALIZADO EN PROGRAMA DE INTERCAMBIO

- TÍTULO: Modelling, optimisation and techno-economic analysis of a process to produce oxygen-enriched air by water desorption. Application and design for a hospital in sub-Saharan Africa
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- FECHA: 01/07/2017
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POLITECNICO DI MILANO School of Industrial and Information Engineering

**BSc Chemical Engineering** 



# MODELLING, OPTIMISATION AND TECHNO-ECONOMIC ANALYSIS OF A PROCESS TO PRODUCE OXYGEN-ENRICHED AIR BY WATER DESORPTION

APPLICATION AND DESIGN FOR A HOSPITAL IN SUB-SAHARAN AFRICA

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# ACKNOWLEDGEMENTS

To all those who have taught me to strive to have an impact on social innovation and human development in all what is done

> Nothing that is worth doing can be achieved in our lifetime; therefore we must be saved by hope. – Reinhold Niebuhr

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## SUMMARY

Oxygen, along with oxygen enriched air, is used in multiple applications, namely chemical industry and healthcare industry. Currently there are three main ways to get oxygen: cryogenic distillation, water electrolysis and membrane separation, being the first the most widely used on industrial scale. It allows the production of highly concentrated oxygen but it has one main downside, which is the high energy spending. The other processes present a lower cost-efficiency.

A new process to produce enriched air was analysed. It is based on the ability of water to absorb and desorb oxygen at different thermodynamic equilibria, varying temperature and pressure.

Firstly, based on empirical tests carried out in laboratory it was attempted to create a mathematical model. The first attempt was modelled with neural networks, but the small available empirical set of information did not allow to get a trustworthy model. The second attempt, adjusted by square errors minimising, outperforms the simulations done with computational software based on theoretical equations.

Secondly, the process was simulated by computer solving the Rachford-Rice equation with an Excel worksheet and with the computer software SimSci PRO/II.

Thirdly, the process model was applied to three different scenarios: chemical industry, ship propulsion and healthcare industry. In the chemical and the oil industry oxidation processes are common practice, ships use large quantities of air to oxidise the fuel in the combustion process that propels them and oxygen is important in healthcare in almost every lung related issue.

Regarding the two first scenarios, the outcomes resulted in flows of water so massive that rendered the whole process unfeasible. The application to healthcare was focused on contexts where there is no possibility to obtain bottled oxygen or electricity supply is unreliable, i.e. sub-Saharan Africa. The process was designed to the Sounon-Sero hospital in Nikki (Benin), as a proxy for any hospital in a similar context.

In fact, based on the information provided by that hospital, after traumatisms and malaria, it is lung-related infections that account for the highest number of patients attended at Sounon-Sero. A special emphasis has been put in designing a simple and reliable system with a demand sizing based on supply side, given the maximum capabilities of the equipment that can be found in Nikki. This opens new research opportunities regarding a more precise demand sizing or budget, which is to be done within an on-field venture.

# **CHAPTER 1: INTRODUCTION**

## 1. Justification

## 1.1. Background | The oxygen industry

Oxygen is the most common and most widespread element on earth. It can be found in the atmosphere, the lithosphere, the hydrosphere and the biosphere. Oxygen has a mass fraction of 50.5% of the earth cover, of 23.16% in the air, being its volume fraction around 20.95%, and of 88.8% in water (seawater: 86%).

In its elementary state, oxygen is dissolved in the form of  $O_2$  in the atmosphere and in the water. In this case, the relatively reactive oxygen will only exist in the form of an equilibrium, since oxygen-producing plants always discharge as much as is constantly consumed by breathing creatures. Without this biological cycle, it would only be found in compounds.

The oxygen allotrope  $O_3$  (ozone) is present in small amounts in the atmosphere. In compounds, oxygen is present all over the earth. In the earth cover almost all minerals and rocks are oxygenated. The most important of these are silicates (silicon-oxygen compounds such as mica), carbonates, for example calcium carbonate in limestone and oxides such as silicon dioxide (quartz).

The use of oxygen is nowadays ubiquitous. Among the main industrial applications one can find, are the following:

- Steel industry: more than half of the world production is devoted to this sector (Emsley, 2001). It is needed in blast furnaces and rotating furnaces where the presence of a higher concentration of oxygen increases the efficiency of the combustion, eliminating sulphur, manganese and phosphor stains as well as excess of carbon. The presence of oxygen favours energy savings as well as reducing polluting emissions.
- 2. Chemical industry: this is second industry, after steel, where the highest amount of oxygen is consumed worldwide, accounting for around a quarter of it (Emsley, 2001). In chemical processes, oxygen is mostly used for the oxidation of various basic materials such as the olefin oxidation of ethene to ethylene oxide and the partial oxidation of heavy oil and coal. Oxygen is also required to produce hydrogen and synthesis gas and the production of sulfuric and nitric acids. Other important products produced by oxidation with oxygen are acetylene, acetaldehyde, acetic acid, vinyl acetate or chlorine.

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Oxygen is also important in the production of sulphuric acid, the most produced chemical substance in the world, using the Claus technique, where oxygen is required to oxidise H<sub>2</sub>S into SO<sub>2</sub>.

- 3. Healthcare industry: this gas is frequently used in the treatment and prevention of hypoxemia and hypoxia, in addition to treatment of obstructive pulmonary diseases, pneumonias, myocardial infarctions and pulmonary emboli. Its application is essential in cases of cardiorespiratory resuscitation, intensive therapy or anaesthesia among others. Oxygen is also commonly used in the medical sector where there are no special sterilization conditions. An example may be in equipment such as the hyperbaric chamber, sealed environments where oxygen is diffused with nitrogen and other gases.
- 4. Ozone production: oxygen is used in systems devoted to the production of ozone. Ozone is produced when oxygen molecules in the feed gas are exposed to a controlled electric discharge in a generator. The instability of ozone, which at first might seem an inconvenience, since it makes it difficult to pack it and requires in-situ production, becomes one of its greatest virtues because after its action as an oxidizer becomes oxygen again and disappears without leaving residues. In this way, it becomes an invaluable tool for hygienic-sanitary control of critical points. It is also used in the biofuel industry to break lignocellulosic structures from agricultural waste and recover the sugars than can be used to get bioalcohols.
- 5. Car industry: oxygen is used in the process of plasma cutting and as an auxiliary gas when laser cutting.
- 6. Energy industry: by working with a higher concentration of oxygen efficiency increases dramatically and facilitates the recovery of greenhouse gases, such as CO<sub>2</sub>.
- 7. Biotech and pharma industries: oxygen is a required gas for cellular growth, being therefore used in bioreactors and fermentations.
- 8. Glass industry: oxygen is an industrial gas capable of improving productivity and it is used to increase combustion in glass baking and to reduce NOx emissions. The use of oxygen in glass production facilities allows high levels of transparency, reduced fuel usage and reduced exhaust volume. It is also used for glass polishing, obtaining high quality products. In this aspect, improvements such as brightness increase or elimination of defects on the surface of the product can be achieved not using acidic substances in the process and being the environmentally friendly.
- 9. Wastewater treatment: oxygen integrates or even replaces air in the aeration tanks, to maximize treatment capacity, minimize emissions of volatile organic compounds, doors, and foam. In some cases, it has been possible to increase to more than double the

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capacity of purification without the realization of civil works and without modification of the biological raft. In other cases, the design of biological purification systems that work with pure oxygen (instead of with aeration systems) allows to reduce the investment needed to be made when studying the installation of a water purification plant. In addition, it has other advantages such as the reduction of iron and manganese in water, oxidation and precipitation reactions, as well as favouring the oxidation of sulphides. Besides, the aggressiveness of water can be reduced or eliminated by the calco-carbon equilibration of the process waters, by addition of soda and CO<sub>2</sub>. An improved control over this water allows less maintenance of the pipes.

10. Paper industry: as an industrial gas, oxygen respects the strict environmental regulations applicable to processes of delignification, oxidative extraction and treatment of waste water. Oxygen is also used for bleaching paper.

Apart from that, it is essential for life, entailing further applications within the healthcare industry. Along history, several approaches have been taken to different way of obtaining oxygen.

# 2. Objectives

The main objective in this project is to evaluate the convenience of a new system to obtain oxygen enriched air by water desorption.

To do this, several steps will be pursued. Firstly, it is necessary to do the modelling of the new alternative proposal. Once this is attained, the next step is to optimise it to get the most cost-efficient possible configuration. This will be done in conjunction with the other last step, which is the economic analysis.

In order to identify if this is indeed an advisable alternative opportunity to current methods, the new proposal will be compared with traditional methods. That way, for a given system or industry, the so-called M-1 will consist on the use of pure oxygen within the process, M-2 will consist on the use of air, and M-3 the proposed alternative method. The comparison will be carried out with either incremental or decremental costs, but not accounting for sunk or common costs to all methods:

	ΔCAPEX		
M-1	0	f(O <sub>2</sub> price, quantity)	0
M-2	f(incremental volume, equipment price)	0	f(energy price, [O <sub>2</sub> ], quantity)
M-3	f(incremental volume, equipment price)	0	f(energy price, [O <sub>2</sub> ], quantity)

As well as evaluating possible gains:

	Δrevenues
M-1	0
M-2	0
M-3	f(residual volume of EA, EA price)

# CHAPTER 2: STATE OF THE ART

## 1. Current oxygen production alternatives

Currently, oxygen is mainly obtained by Distillation of air. The process was first developed by Carl von Linde (Linde method) in 1902 and rendered economically viable by Georges Claude. Another method is Water electrolysis, by which small amounts result as a by-product in the hydrogen production. Oxygen can also be separated from the air by adsorption of other gases: when air flows through molecular sieves, nitrogen and carbon dioxide are adsorbed and only oxygen and argon pass through.

An older process is the chemical-reaction-based barium oxide process. It is not profitable because of the high energy expenditure. Barium oxide is heated up to 500°C in presence of air, forming barium peroxide. When heated to 700°C, the previously absorbed oxygen is released again by thermolysis.

$$2\operatorname{BaO} + \operatorname{O}_2 \xrightarrow{500^{\circ}\mathrm{C}} 2\operatorname{BaO}_2$$
$$2\operatorname{BaO}_2 \xrightarrow{700^{\circ}\mathrm{C}} 2\operatorname{BaO} + \operatorname{O}_2$$

Before the development of the Linde process, this method was the only way to get pure oxygen.

#### 1.1. Distillation of air

Firstly, air is collected and taken to a washing process in large towers by with a solution of water with caustic soda. This process eliminates carbon dioxide. At its exit, it is compressed and subjected to a process of removal of oil and water vapor. After this process the air is passed through cylinders filled with caustic potash, to eliminate any trace of carbon monoxide and water. At the top of these cylinders there are cotton filters that remove any foreign particles from the air preventing them from entering high pressure lines.

Once the air has dried and compressed, it passes to the rectification towers, in which it expands to pressures close to the atmospheric, causing its cooling, and subsequent liquefaction. In the liquid state the air is separable, since the differences between the boiling points between its major elements (nitrogen and oxygen) is approximately 13°C. In addition, there is the extra

advantage that these two compounds do not form azeotropes, which facilitates the separation of components by this method.

The main process for the liquefying of the air and obtaining its separate components is the socalled Linde-Fränkl process (Springmann, 1978). In this process, by the Linde-Hampson method, the air is liquefied by isoenthalp expansion, i.e. cooling occurs due to the Joule-Thomson effect by flow of the fluid through a narrow space, such as a valve.



Figure 1. Schematic drawing of the cryogenic air separation process (Reinhardt, 2015)

Then, the air is compressed at high pressures. This compression process is isothermal. Once the air is compressed, it is cooled in a heat exchanger. This process is critical because the air can contain impurities, such as  $CO_2$  or water, which at this stage could deposit and damage the equipment. To clean the air, it used the above described process, in which water and carbon dioxide were removed.

In the past, shell and tube exchangers were used, which made their construction costly and entailed significant losses, which translated into the replacement with other exchangers, such as Fränkl type exchangers. The low cost of this exchanger and its efficiency for low temperature applications can be explained because of the large surface area per unit volume of packaging (400-1000 ft<sup>2</sup>/ft<sup>3</sup> compared to the 50 ft<sup>2</sup>/ft<sup>3</sup> for the normal type) (Timmerhaus, 1961).

If hot air is introduced, it will cool down as it enters the exchanger, resulting in deposition of solid impurities on the heat exchanger. Heat is retained in the aluminum strips, so when cold air

is introduced, it dissolves those impurities and the resulting product losses can reach up to 60%. Then, using a valve, air expansion occurs due to the pressure drop associated, obtaining a liquidvapor mixture at the outlet of the valve, given the temperature drop associated with the Joule-Thomson effect.

The liquid obtained will be the raw material for the process, while the gas obtained in this isoenthalpic expansion will be used to cool the compressed air in the heat exchanger. Once the gas is used in cooling the air in the heat exchanger, it is emitted back to the atmosphere. After this, the liquefied air will be taken to the rectification tower, where oxygen will be obtained in industrial scale.

The use of rectification towers is possible, as stated above, due to the non-formation of azeotropes and the difference in boiling points between the two compounds. Rectification towers can be of a single column or based in two columns. In the case of using a distillation with a single column, the problem is that the condenser cannot regenerate the reflux, since it is used to cool the incoming air to the process, together with the gas that occurred in the expansion in the valve, resulting in a lower quality nitrogen, though obtained oxygen is practically pure.

The most widely used alternative is the distillation in two columns, in which two columns of rectification are superposed, the lower one works at a higher pressure, around five atmospheres. In this case the steam that rises is enriched in nitrogen, while the liquid is enriched in oxygen. In the head, practically pure nitrogen is obtained, but to purify it, reflux is necessary.

#### 2 | State of the art

## 1.2. Water electrolysis

As it was above stated, this method is far less used than the previous one for cost-effectiveness reasons, however, it is used for some applications, such as oxygen production in the International Space Station due to the high purity of oxygen and hydrogen needs (Robert, 2011). The reactions that occur are the following:

Cathode (reduction): 
$$2H_2O + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$$
;  
Anode (oxidation):  $4OH^-(aq) \rightarrow O_2(g) + 2H_2O + 4e^-$ ;  
Overall reaction:  $2H_2O \rightarrow 2H_2(g) + O_2(g)$ ;



Figure 2. Water electrolysis

## 1.3. Membrane separation

This is the technique used by portable oxygen concentrators used for domestic medical applications and the recommended way to supply oxygen in developing countries (Dobson, 2001) given the high cost and logistical problems associated with using the traditional oxygen cylinders.

Compressed air is fed to the first molecular sieve, where nitrogen is trapped while oxygen follows its way through the system till it is storage in a tank. When the first sieve is saturated with nitrogen, the air flow is directed to the second sieve. The bypass valves open in the second chamber and close in the first. As the second column separates the nitrogen from oxygen, the first sieve releases the trapped molecules of nitrogen into the atmosphere, which is immediately regenerated with ambient air.

Concentrations achieved by this system are about 90% of purity of oxygen.



Figure 3. Ssemi-continuous oxygen production process by membranes

# 2. New proposal for enriched air production

As it has already been mentioned, the main objective of this work is to make an analysis of the viability of a new method proposed for the enrichment of atmospheric air.

This is going to be based on the work by Galli et al. The process flow diagram of the proposed technique at a laboratory scale is displayed in Figure 4.

First, there is a tank (S1) with water at atmospheric pressure that equilibrates thermodynamically with air by bubbling compressed air. Then, the water in equilibrium travels to the degassing unit (R1), which is at a lower pressure than the atmospheric, allowing the water to flow in by depression. There is another pump (G1) that helps in the evacuation of the degassed water that is then discarded.

The resulting gas is compressed (G2) and then sent to a gas cromatograph that analyses the composition. Along the system, pressure, temperature and flow are measured and controlled. There are two rotameters to measure the flow of water and air (K1, K2), as well as thermocouples and valves.

In green it is displayed another line containing helium, which is used to purge the system between one experiment and another. If it was not used, this would result in an underestimation of the final values of the concentration, since the line would be full of atmospheric air before every experiment, and this would cause dilution in the produced air at the beginning.



Figure 4. PFD of the proposed system ((Galli et al., 2016))

## 2 | State of the art

# **CHAPTER 3: MODELLING**

## 1. Multivariable linear empirical model

Given the empirical data this work is based on (Galli et al., 2016) and considering the direct relationship between the final concentration of oxygen in air and the three other variables of operation: pressure, temperature and flow of air, a multivariable model is proposed to empirically simulate the outcome of other operating conditions.

The data on which the model has been built are shown here:

	1	2	3	4	5	6	7	8	9	10	11	12	13
P [mm Hg]	400	400	400	400	400	400	400	400	400	500	500	500	500
F <sub>in</sub> [L/h]	20.8	30.0	29.3	29.3	29.5	19.0	9.2	29.5	29.5	9.6	9.3	20.1	30.0
T [ºC]	41.2	38.8	47.5	39.2	38.9	42.6	48.1	27.9	27.9	54.5	46.3	40.8	38.1
%O <sub>2</sub>	27.9	27.6	28.4	28.5	28.3	28.8	29.6	28.6	28.6	28.2	28.6	27.6	28.6
	14	15	16	17	18	19	20	21	22	23	24	25	
P [mm Hg]	500	500	500	500	500	500	500	500	500	600	600	600	-
F <sub>in</sub> [L/h]	20.3	30.0	20.5	9.5	29.5	29.5	9.5	9.6	20.0	9.3	9.3	21.1	
T [ºC]	50.0	41.0	44.5	49.0	41.2	28.7	67.7	31.5	40.3	54.2	45.8	42.0	
%O <sub>2</sub>	28.5	29.9	28.4	29.3	28.7	29.0	29.8	28.7	28.5	27.0	26.4	28.2	
	1												

#### Table 1. Empirical data (Galli et al., 2016)

The multivariable OLS regression has been calculated using statistics software Gretl and it is the following:

 $\% O_2 = 31 - 0.00973338 * P + 0.0458309 * F_{in} + 0.0365323 * T$ 

## 3 | Modelling

Where:

$$P [mm Hg]$$
$$F_{in} \left[\frac{L}{h}\right]$$
$$T [°C]$$

The paper on which this work is based on had done a simulation with the software PRO/II 9.3 by SimSci-Schneider Electric.

In order to evaluate the convenience of this latter multivariable simulation, a comparison between the two sets of data has been carried out by calculate the relative errors of each model with respect to the actual empirical simulations:



1	2	3	4	5	6	7	8	9	10	11	12	13
27.9	27.6	28.4	28.5	28.3	28.8	29.6	28.6	28.6	28.2	28.6	27.6	28.6
29.9	29.5	30.5	29.5	29.5	29.9	30.5	28.1	28.1	30.0	29.0	28.4	28.0
29.6	29.9	30.2	29.9	29.9	29.5	29.3	29.5	29.5	28.6	28.3	28.5	28.9
1.7	2.3	1.8	1.4	1.6	0.7	-0.3	0.9	0.9	0.4	-0.3	0.9	0.3
2.0	1.9	2.1	1.0	1.2	1.1	0.9	-0.5	-0.5	1.8	0.4	0.8	-0.6
6.0	8.3	6.3	4.8	5.6	2.5	-1.1	3.1	3.1	1.3	-1.2	3.4	1.0
7.2	6.9	7.4	3.5	4.2	3.8	3.0	-1.7	-1.7	6.4	1.4	2.9	-2.1
	1 27.9 29.9 29.6 1.7 2.0 6.0 7.2	1     2       27.9     27.6       29.9     29.5       29.6     29.9       1.7     2.3       2.0     1.9       6.0     8.3       7.2     6.9	1     2     3       27.9     27.6     28.4       29.9     29.5     30.5       29.6     29.9     30.2       1.7     2.3     1.8       2.0     1.9     2.1       6.0     8.3     6.3       7.2     6.9     7.4	1         2         3         4           27.9         27.6         28.4         28.5           29.9         29.5         30.5         29.5           29.6         29.9         30.2         29.9           1.7         2.3         1.8         1.4           2.0         1.9         2.1         1.0           6.0         8.3         6.3         4.8           7.2         6.9         7.4         3.5	1       2       3       4       5         27.9       27.6       28.4       28.5       28.3         29.9       29.5       30.5       29.5       29.5         29.6       29.9       30.2       29.9       29.9         1.7       2.3       1.8       1.4       1.6         2.0       1.9       2.1       1.0       1.2         6.0       8.3       6.3       4.8       5.6         7.2       6.9       7.4       3.5       4.2	1         2         3         4         5         6           27.9         27.6         28.4         28.5         28.3         28.8           29.9         29.5         30.5         29.5         29.9         29.9           29.6         29.9         30.2         29.9         29.9         29.5           1.7         2.3         1.8         1.4         1.6         0.7           20.0         1.9         2.1         1.0         1.2         1.1           6.0         8.3         6.3         4.8         5.6         2.5           7.2         6.9         7.4         3.5         4.2         3.8	1       2       3       4       5       6       7         27.9       27.6       28.4       28.5       28.3       28.8       29.6         29.9       29.5       30.5       29.5       29.9       29.9       30.5         29.6       29.9       30.2       29.9       29.9       29.5       29.3         1.7       2.3       1.8       1.4       1.6       0.7       -0.3         2.0       1.9       2.1       1.0       1.2       1.1       0.9         6.0       8.3       6.3       4.8       5.6       2.5       -1.1         7.2       6.9       7.4       3.5       4.2       3.8       3.0	1       2       3       4       5       6       7       8         27.9       27.6       28.4       28.5       28.3       28.8       29.6       28.6         29.9       29.5       30.5       29.5       29.5       29.9       30.5       28.1         29.6       29.9       30.2       29.9       29.9       29.5       29.3       29.5         1.7       2.3       1.8       1.4       1.6       0.7       -0.3       0.9         2.0       1.9       2.1       1.0       1.2       1.1       0.9       -0.5         6.0       8.3       6.3       4.8       5.6       2.5       -1.1       3.1         7.2       6.9       7.4       3.5       4.2       3.8       3.0       -1.7	1       2       3       4       5       6       7       8       9         27.9       27.6       28.4       28.5       28.3       28.8       29.6       28.6       28.6         29.9       29.5       30.5       29.5       29.5       29.9       30.5       28.1       28.1         29.0       29.9       30.2       29.9       29.9       29.5       29.3       29.5<	1         2         3         4         5         6         7         8         9         10           27.9         27.6         28.4         28.5         28.3         28.8         29.6         28.6         28.6         28.2           29.9         29.5         30.5         29.5         29.9         30.5         28.1         28.1         30.0           29.6         29.9         30.2         29.9         29.9         29.5         29.3         29.5         29.5         29.3         29.5         29.5         28.1         30.0           29.6         29.9         30.2         29.9         29.9         29.5         29.3         29.5         1.4           20.0         1.3         1.4         1.	1       2       3       4       5       6       7       8       9       10       11         27.9       27.6       28.4       28.5       28.3       28.8       29.6       28.6       28.6       28.6       28.7       28.6       28.7       28.6       28.7       28.6       28.7       28.6       28.7       28.6       28.7       28.6       28.7       29.7       29.7       28.7       28.7       29.7       29.7       28.7       29.7 <td>1         2         3         4         5         6         7         8         9         10         11         12           27.9         27.6         28.4         28.5         28.3         28.8         29.6         28.6         28.2         28.2         28.6         27.6           29.9         29.5         30.5         29.5         29.5         29.9         30.5         28.1         28.1         30.0         29.0         28.4           29.6         29.9         30.2         29.9         29.5         29.5         28.1         28.1         30.0         29.0         28.4           29.6         29.9         30.2         29.9         29.9         29.5         28.1         28.1         30.0         28.4           29.6         29.9         30.2         29.9         29.9         29.5         29.5         28.</td>	1         2         3         4         5         6         7         8         9         10         11         12           27.9         27.6         28.4         28.5         28.3         28.8         29.6         28.6         28.2         28.2         28.6         27.6           29.9         29.5         30.5         29.5         29.5         29.9         30.5         28.1         28.1         30.0         29.0         28.4           29.6         29.9         30.2         29.9         29.5         29.5         28.1         28.1         30.0         29.0         28.4           29.6         29.9         30.2         29.9         29.9         29.5         28.1         28.1         30.0         28.4           29.6         29.9         30.2         29.9         29.9         29.5         29.5         28.

I

	14	15	16	17	18	19	20	21	22	23	24	25
%O <sub>2</sub>	29.5	28.4	28.8	29.4	28.4	28.7	31.3	27.1	28.3	28.8	27.8	27.3
%O <sub>2sim</sub>	28.9	29.0	28.7	28.4	29.0	28.5	29.0	27.7	28.5	27.6	27.3	27.7
%O <sub>2MVR</sub>	0.4	-0.9	0.3	-0.9	0.3	-0.5	-0.8	-1.0	0.0	0.6	0.9	-0.5
ABSERR <sub>MVR</sub>	1.0	-1.5	0.4	0.1	-0.3	-0.3	1.5	-1.6	-0.2	1.8	1.4	-0.9
ABSERR <sub>PROII</sub>	1.4	-3.0	1.1	-3.2	1.0	-1.6	-2.5	-3.4	0.1	2.1	3.3	-1.9
RELERR <sub>MVR</sub>	3.5	-5.0	1.4	0.3	-1.0	-1.0	5.0	-5.6	-0.7	6.7	5.3	-3.2
RELERR <sub>PROII</sub>	29.5	28.4	28.8	29.4	28.4	28.7	31.3	27.1	28.3	28.8	27.8	27.3



# 2. Neural network modelling attempt

It was also attempted to make a model of the empirical data using the neural network plugin in Matlab, however, the results did not fit adequately given that there were only 25 sets of data and neural networks need large quantities of information to deliver sound results.

The screenshots of the procedure followed, as well as the final results are shown for illustrative purposes:



#### 3 | Modelling



Figure 5. Results of the first model with neural network where training shows poor results

## 3 | Modelling



 Neural Network Training Regression (plotregression), Epoch 13, Validation stop.
 <u>File Edit View Insert Tools Desktop Window H</u>elp ٥ × \_ Validation: R=0.50474 Training: R=0.98804 O Data Fit ○ Data Fit ······Y = T ○ 29.5 29 28.5 28.5 27.5 27.5 27.5 27 27 27 27 27 27 27 27 27 29.5 29 28.5 28.5 28.5 27.5 27.5 27 27 27 27 27 27 27 26.5 29 £ 0 27 28 Target 29 28 Target 29 All: R=0.72915 Test: R=-0.4581 O Data Fit ° 0 0 O Data 29.5 29 28€**,⊥ardet +3:** 28 27.5 27.5 27.5 27.5 27.5 889 869 29 Y = T 0 28 Target 28 Target 27 29 # 🤤 💿 🗮 🗷 🗷 💽 🔯 📣 🖻 💿 🥥 🛷 ^ 😳 🗁 🦽 ⊄× ENG 15:47 4 S

Figure 6. Results of the second model with neural network

# 3. Computational simulation for the flash with Rachford-Rice equation

## 3.1. Theoretical background

The cornerstone of the simulation is given by the flash tank, whose modelling has been done both using the simulation software SimSci PRO/II and by solving the Rachford-Rice equation with spreadsheets in Microsoft Excel. The scheme of the process is the following:



Figure 7. Scheme of the flash separation process

The Rachford-Rice equation will allow us to calculate the compositions of the two departing streams. It brings together the mass balances and the equations of equilibrium and can be written as follows:

$$\sum_{i=1}^{c} \frac{z_i(K_i - 1)}{1 + \frac{V}{F}(K_i - 1)}$$

Equation 1. Rachford-Rice

Where:

 $z_i$  is the mole fraction of component *i* in the feed  $K_i$  is the equilibrium constant of component *i* 



Figure 8. Ttrustworthiness of Raoult's and Henryy's law for different concentrations

V is the molar flow of vapour F is the total molar flow c is the number of components

Equilibrium constants have been calculated with Henry's law, since they provide a much closer value to the non-ideal solution values than Raoult's law, as can be deduced from Figure 8.

## 3.2. Results

P [mm Hg]	T [ºC]	y2	y2 (dry)	y2 (emp)	AbsErr dry
400	25.0	25.0%	26.6%		
400	27.9	25.2%	27.1%	27.9%	0.82
400	30.0	25.3%	27.4%		
400	35.0	25.3%	28.3%		
400	38.8	25.1%	28.8%	28.4%	0.45
400	40.0	25.0%	29.0%		
400	45.0	24.5%	29.8%		
400	48.0	23.9%	30.3%	28.6%	1.66
400	50.0	23.5%	30.6%		
400	55.0	22.1%	31.3%		
400	60.0	20.1%	32.1%		
400	65.0	17.5%	32.9%		
400	70.0	14.0%	33.7%		
500	25.0	23.5%	24.7%		
500	28.7	23.9%	25.4%	28.2%	2.85
500	30.0	24.0%	25.6%		
500	31.5	24.1%	25.9%	28.6%	2.73
500	35.0	24.3%	26.5%		
500	38.1	24.3%	27.0%	27.6%	0.57
500	40.0	24.4%	27.4%		
500	44.5	24.2%	28.1%	29.3%	1.18
500	45.0	24.2%	28.2%		
500	50.0	23.7%	29.0%	29.8%	0.76
500	55.0	22.8%	29.9%	28.7%	1.17
500	60.0	21.6%	30.7%		
500	65.0	19.7%	31.5%		
500	67.7	18.5%	32.0%	28.5%	3.50

## 3 | Modelling

500	70.0	17.3%	32.4%		
600	25.0	22.1%	23.0%		
600	30.0	22.7%	23.9%		
600	35.0	23.2 %	24.9%		
600	40.0	23.5%	25.8%		
600	42.0	23.5%	26.2%	27.0%	0.82
600	45.0	23.5%	26.7%		
600	45.8	23.5%	26.9%	26.4%	0.47
600	50.0	23.4%	27.6%		
600	54.2	23.0%	28.4%	28.2%	0.17
600	55.0	22.9%	28.5%		
600	60.0	22.1%	29.4%		
600	65.0	20.8%	30.3%		
600	70.0	19.1%	31.2%		

Table 2. Results by solving Rachford-Rice and comparison with experimental results

P [mm Hg]	T [ºC]	HO2 [mol/Lwateratm]	cAO2 [mol/m3water]	HN2 [mol/Lwateratm]	HN2 [atm]	cAN2 [mol/m3water]	XO2 (Z2)	XN2 (Z3)	Z1	P sat water (T) (mm Hg)
400	25	1.3172E-03	0.11065	6.4848E-04	3.5419E-04	0.20233	1.9916E-06	3.6418E-06	9.9999E-01	2.3686E+01
400	27.9	1.2549E-03	0.10541	6.2181E-04	3.3962E-04	0.19400	1.8974E-06	3.4920E-06	9.9999E-01	2.8107E+01
400	30	1.2123E-03	0.10184	6.0348E-04	3.2961E-04	0.18829	1.8330E-06	3.3891E-06	9.9999E-01	3.1740E+01
400	35	1.1188E-03	0.09398	5.6292E-04	3.0745E-04	0.17563	1.6916E-06	3.1613E-06	1.0000E+00	4.2071E+01
400	38.8	1.0544E-03	0.08857	5.3472E-04	2.9205E-04	0.16683	1.5942E-06	3.0030E-06	1.0000E+00	5.1759E+01
400	40	1.0351E-03	0.08695	5.2625E-04	2.8743E-04	0.16419	1.5651E-06	2.9554E-06	1.0000E+00	5.5193E+01
400	45	9.6008E-04	0.08065	4.9301E-04	2.6927E-04	0.15382	1.4516E-06	2.7687E-06	1.0000E+00	7.1705E+01
400	48	9.1871E-04	0.07717	4.7455E-04	2.5919E-04	0.14806	1.3891E-06	2.6650E-06	1.0000E+00	8.3523E+01
400	50	8.9253E-04	0.07497	4.6281E-04	2.5278E-04	0.14440	1.3495E-06	2.5991E-06	1.0000E+00	9.2300E+01
400	55	8.3159E-04	0.06985	4.3529E-04	2.3775E-04	0.13581	1.2574E-06	2.4446E-06	1.0000E+00	1.1778E+02
400	60	7.7645E-04	0.06522	4.1016E-04	2.2402E-04	0.12797	1.1740E-06	2.3035E-06	1.0000E+00	1.4904E+02
400	65	7.2644E-04	0.06102	3.8717E-04	2.1146E-04	0.12080	1.0984E-06	2.1743E-06	1.0000E+00	1.8712E+02
400	70	6.8097E-04	0.05720	3.6608E-04	1.9994E-04	0.11422	1.0296E-06	2.0559E-06	1.0000E+00	2.3317E+02
500	25	1.3172E-03	0.13831	6.4848E-04	3.5419E-04	0.25291	2.4895E-06	4.5523E-06	9.9999E-01	2.3686E+01
500	28.7	1.2384E-03	0.13004	6.1473E-04	3.3575E-04	0.23975	2.3406E-06	4.3154E-06	9.9999E-01	2.9446E+01
500	30	1.2123E-03	0.12730	6.0348E-04	3.2961E-04	0.23536	2.2913E-06	4.2364E-06	9.9999E-01	3.1740E+01
500	31.5	1.1832E-03	0.12423	5.9087E-04	3.2272E-04	0.23044	2.2362E-06	4.1479E-06	9.9999E-01	3.4579E+01
500	35	1.1188E-03	0.11747	5.6292E-04	3.0745E-04	0.21954	2.1145E-06	3.9517E-06	9.9999E-01	4.2071E+01
500	38.1	1.0659E-03	0.11192	5.3976E-04	2.9480E-04	0.21050	2.0145E-06	3.7891E-06	9.9999E-01	4.9842E+01
500	40	1.0351E-03	0.10869	5.2625E-04	2.8743E-04	0.20524	1.9564E-06	3.6942E-06	9.9999E-01	5.5193E+01

P [mm Hg]	T [ºC]	K1	К2	К3	V/F (Ψ)	x1		x2		x3	y1		y2		у3	y2 (dry)
400	25	5.9216E-02	7.9766E+04	1.6203E+05	5.4830E-06		1.0000		0.0000	0.0000		0.0592		0.250	0.69069	0.266
400	27.9	7.0268E-02	8.3727E+04	1.6898E+05	5.9547E-06		1.0000		0.0000	0.0000		0.0703		0.252	0.67801	0.271
400	30	7.9350E-02	8.6667E+04	1.7411E+05	6.2919E-06		1.0000		0.0000	0.0000		0.0794		0.253	0.66884	0.274
400	35	1.0518E-01	9.3913E+04	1.8665E+05	7.1912E-06		1.0000		0.0000	0.0000		0.1052		0.253	0.64149	0.283
400	38.8	1.2940E-01	9.9650E+04	1.9650E+05	7.9045E-06		1.0000		0.0000	0.0000		0.1294		0.251	0.61952	0.288
400	40	1.3798E-01	1.0150E+05	1.9966E+05	8.1478E-06		1.0000		0.0000	0.0000		0.1380		0.250	0.61186	0.290
400	45	1.7926E-01	1.0944E+05	2.1312E+05	9.2642E-06		1.0000		0.0000	0.0000		0.1793		0.245	0.57679	0.298
400	48	2.0881E-01	1.1437E+05	2.2141E+05	1.0072E-05		1.0000		0.0000	0.0000		0.2088		0.239	0.55180	0.303
400	50	2.3075E-01	1.1772E+05	2.2703E+05	1.0649E-05		1.0000		0.0000	0.0000		0.2308		0.235	0.53475	0.306
400	55	2.9444E-01	1.2635E+05	2.4138E+05	1.2469E-05		1.0000		0.0000	0.0000		0.2944		0.221	0.48460	0.313
400	60	3.7260E-01	1.3532E+05	2.5617E+05	1.4982E-05		1.0000		0.0000	0.0000		0.3726		0.201	0.42625	0.321
400	65	4.6780E-01	1.4464E+05	2.7138E+05	1.8813E-05		1.0000		0.0000	0.0000		0.4678		0.175	0.35781	0.329
400	70	5.8293E-01	1.5429E+05	2.8702E+05	2.5606E-05		1.0000		0.0000	0.0000		0.5829		0.140	0.27672	0.337
500	25	4.7373E-02	6.3813E+04	1.2962E+05	3.5059E-06		1.0000		0.0000	0.0000		0.0474		0.235	0.71741	0.247
500	28.7	5.8892E-02	6.7872E+04	1.3674E+05	4.1339E-06		1.0000		0.0000	0.0000		0.0589		0.239	0.70322	0.254
500	30	6.3480E-02	6.9334E+04	1.3929E+05	4.3694E-06		1.0000		0.0000	0.0000		0.0635		0.240	0.69702	0.256
500	31.5	6.9157E-02	7.1044E+04	1.4226E+05	4.6316E-06		1.0000		0.0000	0.0000		0.0692		0.241	0.69032	0.259
500	35	8.4142E-02	7.5130E+04	1.4932E+05	5.2549E-06		1.0000		0.0000	0.0000		0.0841		0.243	0.67352	0.265
500	38.1	9.9683E-02	7.8862E+04	1.5573E+05	5.8316E-06		1.0000		0.0000	0.0000		0.0997		0.243	0.65697	0.270
500	40	1.1039E-01	8.1202E+04	1.5973E+05	6.1882E-06		1.0000		0.0000	0.0000		0.1104		0.244	0.64664	0.274

		T								
P [mm Hg]	T [ºC]	HO2 [mol/Lwateratm]	cAO2 [mol/m3water]	HN2 [mol/Lwateratm]	HN2 [atm]	cAN2 [mol/m3water]	XO2 (Z2)	XN2 (Z3)	<b>Z1</b>	P sat water (T) (mm Hg)
500	44.5	9.6723E-04	0.10156	4.9619E-04	2.7101E-04	0.19352	1.8281E-06	3.4833E-06	9.9999E-01	6.9882E+01
500	45	9.6008E-04	0.10081	4.9301E-04	2.6927E-04	0.19227	1.8145E-06	3.4609E-06	9.9999E-01	7.1705E+01
500	50	8.9253E-04	0.09372	4.6281E-04	2.5278E-04	0.18049	1.6869E-06	3.2489E-06	1.0000E+00	9.2300E+01
500	55	8.3159E-04	0.08732	4.3529E-04	2.3775E-04	0.16976	1.5717E-06	3.0557E-06	1.0000E+00	1.1778E+02
500	60	7.7645E-04	0.08153	4.1016E-04	2.2402E-04	0.15996	1.4675E-06	2.8793E-06	1.0000E+00	1.4904E+02
500	65	7.2644E-04	0.07628	3.8717E-04	2.1146E-04	0.15100	1.3730E-06	2.7179E-06	1.0000E+00	1.8712E+02
500	67.7	7.0136E-04	0.07364	3.7555E-04	2.0512E-04	0.14647	1.3256E-06	2.6364E-06	1.0000E+00	2.1092E+02
500	70	6.8097E-04	0.07150	3.6608E-04	1.9994E-04	0.14277	1.2870E-06	2.5698E-06	1.0000E+00	2.3317E+02
600	25	1.3172E-03	0.16597	6.4848E-04	3.5419E-04	0.30349	2.9874E-06	5.4627E-06	9.9999E-01	2.3686E+01
600	30	1.2123E-03	0.15275	6.0348E-04	3.2961E-04	0.28243	2.7496E-06	5.0837E-06	9.9999E-01	3.1740E+01
600	35	1.1188E-03	0.14097	5.6292E-04	3.0745E-04	0.26345	2.5374E-06	4.7420E-06	9.9999E-01	4.2071E+01
600	40	1.0351E-03	0.13043	5.2625E-04	2.8743E-04	0.24628	2.3477E-06	4.4331E-06	9.9999E-01	5.5193E+01
600	42	1.0041E-03	0.12652	5.1257E-04	2.7995E-04	0.23988	2.2774E-06	4.3178E-06	9.9999E-01	6.1354E+01
600	45	9.6008E-04	0.12097	4.9301E-04	2.6927E-04	0.23073	2.1774E-06	4.1531E-06	9.9999E-01	7.1705E+01
600	45.8	9.4879E-04	0.11955	4.8798E-04	2.6653E-04	0.22838	2.1518E-06	4.1108E-06	9.9999E-01	7.4706E+01
600	50	8.9253E-04	0.11246	4.6281E-04	2.5278E-04	0.21659	2.0243E-06	3.8987E-06	9.9999E-01	9.2300E+01
600	54.2	8.4093E-04	0.10596	4.3952E-04	2.4006E-04	0.20570	1.9072E-06	3.7025E-06	9.9999E-01	1.1334E+02
600	55	8.3159E-04	0.10478	4.3529E-04	2.3775E-04	0.20372	1.8860E-06	3.6669E-06	9.9999E-01	1.1778E+02
600	60	7.7645E-04	0.09783	4.1016E-04	2.2402E-04	0.19196	1.7610E-06	3.4552E-06	9.9999E-01	1.4904E+02
600	65	7.2644E-04	0.09153	3.8717E-04	2.1146E-04	0.18119	1.6476E-06	3.2615E-06	1.0000E+00	1.8712E+02
600	70	6.8097E-04	0.08580	3.6608E-04	1.9994E-04	0.17132	1.5444E-06	3.0838E-06	1.0000E+00	2.3317E+02

P [mm Hg]	T [ºC]	К1	K2	КЗ	V/F (Ψ)	x1		x2		x3	y1	у2	2	у3	y2 (dry)
500	44.5	1.3976E-01	8.6904E+04	1.6940E+05	7.1011E-06		1.0000		0.0000	0.0000	0	.1398	0.242	0.61902	0.281
500	45	1.4341E-01	8.7551E+04	1.7049E+05	7.2247E-06		1.0000		0.0000	0.0000	0	.1434	0.242	0.61497	0.282
500	50	1.8460E-01	9.4177E+04	1.8162E+05	8.4068E-06		1.0000		0.0000	0.0000	0	.1846	0.237	0.57860	0.290
500	55	2.3555E-01	1.0108E+05	1.9310E+05	9.8363E-06		1.0000		0.0000	0.0000	0	.2356	0.228	0.53613	0.299
500	60	2.9808E-01	1.0826E+05	2.0493E+05	1.1667E-05		1.0000		0.0000	0.0000	0	.2981	0.216	0.48650	0.307
500	65	3.7424E-01	1.1571E+05	2.1710E+05	1.4176E-05		1.0000		0.0000	0.0000	0	.3742	0.197	0.42859	0.315
500	67.7	4.2184E-01	1.1985E+05	2.2382E+05	1.5987E-05		1.0000		0.0000	0.0000	0	.4218	0.185	0.39355	0.320
500	70	4.6635E-01	1.2343E+05	2.2961E+05	1.7942E-05		1.0000		0.0000	0.0000	0	.4663	0.173	0.36102	0.324
600	25	3.9477E-02	5.3177E+04	1.0802E+05	1.6220E-06		1.0000		0.0000	0.0000	0	.0395	0.221	0.73989	0.230
600	30	5.2900E-02	5.7778E+04	1.1607E+05	2.5592E-06		1.0000		0.0000	0.0000	0	.0529	0.227	0.72037	0.239
600	35	7.0118E-02	6.2608E+04	1.2443E+05	3.4832E-06		1.0000		0.0000	0.0000	0	.0701	0.232	0.69880	0.249
600	40	9.1988E-02	6.7669E+04	1.3311E+05	4.4371E-06		1.0000		0.0000	0.0000	0	.0920	0.235	0.67364	0.258
600	42	1.0226E-01	6.9757E+04	1.3666E+05	4.8201E-06		1.0000		0.0000	0.0000	0	.1023	0.235	0.66322	0.262
600	45	1.1951E-01	7.2959E+04	1.4208E+05	5.4356E-06		1.0000		0.0000	0.0000	0	.1195	0.235	0.64534	0.267
600	45.8	1.2451E-01	7.3827E+04	1.4354E+05	5.6056E-06		1.0000		0.0000	0.0000	0	.1245	0.235	0.64030	0.269
600	50	1.5383E-01	7.8481E+04	1.5135E+05	6.5364E-06		1.0000		0.0000	0.0000	0	.1538	0.234	0.61246	0.276
600	54.2	1.8889E-01	8.3297E+04	1.5937E+05	7.5792E-06		1.0000		0.0000	0.0000	0	.1889	0.230	0.58106	0.284
600	55	1.9629E-01	8.4232E+04	1.6092E+05	7.7933E-06		1.0000		0.0000	0.0000	0	.1963	0.229	0.57468	0.285
600	60	2.4840E-01	9.0214E+04	1.7078E+05	9.3105E-06		1.0000		0.0000	0.0000	0	.2484	0.221	0.53078	0.294
600	65	3.1186E-01	9.6424E+04	1.8092E+05	1.1247E-05		1.0000		0.0000	0.0000	0	.3119	0.208	0.47989	0.303
600	70	3.8862E-01	1.0286E+05	1.9134E+05	1.3896E-05		1.0000		0.0000	0.0000	0	.3886	0.191	0.42097	0.312

Table 3. Compilation of results of the general simulation

## 3 | Modelling



Figure 9. Graphical representation of theoretical and empirical data

# **CHAPTER 4: POSSIBLE APPLICATIONS**

## 1. Chemical industry

Industrially, oxygen is mainly used in metallurgy for the production of iron and steel, as well as for copper refining. Pure oxygen or oxygen-enriched air serves here on the one hand to reach high temperatures, on the other hand for the refining of the crude steel.

It is also used to remove undesired carbon, silicon, manganese and phosphorous deposits, which are oxidized and separated. In chemical processes, oxygen is mostly used for the oxidation of various basic materials such as the olefin oxidation of ethene to ethylene oxide and the partial oxidation of heavy oil and coal. Oxygen is also required to produce hydrogen and synthesis gas and the production of sulfuric and nitric acids.

Other important products obtained by oxidation with oxygen are acetylene, acetaldehyde, acetic acid, vinyl acetate and chlorine. In the glass industry, as well as in the welding and cutting of concrete, the oxygen serves to achieve the needed high temperatures. Oxygen is also used to get ozone, used as an oxidizing agent in fuel cells, and in semiconductor technology. In rocket technology, liquid oxygen is used as the oxidizing agent and is abbreviated by LOX (liquid oxygen). In environmental technology, effluents are freed from organic pollutants and toxins by the introduction of oxygen.

## 2. Ship engines

Environmental impact awareness of industrial applications is gaining more and more momentum. In Europe alone, the Institute for European Environmental Policy estimates the body of EU environmental law amounts to well over 500 Directives, Regulations and Decisions.

As a consequence, great effort is being put, among other areas, on improving the efficiency and pollution emitted by diesel engines. And oxygen enriched combustion is one of the attractive combustion technologies to control pollution and improve combustion in this type of engines. (Baskar & Senthilkumar, 2016).

An application for ship engines was proposed, considering ship engine model Wärtsilä 16V46F. Calculations were performed for this engine capable of delivering 26100HP at 100% capacity.



The following equation sums up the factors that contribute to the power delivered by an internal combustion engine:

$$P = \dot{m_f} H_L \eta_t;$$

Equation 2

Where:

P: power  $\dot{m}_f$ : mass flow of fuel  $H_L$ : heat power, dependent on the type of fuel introduced  $\eta_t$ : total efficiency, dependent on mechanical and thermal efficiency

The increase in oxygen concentration in the inlet air flow would improve efficiency in the following areas:

 Fuel flow: this is by far the main contribution. The power an engine is able to deliver is function of the quantity of fuel burned, which keeps a constant ratio with the oxygen (air) with which it reacts (keeping efficiency factors aside). The constraint here is the volume of the cylinder where the combustion takes place, in this case, 96.4L. Usually the volume occupied by air in the cylinder is more than 99% of the total volume. If the

#### 4 | Possible applications

quantity of air needed is lower because the concentration of oxygen is higher, this allows to introduce a larger volume of fuel, eventually delivering a higher power.

- Chemical efficiency, deemed thermal efficiency in Equation 2: the surface of contact among molecules of oxygen and of fuel will be larger given the higher oxygen concentration. This contribution is difficult to quantify without empirical analysis.
- Mechanical efficiency: for a given power, working with higher quantities of fuel entails reduction in rpm, which may decrease losses due to mechanical friction. This contribution is also difficult to quantify without empirical analysis.
- Exergy: energy recovery is more difficult if the energy of the exhausts is dispersed in a larger volume of gas. Higher oxygen concentration allows for a reduction in this volume and therefore a higher conservation of the available exergy.

Since the highest concentration achieved by the new proposed technique is about 25-29%, which is not a big difference from the 21% present in atmospheric air, the calculations are done supposing all the enriched air is directly introduced in the engine, and it is not contemplated the possibility of mixing enriched air with atmospheric air.

A flow of 33.3kg/s of air means 1.15kmol/s (or 0.86kmol/s of EA @28%). Given the results showed in Table 3, the relation V/F varies, but is always around  $10^{-5}$ . This would entail around  $10^{5}$  kilomoles of water every second, which translates into around **15.10<sup>5</sup> kg/s of water**.

Therefore, this application is deemed as unfeasible because of the large flows of water needed.

# 3. Medical application

## 3.1. Generic application

Injuries and many lung infections, as well as some cardiac diseases can lead to an oxygen deficiency (hypoxia) in the arteries and in the tissue of vital organs. For this reason, additional oxygen is often given to patients in emergency and intensive care medicine. In the case of self-breathing patients, the ambient air is enriched with oxygen using various probes and masks

In the case of artificially ventilated patients, the oxygen is admixed in the breathing apparatus. The effect of oxygen accumulation in the blood is measurable by means of pulse oximetry or by means of blood gas analysis.

For diseases with a severe chronic oxygen deficiency, both the quality of life and survival rate are improved by a long-term and daily long-term supply of oxygen.

The inhalation of 100% pure oxygen via a mask (7-15 lpm over 15-20 min) is the first choice for the acute treatment of cluster headache. Pure 100% oxygen can lead to problems an undesirable increase in brain activity in the hypothalamus. These negative effects are avoided by the addition of carbon dioxide.

## 3.2. Motivation

Among the more than 10 million children who die every year, most die from pneumonia or diarrhoea, preventable and curable illnesses (Black, Morris, & Bryce, 2003). In an acute context, pneumonia can eventually cause hypoxaemia, an abnormally low level of oxygen in blood.

Oxygen is carried inside the human body mainly by a protein called haemoglobin, transporting 20 ml of  $O_2/100$  ml of blood. When oxygen binds to hemoglobin, oxyhemoglobin (HbO<sub>2</sub>) is formed, while the deoxygenated form is called deoxyhemoglobin (Hb). The binding of oxygen to hemoglobin is reversible and depends on the partial pressure of oxygen in the blood.

The hemoglobin saturation is defined as the percentage ratio between oxygen content and maximum binding capacity. Arterial blood is usually saturated with oxygen at 97%, while venous blood is at 75%.

Figure 10 shows the relation between the partial pressure of oxygen in blood and the haemoglobin saturation previously defined (which is in turn a function of the actual quantity of oxygen being transported). An increase in temperature, caused for instance by a serious

infection such as pneumonia, makes the curve move to the right, and provided the sigmoidal shape of the curve, this entails a life-threatening massive drop in oxygen transport.



Figure 10. Curve of dissociation for the haemoglobin

One way to alleviate this effect is by artificially increasing the partial pressure of oxygen, which is achieved with the use of concentrated medical oxygen. However, in underdeveloped countries this is not available. A proposed solution is the use of portable concentrators that use PSA techniques to get enriched air. However, these devices require a maintenance schedule which is, again, difficult to be met in these countries.

The current proposal is going to be designed for the hospital Sounon-Sero located in Nikki (Benin). The population of Nikki is of around 150,000 inhabitants, however, this hospital is located at a crossroad between Nigeria, Burkina Faso and Benin, resulting in a served population of more than 300,000 people ("Hôpital Sounon Sero, Nikki | Site Medics Without Vacations," n.d.).

#### Geographical and economic context

Benin, and formerly Dahomey, is a country in West Africa. It is bordered by Togo to the West, Nigeria to the East, and Burkina Faso and Niger to the North. A majority of the population live on its small southern coastline on the Bight of Benin, part of the Gulf of Guinea in the northernmost tropical portion of the Atlantic Ocean.



Figure 11. Geographical location of Nikki

The capital of Benin is Porto-Novo, but the seat of government is in Cotonou, the country's largest city and economic capital. Benin covers an area of approximately 115,000 square kilometres (42,000 sq mi), with a population of approximately 9.98 million. Benin is a tropical, sub-Saharan nation, highly dependent on agriculture, with substantial employment and income arising from subsistence farming.

The official language of Benin is French. However, indigenous languages such as Fon and Yoruba, or Bariba in the north, are commonly spoken.

Benin is divided into 12 departments and subdivided into 77 communes. In 1999 the six former departments were divided into two halves, forming the current 12.

Nikki is one of the communes of the department of Borgou, it has a population of 150,000, but it also has a high population growth rate, and an area of about 3,000 km<sup>2</sup> (similar to the province of Álava in Spain, or Valle d'Aosta in Italy). The commune is divided into the *arrondissements* of Biro, Gnonkourokali, Ouénou, Sérékalé, Suya, Tasso and Nikki.

As for population, it is evenly distributed among all the villages but Nikki, which has a population of 70,000. Suya has around 8,000, and the others 15,000 people each.

As president of each of these *arrondissements* there is a Chef d'Arrondissement (CA) and as lord major of every *village*, a delegate democratically elected in elections held every 4 or 5 years (Gimeno, 2016).

## 3.3. Insights into medical oxygen therapy

As it was stated above, the main objective of oxygen therapy is to re-establish the adequate levels of oxygen to the body tissues. It is necessary to check the amount of oxygen in the blood with the help of a pulse oximeter, which measures the oxygen saturation, or a blood gas analysis, which is done by extracting arterial blood and analysed in laboratory to know the concentrations of gases in the sample: mainly by measuring the arterial pressure of oxygen, Pa<sub>02</sub>, and arterial carbon dioxide pressure, Pa<sub>co2</sub>).

In order to be able to prescribe oxygen therapy, it is necessary to comply with the following requirements:

- 1. Trained staff to take blood samples
- 2. Laboratory where the samples can be processed by trained laboratory staff

Excess oxygen in blood can generate oxygen poisoning, causing a fatal multiorgan failure.

The situations in which oxygen therapy necessary are the following (in bold those most frequently found in Nikki):

- 1. Arterial hypoxemia. It is the most frequent indication. It occurs in cases of:
  - a. Chronic obstructive pulmonary disease (COPD)
  - b. Asthma
  - c. Atelectasis
  - d. **Pneumonia**: respiratory infections are very common as seen in the hospital report
  - e. High altitude sickness
  - f. Interstitial pneumonitis: caused by fumes from the kitchens
  - g. Arteriovenous fistulas

## h. Pulmonary thromboembolisms

- 2. Tissue hypoxia without hypoxemia: Occurs in cases of:
  - a. Anemia
  - b. Cyanide poisoning
  - c. Hypermetabolic states

## d. Hemoglobinopathies

3. Special situations (where oxygen is recommended):

## a. Acute myocardial infarction (AMI)

b. Heart failure

## 4 | Possible applications

- c. Hypovolemic shock: bleeding from accidents or childbirth
- d. Carbon monoxide poisoning

#### Additional Considerations

Depending on the time it takes for them to appear, secondary effects of oxygen administration are classified as *early* and *late*. Among the *early* side effects are the following:

- Hypercapnia: it occurs in some patients who are already chronic CO2 retention when oxygen is administered at high doses, as it attenuates the stimulus that exerts on the respiratory center
- Atelectasis. The administration of oxygen at high concentrations (greater than 80%) for more than 24 hours causes denervation of the alveoli, which can lead to collapses in them by decreasing volume
- 3. Infections: Hygiene should be respected in the handling of the devices and in the maintenance of the same, in order to prevent infections secondary to their use. The use of nebulizers and humidifiers increases the risk of bacterial contamination.

## 3.4. Process flow diagram



Figure 12. Process Flow Diagram

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## 3.5. Demand sizing

It is important to keep in mind that the oxygen flow delivered to patients has to be kept under strict control within a given range because an overdose can result in and multiorgan failure, with fatal results.

However, the aim of this section is to make a preliminary feasibility analysis by testing oversized upper boundary conditions, therefore after all the mathematical operations the result has been rounded to larger numbers and all the parameters used have been slightly oversized.

## Identification of needs

The main illnesses found at Sounon-Sero are presented in the following table (Pascual, Rojo, & De Arístegui, 2015):

ILLNESS	2011	2012	2013	2014
MALARIA	4880	6047	5577	2419
UPPER RESPIRATORY TRACT INFECTION	627	1663	1610	820
HYPERTENSION	486	1182	1759	838
TRAUMATISM	715	771	708	434
DIABETES	156	352	497	280
ANAEMIA	914	136	103	110

Table 4. Illnesses at Sounon-Sero 2011-2014

There is no available information on the exact requirements of oxygen for the patients of Sounon-Sero.

Therefore, it is decided to perform two sizing approaches:

- 4. From the demand side: considering all patients with lung problems need the highest concentration of oxygen delivered by commercial oxygen concentrators 24/7, being aware that this figure will be over scaled.
- 5. From the supply side: considering the maximum capabilities of the equipment that could be used in the proposed context.

After both analyses are done, it will be decided which one represents the best approach.

#### Demand side

Regarding lung-related infections, these figures present large differences, so for safety reasons the highest figure will be chosen as basis of calculus for nominal conditions, rounding up to the nearest thousands (2000 patients).

The average duration of stay at Sounon-Sero changed from 4.0 to 4.8 days from 2011 to 2014. Again, rounding up for safety reasons, an average stay of 7 days will be considered.

The demand needs will therefore be (on a daily basis):

$$\frac{2000 patients * \frac{7 days}{patient}}{\frac{365 days}{year}} = 38.36 \approx 40 simultaneous spots of oxygen;$$

The average amount of air inhaled by a person is 7.5lpm (litres per minute), which means (considering 21% concentration of oxygen in air) an oxygen flow of 1.60lpm.

Designing for 40 spots, would entail an EA flow of 40\*7.5lpm=300lpm of EA.

$$P\dot{V} = nRT \rightarrow 1atm * 300lpm = \dot{n} * 0.082 * 298.15 \rightarrow \dot{n} = 12.27mol EA/min$$
;

#### Feasibility study

Considering the Results obtained in section 3.2, for a concentration of around 30%, the conditions need to be one of these:

Pressure (mm Hg)	Temperature ( <sup>o</sup> C)
400	48
500	55
600	65

Table 5. Conditions that produce 30% oxygen concentration of EA

Taking into account the context where the system will be installed, the critical point is electricity access, used to produce vacuum since temperature can be increased directly with sun radiation. Therefore, the recommended combination would be the latter.

For these conditions, the ratio V/F is  $1.1247 \cdot 10^{-5}$ . Given that V is 12.27 mol/min, this implies F is 1090.96 kmol/min, translating into 22336.8 kg/min or 372.28 kg/s, which is a very large flow.

## Supply side

It was considered that the bottleneck from the supply side is caused by the power of the on field available water pumps. These are irrigation pumps. It was found that an average diesel-powered irrigation pump of 22HP can lift 65m<sup>3</sup>/h of water 25m (Kobuta KDZN80-65-25). This translates in 18kg/s or 1kmol/s.

Tag			AIR	RAINWATER	EXCESS_AIR	03	08	02	10	EA_COND	06	07
Total S	tream Properties											
Rate		G-MOL/MIN	1800000.000	79178.870	1878762.810	59998.447	417.623	138761.257	417.623	417.623	59998.447	59998.447
		G/MIN	51930713.974	1426429.494	53349639.397	1080897.453	7532.230	2499822.877	7532.230	7532.230	1080897.453	1080897.453
Std. Lic	uid Rate	LIT/MIN	59895.733	1427.837	61316.057	1081.967	7.542	2502.290	7.542	7.542	1081.967	1081.967
Total Adj.Liq.Vol.Rate		LIT/MIN	154546.041	1423.523	155962.034	1078.736	7.558	2494.729	7.558	7.558	1078.736	1078.736
Total A	dj.Vap.Vol. Rate	LIT/MIN	40345185.853	1774714.569	42110574.863	1344804.720	9360.594	3110193.730	9360.594	9360.594	1344804.720	1344804.720
Tempe	rature	°C	30.000	30.000	30.000	30.000	76.150	30.000	163.742	10.000	60.979	80.000
Pressu	re	ATM	1.000	1.000	1.000	1.000	0.400	1.000	1.000	1.000	2.000	2.000
Molecu	ılar Weight		28.850	18.015	28.396	18.015	18.036	18.015	18.036	18.036	18.015	18.015
Enthalp	ру	M*KJ/MIN	2.096	0.180	5.715	0.136	0.020	0.315	0.021	0.000	0.276	0.362
		КJ/G	0.040	0.126	0.107	0.126	2.635	0.126	2.760	0.042	0.255	0.335
Total L	iquid Fraction		0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	0.9982	1.0000	1.0000
Reduce	ed Temp.		2.2938	0.4685	1.9717	0.4685	0.5405	0.4685	0.6761	0.4382	0.5163	0.5457
	Pres.		0.0271	0.0046	0.0225	0.0046	0.0018	0.0046	0.0046	0.0046	0.0092	0.0092
Acentri	ic Factor		0.0345	0.3449	0.0475	0.3449	0.3443	0.3449	0.3443	0.3443	0.3449	0.3449
Watso	n K (UOPK)		6.027	8.758	6.100	8.758	8.749	8.758	8.749	8.749	8.758	8.758
Standa	rd Liquid Density	G/LIT	867.019	999.014	870.076	999.012	998.709	999.014	998.709	998.709	999.012	999.012
	Specific Gravity		0.8679	1.0000	0.8709	1.0000	0.9997	1.0000	0.9997	0.9997	1.0000	1.0000
API Gravity			31.542	10.000	30.969	10.000	10.043	10.000	10.043	10.043	10.000	10.000
Total A	Total Adj. Liq. Density G/LIT		336.021	1002.042	342.068	1002.003	996.538	1002.042	996.538	996.538	1002.003	1002.003
Latent	Latent Heat KJ/		n/a	n/a	n/a	n/a	n/a	n/a	n/a	1.706	n/a	n/a

Stream Name			EA	WASTE	07A	09	11	05	01	04	MIXAIR	ENDPROD
Total St	tream Properties											
Rate		G-MOL/MIN	0.762	416.861	59998.447	59580.824	59580.824	59580.824	59580.824	59998.447	1.111	1.873
		G/MIN	22.270	7509.960	1080897.453	1073365.223	1073365.224	1073365.224	1073365.224	1080897.453	32.057	54.327
Std. Liq	uid Rate	LIT/MIN	0.025	7.517	1081.967	1074.425	1074.425	1074.425	1074.425	1081.967	0.037	0.062
Total Adj.Liq.Vol.Rate		LIT/MIN	0.063	7.495	1078.736	1071.178	1071.178	1071.178	1071.178	1078.736	0.095	0.159
Total A	dj.Vap.Vol. Rate	LIT/MIN	17.084	9343.511	1344804.720	1335444.126	1335444.127	1335444.127	1335444.127	1344804.720	24.905	41.989
Tempe	rature	₽C	10.000	10.000	76.150	76.150	76.165	45.024	30.000	30.024	10.000	10.000
Pressur	е	ATM	1.000	1.000	0.400	0.400	1.000	1.000	1.000	2.000	1.000	1.000
Molecu	ılar Weight	·	29.219	18.016	18.015	18.015	18.015	18.015	18.015	18.015	28.850	29.000
Enthalp	у	M*KJ/MIN	0.000	0.000	0.362	0.342	0.342	0.203	0.135	0.136	0.000	0.000
		KJ/G	0.020	0.042	0.335	0.319	0.319	0.189	0.126	0.126	0.001	0.009
Total Li	quid Fraction		0.0000	1.0000	0.9930	1.0000	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000
Reduce	d Temp.		1.9946	0.4376	0.5398	0.5398	0.5398	0.4917	0.4685	0.4685	2.1425	2.0797
	Pres.		0.0046	0.0018	0.0018	0.0046	0.0046	0.0046	0.0092	0.0271	0.0259	0.0092
Acentri	c Factor		0.0363	0.3449	0.3449	0.3449	0.3449	0.3449	0.3449	0.3449	0.0345	0.0352
Watsor	n K (UOPK)		5.830	8.757	8.758	8.758	8.758	8.758	8.758	8.758	6.027	5.946
Standa	rd Liquid Density	G/LIT	905.832	999.013	999.012	999.014	999.014	999.014	999.014	999.012	867.019	882.520
	Specific Gravity		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.8679	0.8834	1.0000
	API Gravity		10.000	10.000	10.000	10.000	10.000	10.000	10.000	31.542	28.678	10.000
Total A	Total Adj. Liq. Density G/LIT		351.724	1001.986	1002.003	1002.042	1002.042	1002.042	1002.042	1002.003	336.021	342.285
Latent	Heat	KJ/G	n/a	n/a	2.320	n/a	n/a	n/a	n/a	n/a	n/a	n/a

#### 4 | Possible applications

#### Pipe Sizing

To calculate the diameter of the pipes the following criteria have been used:

For liquids:

- 6. Pump suction:
  - Bubble point: DP < 0.5 bar/km , u < 1 m/s
  - $\circ$  Undercooled: DP < 2 bar/km , u < 1.5 m/s
- 7. Impulsion: DP < 5 bar/km , u < 3 m/s
- 8. Gravity: DP < 0.3 bar/km , u < 0.5 m/s

For gases:  $DP < 0.5 * P^{0.5}$ , P |=| bara, DP |=| bar/km P < 10 bara  $\rightarrow u < 30$  m/s P > 10 bara  $\rightarrow u < 60$  m/s

Where: DP: permissible loss of pressure every 1000km u: speed

The equation of loss of pressure being:

$$(-\Delta P) = f \frac{L}{D} \frac{\rho u^2}{2};$$

Equation 3. Loss of pressure

And the factor friction is determined by explicit correlations such as the Chen's equation:

For turbulent flow (Re>4200):

$$\frac{1}{\sqrt{f}} = 2 \cdot \log_{10} \left[ \frac{\left(\frac{\varepsilon}{D}\right)}{3.7065} - \frac{5.0452}{\text{Re}} \cdot \log_{10} \left[ \frac{\left(\frac{\varepsilon}{D}\right)^{1.1098}}{2.8257} + \frac{5.8506}{\text{Re}^{0.8981}} \right] \right]$$

Equation 4. Chen's equation for turbulent flow

And for laminar flow (Re<2100):

$$f=\frac{64}{Re};$$

Equation 5. Chen's equation for laminar flow

The results are presented in the following table:

Тад	Temp	Press	Mass flow	OD	Sch	Phase	Cond	Delta P perm	Delta P		Veloc	Flow	G- design	Density	Visc	ID	Re	Flow Reg	E/D	f
	°C	atm	kg/s	(in)				bar/km	bar/km		(m/s)	(m³/h)	(kg/h)	(kg/m <sup>3</sup> )	(cp)	(in)				
01	30.00	1.00	17.89	6	40	Liquid	IMP	5.00	0.931	0	1.20	64.84	64402	993.2	0.820	5.4	201117	TURB.	0.00033	0.018
02	30.00	1.00	41.66	12	40	Liquid	GRV	0.30	0.123	0	0.65	151.02	149989	993.2	0.820	11.2	226509	TURB.	0.00016	0.017
03	30.00	1.00	18.01	8	40	Liquid	SUC	0.50	0.211	0	0.66	65.30	64854	993.2	0.820	7.4	149787	TURB.	0.00025	0.018
04	30.02	2.00	18.01	6	40	Liquid	IMP	5.00	0.943	0	1.21	65.30	64854	993.2	0.819	5.4	202638	TURB.	0.00033	0.018
05	45.02	1.00	17.89	6	40	Liquid	IMP	5.00	0.908	0	1.21	65.23	64402	987.4	0.611	5.4	269690	TURB.	0.00033	0.017
06	60.98	2.00	18.01	6	40	Liquid	IMP	5.00	0.905	0	1.23	66.17	64854	980.0	0.467	5.4	355488	TURB.	0.00033	0.017
07	80.00	2.00	18.01	6	40	Liquid	IMP	5.00	0.896	0	1.24	66.87	64854	969.9	0.355	5.4	467074	TURB.	0.00033	0.017
08	76.15	0.40	0.13	6	40	Vapor	GAS	0.59	0.198	0	33.26	1795.53	452	0.252	0.012	5.4	99443	TURB.	0.00033	0.020
09	76.15	0.40	17.89	8	40	Liquid	SUC	0.50	0.193	0	0.67	66.25	64402	972.1	0.374	7.4	325805	TURB.	0.00025	0.017
10	163.74	1.00	0.13	6	40	Vapor	GAS	0.71	0.103	0	16.64	898.31	452	0.503	0.015	5.4	77364	TURB.	0.00033	0.020
11	76.16	1.00	17.89	6	40	Liquid	IMP	5.00	0.885	0	1.23	66.25	64402	972.1	0.374	5.4	440625	TURB.	0.00033	0.017

Table 6. Pipe sizing

4 | Possible applications

# **CHAPTER 5: ECONOMIC ANALYSIS**

## 1. Incremental cost functions

## 1.1. Chemical industry

The total cost will be calculated based on (Turton, 2012), which means that the costs calculated will have to be updated with the CEPCI index.

Recapitulating the objectives, the comparison among methods will be carried out with either incremental or decremental costs, but not accounting for sunk or common costs to all methods:

	ΔСΑΡΕΧ	$\Delta OPEX_{raw material}$	
M-1	0	$f(O_2 \text{ price, quantity})$ $f_3$	0
M-2	f(incremental volume, equipment price) f <sub>1</sub>	0	f(energy price, [O <sub>2</sub> ], quantity) f <sub>4</sub>
M-3	f(incremental volume, equipment price) f <sub>2</sub>	0	f(energy price, [O <sub>2</sub> ], quantity) f <sub>5</sub>

Let's start analysing operational costs:

For the first cost function, the main additional cost associated with capital expenditure is that of larger compressors.

According to (Turton, 2012), the extra capacity for a centrifugal blower has an economies of scale diminishing factor of 0,6:

$$\frac{c_a}{c_b} = \left(\frac{A_a}{A_b}\right)^n \to c_a = 2,55c_b;$$

And, given the information on (Turton, 2012), the required capital expenditure per cubic meter of gas blowed every second is \$40000, entailing incremental costs of:

$$f_1[\$] = 1,55 * 40000 = 62000;$$

Assume an industry with needs of oxygen supply of 1 stdm<sup>3</sup>/s. Given the average price of industrial oxygen:

$$f_3[\frac{\epsilon}{s}] = p;$$

Supposing an average operation of 250 days a year and 24 hours a day, this gives 6000 hours a year.

$$f_3\left[\frac{\epsilon}{y}\right] = p * 6000 * 3600;$$

Now, if an industry with needs of 1 stdm<sup>3</sup>/s is fed with normal air, the extra gas quantity to be compressed will be (1/0.21-1) stdm<sup>3</sup>/s, provided an average concentration of oxygen of 21%. The work this compression entails is the following:

$$W = \int_{V_1}^{V_2} P(V) dV = \int_{V_1}^{V_2} \frac{nRT}{V} dV \to P = \dot{n}RT \ln\left(\frac{V_2}{V_1}\right) = 40,90 * 8,314 * 298,15 * \ln(0,25)$$
$$= 140,53kW$$

Supposing an average operation of 250 days a year and 24 hours a day, this gives 6000 hours a year.

The average price of electricity is considered to be 0.15€/kWh according to the Italian Energy Authority Autorità per l'energia elettrica, il gas e il sistema idrico.

$$f_4\left[\frac{\notin}{y}\right] = 0,15 * 140,53 * 6000 = 126477;$$

# 2. List of equipment and CAPEX estimation

## 2.1. Medical application

	ΔСΑΡΕΧ		
M-1	f(incremental volume, equipment price) $f_1$	0	f(energy price, [O <sub>2</sub> ], quantity) f <sub>4</sub>
M-2	f(incremental volume, equipment price) $f_2$	0	f(energy price, [O <sub>2</sub> ], quantity) f <sub>5</sub>

## 2.2. Shell and tube heat exchanger

The exchanged heat is the following:



 $q = \dot{m}c_p \Delta T = 18 * 4.18 * 31 = 2332kW.$ 

The recommended value for the global coefficient U is 800-1500W/m<sup>2</sup> C for water flowing through both the shell and the tubes. An intermediate value of 1000W/m<sup>2</sup> C will be considered.

For counter-current flow, Figure 14, the logarithmic mean temperature is given by (R. K. SINNOTT, 2005):

$$\Delta T_m = \Delta T_{Ln} = \frac{\Delta T_1 - \Delta T_2}{\ln \frac{\Delta T_1}{\Delta T_2}} = \frac{15 - 15.186}{\ln \left(\frac{15}{15.186}\right)} = 15.092^{\circ}C_{2}$$

Applying the equation for heat transfer:

$$q = US\Delta T_m \to S = \frac{2332000}{15.092 * 1000} = 154.52m^2;$$

Which translates into a cost of around \$250/m<sup>2</sup> (Figure 15), implying a total cost of **\$38630**.



Figure 14. Shell and tubes heat exchanger scheme



#### 2.3. Flash tank

The sizing of the flash tank will be done following the proposed method in (Wankat, 2011).

Firstly, the permissible vapor velocity is calculated:

$$u_{perm} = K_{drum} \sqrt{\frac{\rho_L - \rho_V}{\rho_V}};$$

Equation 6

Where

$$K_{drum} = e^{A + B \ln F_{lv} + C (\ln F_{lv})^2 + D (\ln F_{lv})^3 + E (\ln F_{lv})^4};$$

Equation 7

The constants A to E are defined in (Blackwell, 2003), and

$$F_{lv} = \frac{W_L}{W_V} \sqrt{\frac{\rho_V}{\rho_L}};$$

Equation 8

Being  $W_L$  and  $W_V$  the liquid and vapor flow rates in weight units per hour.

$$F_{lv} = \frac{18}{0.1255} \sqrt{\frac{0.252}{972.14}} = 2.31;$$
  

$$K_{drum} = 0.0672;$$
  

$$u_{perm} = 0.0672 \sqrt{\frac{972.14 - 0.252}{0.252}} = 4.17 ft/s;$$

From this data, the cross-sectional area can be calculated as:

$$A_{c} = \frac{V\left[\frac{lbmol}{h}\right] * MW_{V}\left[\frac{lbm}{lbmol}\right]}{u_{perm}\left[\frac{ft}{s}\right] * 3600 * \rho_{V}\left[\frac{lbm}{ft^{3}}\right]} = \frac{997.64}{4.17 * 3600 * 0.0157} = 4.21ft^{2} \rightarrow r = 1.15ft$$
$$= 35.31cm;$$

Rounding to the next integer, diameter will be 3ft.

As rule of thumb, h/D must be 3.0-5.0. Therefore, in the worst case, h will be 15ft, and volume of  $3m^3$ .

The cost of which being:

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10} A + K_3 [\log_{10} A]^2;$$
Equation 9

Where A is the capacity of the equipment, and the constants  $K_i$  are considered such of a vertical process vessel found in (Turton, 2012):

$$\log_{10} C_p^0 = 3.4974 + 0.4485 \log_{10} 3 + 0.1074 [\log_{10} 3]^2 = 3.4974 + 0.2140 + 0.0244$$
  
= 3.7358 \rightarrow C\_p^0 = \$5443;

2.4. Solar heat exchanger

The exchanged heat is the following:

$$q = \dot{m}c_p \Delta T = 18 * 4.18 * 19 = 1430 kW.$$

The sizing of the solar heater will be calculated assuming a single pipe exposed to the sunlight that heats up to 90°C.

The heat transfer coefficient is calculated with the Dittus-Bölter equation:

$$Nu = 0.023 * Re^{0.8} * Pr^{0.4}$$

Equation 10. Dittus-Bölter Equation

Applying the equation for heat transfer:

$$\Delta T_m = \Delta T_{Ln} = \frac{\Delta T_1 - \Delta T_2}{\ln \frac{\Delta T_1}{\Delta T_2}} = \frac{29 - 10}{\ln \left(\frac{29}{10}\right)} = 17.85^{\circ}C$$

$$q = US\Delta T_m \to S = \frac{1430000}{4659.64 * 17.85} = 17.19m^2;$$

Given the diameter considered, the length of the tubes will have to be:

$$\frac{17.19m^2}{\pi * 0.137} = 39.95m = 131.05ft$$

The cost of the pipe is given by (Turton, 2012):

$$PC_{pipe} = 10 * d_{pipe} + 2 * d_{pipe}^{1.4} = 84.57$$
feet  $\rightarrow$  \$11084

Now, let's calculate, given the average solar radiation, the necessary surface to be exposed to collect the necessary amount of power.



Figure 16. Solar radiation in Africa

$$S = \frac{1430kW}{5.5kWh/(m^2d) * 1d/24h} = 6240m^2;$$

One of the main parameters that define parabolic troughs is the geometrical concentration ratio, whose maximal value in real systems, accepting the projected absorber tube area as  $A_{ap,r}$ , is 82. (Günther, Joemann, & Csambor, 2011):





Therefore, it is possible to assume one of the sides of the projected reflective surface to be 2m, constraint given by local manufacturing capabilities. This entails a mirror length of 3140m.

The average cost per square meter of trough is 220€ (Morin, 2004), what would entail a total cost of **1381600€**. The cost of the pipe should be updated given the new distance.

$$3140m * 3.28 \frac{ft}{m} * \frac{\$84.57\$}{ft} = \$871000 = 1067598 \notin (CEPCI updated);$$

Rendering a total cost of **2.5M€**.

However, this is a very large figure and an alternative heating method is considered, a hot water heater, whose cost can be estimated with Equation 9:

$$log_{10} C_p^0 = 2.0829 + 0.9074 log_{10} 1430 - 0.0243 [log_{10} 1430]^2$$
  
= 2.0829 + 2.8631 - 0.2419 = 4.7040 →  $C_p^0 =$ \$50590  
= 62010€ (CEPCI updated);

In this case OPEX will not be negligible in comparison with the CAPEX:

For every operating journey (considering 12h/day of powerful sunlight).

$$\frac{1430kW}{43000kJ/kg} * 12h * \frac{3600s}{h} = 1436kg \text{ of diesel/operating journey};$$

$$1436kg \text{ diesel} = 1690l \text{ diesel} = 1320 \notin \text{op. journey}$$

It has been assumed a price of 0.78€/L, using the 2012 benchmark results from the German Development Agency.



It can be seen that after 5 years the solar heater is a more cost-efficient alternative.

## 2.5. Compressor

The volumetric flow of air is going to be 0.171std m<sup>3</sup>/s, which entails a cost of around **\$10000** extrapolating from the curve in Figure 18:



Figure 18. Purchased equipment cost of a compressor

## 2.6. Water tank (x2)

Based on the actual cost of construction of water tanks developed by OAN International in 2016, it can be assumed a cost of each water tank of 3000€.

## 2.7. Pump (x2)

The cost of the pump has been taken from the retail website www.alibaba.com.

## 2.8. Summary and cost updates

Concept	Cost (\$)	CEPCI	Cost (\$)	Cost (€)	
			CEPCI updated	1€ = 1.12\$	
			545 – 07/2016		
Shell and tube exchanger	38630	397	53030	47350	
Flash tank	5443	397	7473	6675	
Solar heat exchanger	-	-	-	2500000	
Compressor	10000	500	10900	9735	
Water tank	-	-	-	6000	
Pump	-	-	3000	2680	
TOTAL (€)	-	-	-	2572440	

# 3. Comparative with traditional equipment

Following the incremental cost functions set forth at the beginning of this chapter, this method will be compared with an already existing alternative.

The alternative would be to use a domestic oxygen concentrator such the *DeVilbiss Oxygen Concentrator 5 Liter*, that produces a flow of 5lpm of oxygen at 90% purity, making it possible to produce an airflow of 15lpm of EA at 30% oxygen concentration, similar to the enriched air production modelled along the development of this project.

The cost of this equipment was found to be around \$600/unit. It consumes 310W when used at design conditions. This electricity would have to be supplied by an auxiliary generator. The design has been based on the *Honda EU2000i*, that can provide up to 2000W, and when used at 25% of maximum capacity lasts for 8 hours. The operating journey was considered to be 10 hours for the preceding calculations, and so will be for these. The tank has a capacity of 1 gallon, which translates into 3.6litres.

In order to be used for 10 hours, the consumption will be 4.5 litres. The cost of this equipment was found to be around \$1000/unit. Using the same cost for diesel as for the preceding sections, the cost for every operating journey will be  $4.5 * 0.78 = 3.51 \notin$  operating journey.

A priori, the differences in cost seems huge. The CAPEX of the new alternative will be compared with the CAPEX+OPEX of the traditional method. If there is already a big difference, the alternative method must be discarded.

It has been considered a 100% replacement of the equipment (additional CapEx) every three years.

The simulation was done for 30 years of operation.



Figure 19. Cost comparison alternative-traditional

It can be concluded that the process is not more efficient that the traditional approaches.

Besides, even if the solar heater is not considered, that involves 95% of the cost of the equipment, after 30 years of operation it does not present any cost efficiency compared with the traditional method.



Figure 20. Cost comparison alternative (without solar concentrator)-traditional

It has been modelled an innovative process for the production of oxygen enriched air by desorbing the oxygen contained in a stream of water. Afterwards, an analysis of possible applications for this process has been carried out.

Three main scenarios have been identified: chemical industry, ship propulsion and healthcare industry. The high water flows necessary for the first two scenarios make its construction unfeasible. The application to the healthcare industry shows needs of water flow are feasible figures and a case study has been developed for a hospital in Benin (Africa).

In terms of design, the demand sizing has been done considering as bottleneck the maximum local water pumping capabilities, which are provided by irrigation pumps. It has been shown that the proposal is far less cost-efficient than the traditional PSA separation method considering a time-frame of 30 years of operation for the facilities. It is remarkable that the cost dedicated to heating water represent more than 95% in capital expenditure, so there is potential to open a new path of research in an economic solution that makes this process attractive.

In terms of next steps, five main points have been identified for future development:

- 1. More precise demand sizing: given the lack of information, the demand has been sized considering as bottleneck local pumping capabilities. A deeper on field study in hospitals is necessary to assess whether this forecast is in keeping with actual requirements.
- 2. More precise budget forecast: the method used to calculate capital expenditures has been extrapolated from mathematical models based on empirical information from Europe and USA. Price levels in Africa are far lower and therefore on field research on local prices with domestic solutions and production capabilities is to be carried out to get a more precise budget.
- 3. Analysis of the water heating process: as earlier stated, this part of the system accounts for more than 90% of the capital expenditure for a solar system, and provides similar results when both capital and operational costs are considered for a diesel heater. But the budget for this project has been done considering commercial solutions already existing in Europe. Therefore, it could be possible to design a system of solar parabolical troughs with local materials that might plummet the capital expenditure.

- 4. Analysis of other substances for oxygen desorption: maximum solubility of oxygen in water is still extremely low, this causes required water flows to be massive. The use of other substances could be considered to decrease this necessary mass flow.
- 5. Study of process performance at different operating conditions. All the simulations were carried out considering the water was at equilibrium at atmospheric pressure and then oxygen was desorbed with lower-than-atmospheric pressures. An alternative would be to make the water reach the equilibrium at higher-than-atmospheric pressures and desorb oxygen at atmospheric pressure.

- Baskar, P., & Senthilkumar, A. (2016). Effects of oxygen enriched combustion on pollution and performance characteristics of a diesel engine. *Engineering Science and Technology, an International Journal*, 19(1), 438–443. http://doi.org/10.1016/j.jestch.2015.08.011
- Black, R. E., Morris, S. S., & Bryce, J. (2003). Where and why are 10 million children dying every year? *The Lancet*, *361*(9376), 2226–2234. http://doi.org/10.1016/S0140-6736(03)13779-8
- Blackwell, W. (2003). *Chemical Process Design on a Programmable Calculator*. New York: McGraw-Hill.
- Dobson, M. B. (2001). Oxygen concentrators and cylinders. The International Journal of Tuberculosis and Lung Disease : The Official Journal of the International Union against Tuberculosis and Lung Disease, 5(6), 520–3. Retrieved from http://www.ncbi.nlm.nih.gov/pubmed/11409577
- Emsley, J. (2001). *Nature's Building Blocks: An A-Z Guide to the Elements*. Oxford: Oxford University Press.
- Galli, F., Comazzi, A., Previtali, D., Manenti, F., Bozzano, G., Bianchi, C. L., & Pirola, C. (2016).
   Production of oxygen-enriched air via desorption from water: Experimental data, simulations and economic assessment. *Computers and Chemical Engineering*. http://doi.org/10.1016/j.compchemeng.2016.07.031
- Gimeno, A. (OAN I. (2016). Informe Anual OAN International 2016. Madrid (Spain).
- Günther, M., Joemann, M., & Csambor, S. (2011). Advanced CSP Teaching Materials Chapter 5 Parabolic Trough Technology Authors. *2011*, 1–43.
- Hôpital Sounon Sero, Nikki | Site Medics Without Vacations. (n.d.). Retrieved June 4, 2017, from http://www.msv.be/hospital/hôpital-sounon-sero-nikki
- Morin, G. (2004). Technologievergleich im Vergleich.
- Pascual, Á., Rojo, M. Á., & De Arístegui, J. (2015). *Informe Biosanitario OAN International*. Madrid (Spain).
- R. K. SINNOTT. (2005). Coulson Richardson's Chemical Engineering Vol.6 Chemical Engineering Design 4th Edition, volume 6. http://doi.org/10.1017/CBO9781107415324.004

Reinhardt, H.-J. (2015). Oxygen enrichment for intensification of air oxidation reactions. Linde.

Robert, R. (2011). Making Space Safer with Electrolysis. Retrieved March 11, 2017, from https://www.asme.org/engineering-topics/articles/aerospace-defense/making-space-safer-with-electrolysis

Springmann, H. (1978). United States Patent [ 191. USA.

Timmerhaus, K. D. (1961). *Advances in Cryogenic Engineering*. Colorado: Springer Science+Business Media.

Turton, R. (2012). Analysis, Synthesis and Design of Chemical Processes (4th ed.). Prentice Hall.

Wankat, P. C. (2011). Separation process engineering : includes mass transfer analysis.