MOTORVALLEY UNIVERSITY OF EMILIA ROMAGNA

ADVANCED AUTOMOTIVE ENGINEERING

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MASTER DEGREE THESIS

MODELLING OF A REACTOR FOR H2 PRODUCTION FROM Al IN NaOH SOLUTION FOR VEHICLE APPLICATIONS

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Alla mia famiglia sparsa per l'Italia.

Contents

Abstract

This thesis presents the design process of a hydrogen production system to be used for both stationary applications and onboard use in moving vehicles, aimed at the generation of clean energy through fuel cell technology without the problems related to hydrogen storage.

Introduction

The consequences of the pollution caused by the human activity on heart have been studied for years, nevertheless the causes have not been solved and the need for actions that can improve our society and lead it to a sustainable equilibrium is higher than ever.

Indeed the impact of the climate and environmental problems experienced in the world with the industrial revolution has prominently begun to be felt today, and the consequences of climate change on the environment and public health have now become visible. The increase in greenhouse gas emissions resulting from human activities, which is the main cause of global climate change, caused the global surface temperature to be 1.1 $^{\circ}C$ higher between 2011 and 2020 compared to 1850–1900. [14]

In parallel with the environmental problem caused by the industries and the human activities in general, the urgency for a transition to different kinds of energy has increased significantly with technological developments together with the recent global geopolitical situation. Indeed the consequent increasing of concerns about energy security is leading many countries to more aggressive energy policies.

One of the main causes of the global warning can be tracked down to the *Greenhouse Gases* , and in particular to the CO_2 emissions.

As a matter of fact the dangerous trend of constant rise in surface and ocean temperatures worldwide, generally known as *global warming*, is caused by the build-up of CO_2 in the atmosphere, which traps the infrared radiation released from the Earth's surface after sunlight is absorbed. [25]

In this context the topic of this thesis is the study of a system to use an energy medium different to the traditional ones to generate clean energy that can be exploited for a dual use, both for stationary energy usage and on board moving vehicles: **Hydrogen**.

Chapter 1

Introduction to Hydrogen

Hydrogen is the most abundant element in the observable universe. It forms up to 75% of matter, by mass, and more than 90% by number of atoms in the Milky Way Galaxy. In our solar system Jupiter and Saturn are composed of about 80% hydrogen and the Sun by 90%. [22]

1.1 Hydrogen characteristics

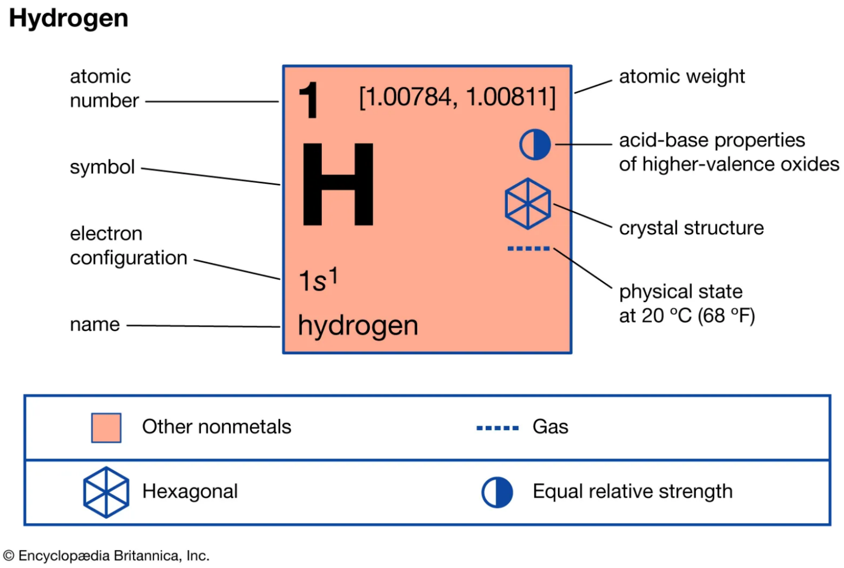


Figure 1.1: Hydrogen periodic table [9]

Hydrogen (that literally means «water generator») is the first chemical element in the periodic table. Beyond being the most abundant element in the whole universe it is also the lightest, has atomic number 1 and its symbol is H.

Hydrogen is consider a vector of energy and not an energy source because, despite it can be obtained in many ways, it is not available in nature in usable quantities. Consequently is used as a vector to transport and store energy for subsequent use. Furthermore it's formed by two atoms and it's necessary to use energy to brake their bounds to isolate them to obtain pure hydrogen.

Hydrogen main characteristics are:

- Under normal conditions it is a colourless, very light, odourless gas.
- It's non toxic and non corrosive.
- Has a density way lower than that of air thus in case of dispersion in open atmosphere it goes away very fast avoiding accumulations and consequent problems.
- When liquid, it is colourless, clear.
- T_s boiling point is at - 252,7 C.
- It has a big flammability range (between 4% and 75 %).
- The auto-ignition temperature of hydrogen is twice that of gasoline vapour.
- The molecule is very stable.

As a matter of fact the use of the hydrogen not only it's important for the environment and the purpose of reducing the harmful emission, but also it can have a pivotal role in the reduction of the dependency of a country on foreign oil or other energy sources.

1.2 Hydrogen production

Hydrogen is not the only fuel that can be used in a fuel cell but is the most interesting because it can be produced in many different ways [16] as shown also in the following figure1.2 and because the only product of the reaction is pure water.

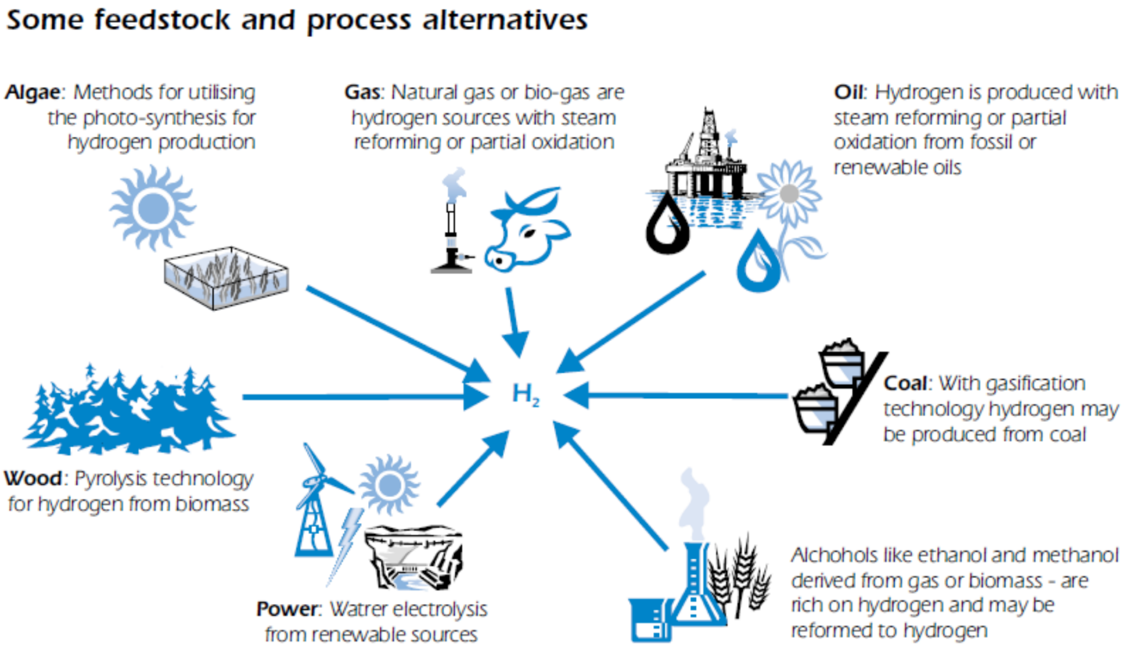


Figure 1.2: Hydrogen production techniques [16]

Based on the way it is produced commonly, the following names are designated:

- **’Black’ hydrogen** if it is produced from fossil fuels, without capture of CO_2 emissions from the process;
- **‘Grey’ hydrogen** if it is produced with partial sequestration of CO_2 emissions;
- **‘Blue’ hydrogen** if it is obtained from non-renewable energy sources, where, however, the total CO_2 produced is captured downstream, or if it is obtained by electrolysis of water using electricity obtained from nuclear power;
- **‘Green’ hydrogen** if it is produced entirely from renewable energies without CO_2 emissions.

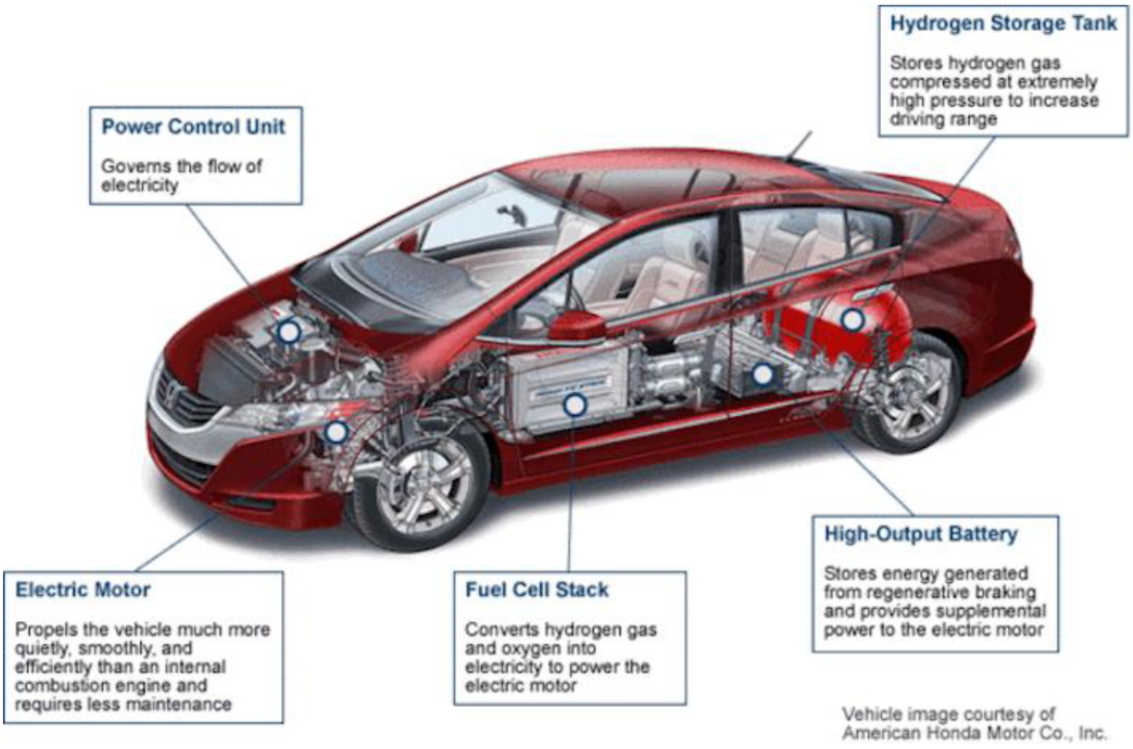
The green hydrogen is of particular interest because its usage doesn’t generate CO_2 at all in its usage chain from the production to after the usage.

Chapter 2

Hydrogen applications

2.1 State of art for hydrogen vehicles

In figure 2.1 it is possible to observ the architecture of a fuel cell vehicle using hydrogen as fuel, many car manufacturers are nowadays offering solutions like this for their fuel cell vehicles (FCV) as for example the Toyota Mirai.



Power Control Unit

Governs the flow of electricity

Hydrogen Storage Tank

Stores hydrogen gas compressed at extremely high pressure to increase driving range

Electric Motor

Propels the vehicle much more quietly, smoothly, and efficiently than an internal combustion engine and requires less maintenance

Fuel Cell Stack

Converts hydrogen gas and oxygen into electricity to power the electric motor

High-Output Battery

Stores energy generated from regenerative braking and provides supplemental power to the electric motor

Vehicle image courtesy of American Honda Motor Co., Inc.

Figure 2.1: Fuel cell concept car (manufacturer Honda, type FCX Clarity)

In figure 2.1 starting from the left to the right it is possible to see:

1. **An electric motor.** As a matter of fact the fuel cell vehicle is an electric vehicle that uses electric motors, buffer batteries and fuel cells to feed them. The electric motors allow to have a more quietly, smoothly, and efficient transportation with respect to do a a combustion engine, furthermore they also require less maintenance.
2. **A power control unit,** that is necessary to govern the flow of electricity to optimise the usage and reduce the fuel consumption. Indeed it is also possible to transform the kinetic energy of the vehicle during the decelerations in electric energy, that must be stored in the buffer batteries, to reduce even more the need of on board energy generation.
3. Then, as can be seen, in traditional Fuel Cell Vehicles there is the need to have an **hydrogen storage unit** that can be done in one or more tanks. Based on the type vehicle and thus the amount of energy needed pressure vessels that can reach up to 700 bar are used. [22] There is also a battery that can store the energy generated from regenerative braking and the energy produced by the fuel cell stack, when the electric motor requires less energy than the one produced by the fuel cell.
4. Finally there is the **fuel cell stack** that converts hydrogen and the oxygen contained in the air into electricity to power the electric motor. For the automotive applications the most used fuel cells are polymer electrolyte membrane fuel cell (PEM). This kind of fuel cell was developed by General Electric in the 1960 for NASA that has used it in space mission. The PEM fuel cell, works at low temperature in the range of 70-100 degrees, thus is the most appropriate to be used in this field, being able to guarantee frequent switches on and off of the vehicles.

2.1.1 PEM fuel cells

The polymer electrolyte membrane fuel cell (PEM) fuel cell is probably the most important fuel cell in the field of the transport. The PEM fuel cell is also known as proton exchange membrane fuel cell(PEMFC) also known as solid polymer fuel cell (SPFC).

The global reaction that takes place inside a PEM fuel cell is:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O + 286\frac{kJ}{mol} \tag{2.1.1}$$

In figure 2.2 it can be seen a schematic representation of the PEM fuel cell.

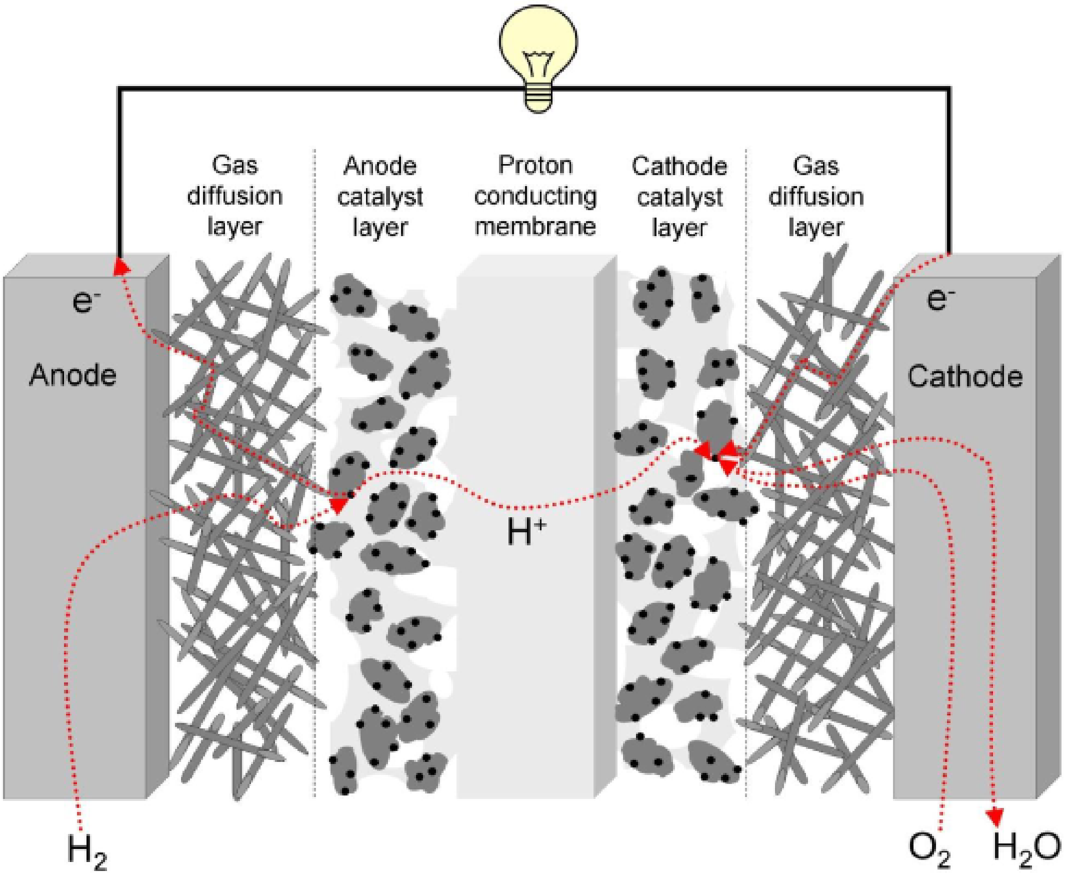


Figure 2.2: PEM fuel cell scheme

From the left to right, we have:

1. The anode.
2. The gas diffusion layer, that is a porous layer, made using carbon fibers necessary to distribute the gas (hydrogen in this case), on the anode catalyst layer.
3. The anode catalyst layer, that is made by 3 main materials: Unomer, Particles of Carbons and the Catalysts. Here we can see in a light gray the Unomer, in gray the particle of carbon and in black the nanoparticle of catalyst.

4. The membrane (electrolyte) that must maintain separated the 2 gases, hydrogen and oxygen but also must permit the transfer of the hydrogen ions from the anode to the cathode and must avoid the transfer of the electron produced in the anode to the cathode directly.
5. Cathode catalyst layer. The composition is similar to the anode, but the concentration of a catalyst is higher than the anode one, because the reaction that is at the cathode has a rate lower than the one present in the anode.
6. A second gas diffusion layer
7. The cathode

2.2 Hydrogen transportation

The transportation of hydrogen presents some complications mainly related to its low density and the hydrogen embrittlement (HE).

As can be seen in the graph in fig. 2.3 hydrogen presents some challenges with respect to the transport and the storage since, as can be noticed, in different conditions as a liquid or at different pressures, is in the bottom right part of the diagram. This means that hydrogen contains a lot of energy per kilogram, more than all the other fuel considered in the graph (gasoline, diesel, methane, methanol, methane,ecc...) but has an extremely low volumetric density.

As a consequence of this it is needed more space to store hydrogen in a tank or a pipeline with a big diameter to transport it.

As can be seen also in figure 2.4 , considered the characteristic of hydrogen it can be stored in mainly 3 different ways:

- As a compressed gas in high pressure vessels.
- As a liquid in dewars or tanks, but this requires to store it at -253° C, so $20^\circ K$, an extremely low temperature, difficult to obtain and maintain.

- As a solid by either absorption or reaction with metals or chemical compounds or in a alternative chemical forms.
- Cryo-compressed hydrogen, at a super critical cryogenic gas condition.

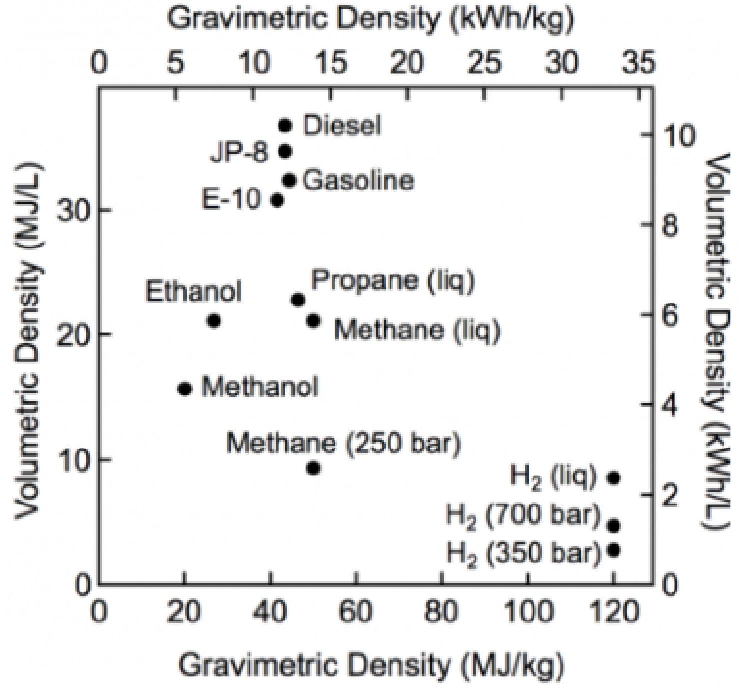


Figure 2.3: Energy sources and carriers density comparison [22]

The compression of the hydrogen can be a solution that allows to carry more hydrogen in the same volume, but this means that it is necessary to spend energy for the compression consequently reducing the efficiency of the whole process of storage. Furthermore this solution can be dangerous in the event of a crash or system failure due to the fact that the pressure inside the tanks can reach up yo 700 bar.

It is also possible to store hydrogen as a liquid, but this require to spend a lot of time and energy to transform the hydrogen from gas to liquid and then a lot of energy would be needed to ensure the proper temperature (-253 °C) from the moment of the transformation to the moment of the usage. Liquification has is the main drawback its high consumption of power, accounting for roughly 20 % to 40% percent of the hydrogen energy content in the liquefaction process, in addition to eventual hydrogen loss due to boil off [22]. In all the phases there is an high cost for the tanks and for the reduction of the heat transmission among the surfaces of the tanks.

An alternative is cryo-compressed hydrogen that is a super critical cryogenic gas. Liquefaction does not happen and gaseous hydrogen will be compressed at about $-233°C$. It has proven promising with respect to storage and safety level. Cryo-compressed storage provides high storage density (80 g/L, which is about 10 g/L more than liquid storage), quick and efficient refuelling, and high safety level due to the existence of a vacuum enclosure [15], however the need of such low temperatures is still a big limitation to this system.

Hydrogen absorption is a solution not feasible for transportation since it requires high pressures and long charge/discharge times.

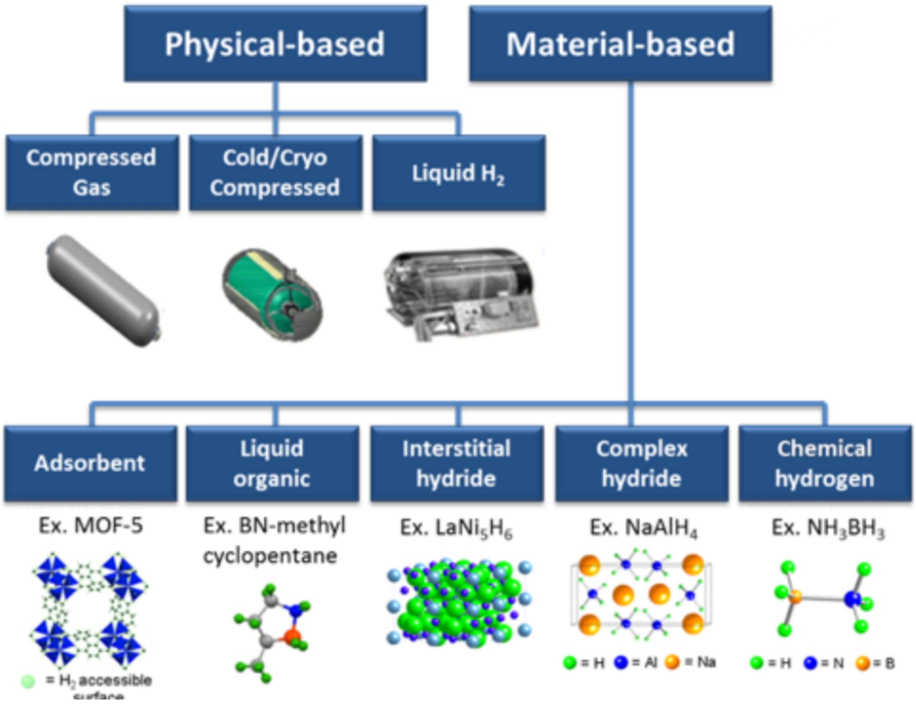


Figure 2.4: Hydrogen storage solutions [22]

All these possible storage solutions face many issues, such as:

- Operating pressure and temperature for high pressure vessels (for a quick recharge of an high pressure tank the temperature can reach high values due to the quasi adiabatic nature of the compression is quasi adiabatic);

- High hydrogen purity required by the fuel cell (difficult to guarantee during hydrogen transportation and storage);
- Reversibility of hydrogen uptake and release;
- Refuelling conditions of rate and time;
- Hydrogen safety, toxicity, and system-efficiency

No material available today comes close to meeting all the requirements for on-board storage of hydrogen for fuelling a fuel cell/electric vehicle.

In summary all the possible solutions for hydrogen storage and transportation require very expensive tanks and energy usage, and up to now it has not be found a solution that satisfies all the requirements.

It is also clear that many problems of the use of hydrogen can be solved generating the needed hydrogen directly on board both for cars and lightweight vehicles such as bicycles.

Hydrogen Embrittlement(HE)

Another advantage of not having to store big quantities of hydrogen for long time is the reduction of components that have to stay continuously in touch with hydrogen thus reducing the risk of *Hydrogen Embrittlement* (HE) also known as *hydrogen assisted cracking (HAC)* and *hydrogen-induced cracking (HIC)*.

Hydrogen embrittlement is a process originated from the small size of hydrogen's atoms. The small size of hydrogen's atoms compared to the the size of the atoms of the alloys and their crystal lattice makes possible their infiltration inside the metals structure, leading to a premature failure under stress due to the reduced ductility of the material caused by the dispersion of hydrogen and the way it interacts with the alloy elements. An example of a crack originated by hydrogen embrittlement is shown in figure 2.5

Figure 2.5: HE cracking.
Photo by CEphoto, Uwe Aranas

Many metals are susceptible to hydrogen embrittlement, and in particular high strength steels (HSS) such as dual phase (DP) steels and martensitic steels.

Aluminium alloys instead have a good resistance to hydrogen embrittlement, especially at low temperature. For this reason they are more suitable for applications related to hydrogen, combined to a design intended to reduce temperature growth during the usage.

Furthermore to reduce the risk of hydrogen embrittlements it is possible to take some precautions to protect the components, the main and most used ones are various types of coatings [13]:

- **Electrodeposition/Electroplating**, that is a commonly used method to deposit a protective layer onto the metal surface. This process involves immersing the metal substrate into an electrolyte solution containing metal ions. By applying an electric current, the metal ions are reduced and form a metallic coating on the substrate. Electroplating can provide an excellent protective layer that enhances corrosion resistance and reduces the susceptibility to hydrogen embrittlement. This process is suitable to get uniform, decorative and dense coating.
- **Chemical conversion coatings**, that are typically formed through chemical reactions between the metal substrate and a chemical solution. The conversion coating chemically reacts with the metal surface, resulting in a thin, tightly adhering protective layer. Examples of conversion coatings include chromate, phosphate, and oxide coatings. These coatings not only provide a barrier against

hydrogen diffusion but also enhance the metal's corrosion resistance. This process is suitable to get thin, cost-effective and uniform coating.

- **Chemical Vapour Deposition (CVD)**, in this process chemical precursors are introduced into a vacuum chamber where they react with a hot surface substrate, depositing a solid film. This process is suitable to get thin, dense and adherent film.

Another helpful solution, used also in pressure vessels, is the use of a polymer layer to protect the metal. Nevertheless hydrogen permeation barrier coatings have been considered the most common way to resist hydrogen embrittlement. They offer a possibility to ensure long-term integrity and safety of the metal and alloy components in a hydrogen-rich environment. [13]

2.3 Hydrogen use for stationary electricity generation

The fuel cell technology can and is used not only for transportation but also for stationary electricity generation. Different types of fuel cells are used for these applications, using alternative working principles that enable to achieve higher efficiencies.

The main types of fuel cells used for power plants are:

- Molten Carbonate Fuel Cell (MCFC)
- Solid Oxide Fuel Cell (SOFC)

Due to the high temperature that they need to work a lot of time (hours) is necessary to reach the working range. Moreover, during the transient, so when we start or stop the production of energy, the variation of temperature generates strong mechanical stress on the different materials (anode, cathode and electrolyte) and this can produce cracks that not only reduce the efficiency of the fuel cell, but they can also let hydrogen flow between the anode and the cathode.

Thus both the Molten Carbonate Fuel Cell (MCFC) and the Solid Oxide Fuel Cell (SOFC) are not suitable for systems that need frequent switch off and switch on. These solutions are used for power generation for medium or big dimensions, with a range from 50 kilowatt to 5 megawatt. [22]

These fuel cells can be used to power big infrastructures like universities, production plants or hospitals but as the other fuel cells also these solutions require hydrogen to generate electricity and thus have to face the same supply problems.

2.3.1 Power generation for emergency situations

Beside the everyday usage for power generation fuel cells can play a key role in emergency response where the normal power supply is cut off, like for example in the event of an earthquake.

In this situations portable fuel cells like Polymer electrolyte membrane fuel cell (PEM) fuelled by a portable hydrogen generation unit can allow rescue teams to have access to electricity where otherwise would be difficult, giving an alternative to traditional emergency power generators based on internal combustion engines.

Chapter 3

Product planning

In order to start the development of a new system it's important to analyse the baseline context in order to identify possible needs and consequently find the best way to satisfy them.

In this case it has been pivotal the analysis of the status of the art of energy delivery in the field of fuel cells vehicles (FCV) in order to find room for possible improvements.

3.1 Analysis and summary of the current situation

Taking into consideration all the observations related to hydrogen production (paragraph 1.2 and hydrogen applications (paragraph 2.2) it has been possible to understand that fuel cells are a mature technology capable to generate electricity with high efficiency and low or zero impact on the environment, however the supply of hydrogen and even more its storage(paragraph 2.2) presents some limitations that are restricting the diffusion of this technology.

For these reasons it has been identified the need for a different way to feed the fuel cells, eliminating the problems related to the storage of hydrogen.

3.1.1 The need for different solutions for hydrogen fuel cell vehicles

The need to find different solutions for hydrogen storage is even more clear for fuel cell vehicles because the problems related to the storage sum up with:

- the need to have a a lightweight system
- the possibility to ensure safety also in the eventuality of a crash

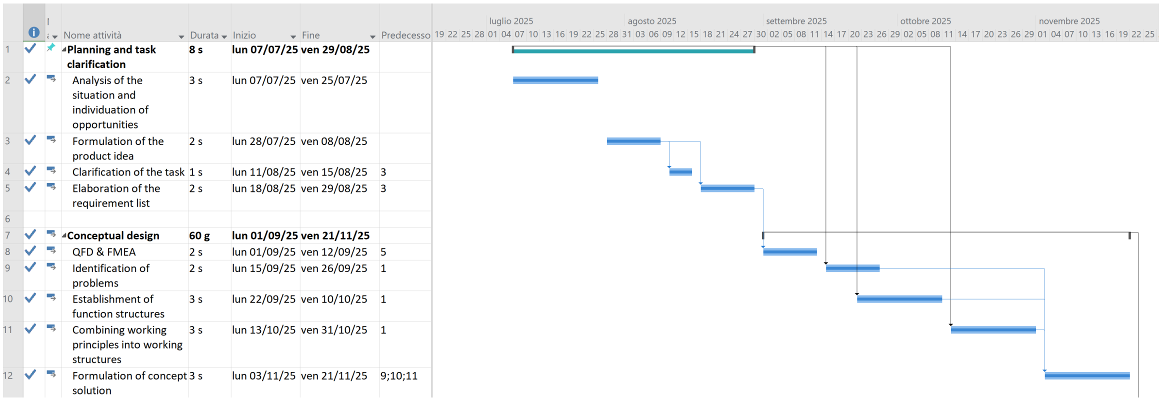
The first need is not compatible with the liquid form storage that needs several auxiliary systems to guarantee the required temperature, it is not compatible neither with the absorption/adsorption due to the high weight of the materials needed.

The second need instead becomes crucial when considering high pressure vessels, indeed although nowadays there are tanks capable of suffer huge crashes or shocks without failing it is still considered a potential risk in the event of an high speed crash involving fuel cell vehicles.

Furthermore this is a crucial aspect also for what regards the marketing of these kind of vehicles because it is not easy to sell a car if the customers are scared by the need of carrying vessels that can reach up to 700 bar.

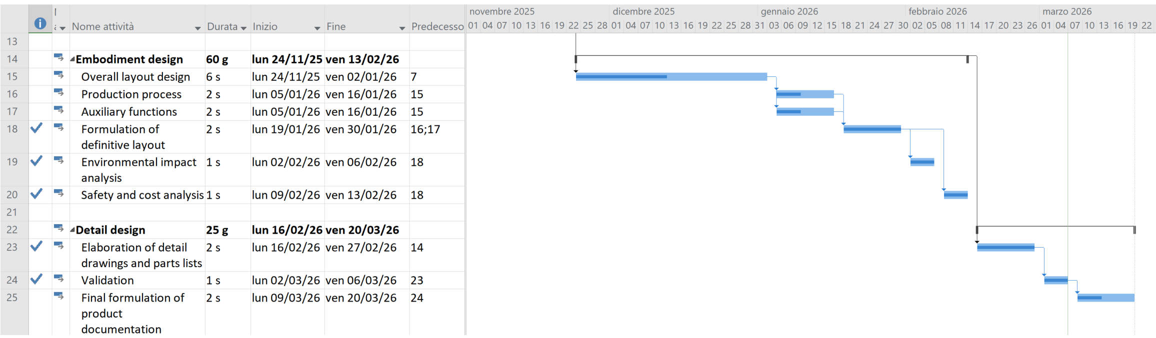
3.2 Product planning (Gantt diagram) for task clarification

At the beginning of this work a Gantt diagram has been developed to manage the engineering process. Milestones have been defined and the time necessary to complete each step has been evaluated. Each step has then been analysed to understand if it was necessary to complete it before going on or if it was possible to work on activities in parallel. Consequently all the task have been ordered to formulate the product planning as shown in fig. 3.1 and 3.2.



		Nome attività	Durata	Inizio	Fine	Predecesso
1	✓	**Planning and task clarification**	**8 s**	**lun 07/07/25**	**ven 29/08/25**	
2	✓	Analysis of the situation and individuation of opportunities	3 s	lun 07/07/25	ven 25/07/25	
3	✓	Formulation of the product idea	2 s	lun 28/07/25	ven 08/08/25	
4	✓	Clarification of the task	1 s	lun 11/08/25	ven 15/08/25	3
5	✓	Elaboration of the requirement list	2 s	lun 18/08/25	ven 29/08/25	3
6						
7	✓	**Conceptual design**	**60 g**	**lun 01/09/25**	**ven 21/11/25**	
8	✓	QFD & FMEA	2 s	lun 01/09/25	ven 12/09/25	5
9	✓	Identification of problems	2 s	lun 15/09/25	ven 26/09/25	1
10	✓	Establishment of function structures	3 s	lun 22/09/25	ven 10/10/25	1
11	✓	Combining working principles into working structures	3 s	lun 13/10/25	ven 31/10/25	1
12	✓	Formulation of concept solution	3 s	lun 03/11/25	ven 21/11/25	9;10;11

Figure 3.1: Gantt part one



		Nome attività	Durata	Inizio	Fine	Predecesso
13						
14		**Embodiment design**	**60 g**	**lun 24/11/25**	**ven 13/02/26**	
15		Overall layout design	6 s	lun 24/11/25	ven 02/01/26	7
16		Production process	2 s	lun 05/01/26	ven 16/01/26	15
17		Auxiliary functions	2 s	lun 05/01/26	ven 16/01/26	15
18	✓	Formulation of definitive layout	2 s	lun 19/01/26	ven 30/01/26	16;17
19	✓	Environmental impact analysis	1 s	lun 02/02/26	ven 06/02/26	18
20	✓	Safety and cost analysis	1 s	lun 09/02/26	ven 13/02/26	18
21						
22		**Detail design**	**25 g**	**lun 16/02/26**	**ven 20/03/26**	
23	✓	Elaboration of detail drawings and parts lists	2 s	lun 16/02/26	ven 27/02/26	14
24	✓	Validation	1 s	lun 02/03/26	ven 06/03/26	23
25		Final formulation of product documentation	2 s	lun 09/03/26	ven 20/03/26	24

Figure 3.2: Gantt part two

3.3 Selection of product ideas

As outlined in the previous paragraphs the aim of this work is to identify solutions that allow hydrogen generation on board (or on site in the case of stationary applications) in order to remove all the problems related to hydrogen storage from fuel cells usage.

Between all the possible hydrogen production methods, the sorting for viable product ideas starts discarding all the production processes that need big infrastructures, that wouldn't be feasible to suppose to carry wherever the fuel cell is needed. Discarded solutions are:

- Steam reforming (steam methane reforming SMR)
- Partial oxidation (POX)

- Auto-thermal reforming (ATR)
- Water electrolysis

The first three processes not only wouldn't satisfy the need to have the opportunity to produce hydrogen with the use of few and simple systems but would lead to the production of the so called **black hydrogen**, that takes this name due to the fact that it is produced starting from fossil fuels without the capture of CO_2 emissions from the process. However in the eventuality that the CO_2 produced with these processes is captured they would lead to the production of **blue hydrogen** (as seen in paragraph 1.2). These solutions would consequently be detrimental also from the environmental protection point of view.

Despite water electrolysis could be a great solution for hydrogen generation when or where energy sources like solar energy are available, is to be discarded for the desired applications because in the usage scenario it is not possible to have "free" energy to carry out the electrolysis. Thus a battery would be needed to perform the electrolysis making wasteful the use of this system to obtain hydrogen. Indeed due to the non unitary efficiency of the processes in the end the energy balance would be negative and it would be necessary to have more energy to generate the hydrogen than that retrieved after from the fuel cell to actuate the electric motors, in the example case of a moving vehicle.

Other solutions, more practical for the needs of the desired cases (chapter 2.3.1), but also more environmental friendly, consequently have been explored:

- **Bio-Hydrogen:** the biological production of hydrogen is mainly done in bioreactors and is based on the production of hydrogen by some algae or bacteria, the possible processes are:
  - Direct bio-photolysis
  - Indirect bio-photolysis
  - Photo fermentations
  - Dark fermentations
- **Inorganic chemical reactions** that lead to hydrogen generation

- NaOH and Al
- KOH and Al
- $Al + 3H2O \longrightarrow Al(OH)_3 + \frac{3}{2}H_2$

3.3.1 Direct bio-photolysis

In direct bio-photolysis green algae break the bond between H and O in the water molecules using the sun energy, the hydrogen ions are then converted in hydrogen gas by hydrogenase enzyme.[22]

The conversion of water to hydrogen by green algae can be represented by the following general reaction:

$$2H_2O + \text{ light energy } \longrightarrow 2H_2 + O_2 \tag{3.3.1}$$

3.3.2 Indirect bio-photolysis

In indirect bio-photolysis, the water reacts with cyanobacteria or blue-green algae according with the reactions [22]:

$$6\mathrm{H_2O} + 6\mathrm{CO_2} + \text{light energy} \rightarrow \mathrm{C_6H_{12}O_6} + 6\mathrm{O_2} \tag{3.3.2}$$

The result of these reactions are oxygen and a glucose molecule, glucose react then with water again in presence of light energy to obtain hydrogen and CO_2.

$$\mathrm{C_6H_{12}O_6} + 12\mathrm{H_2O} + \text{light energy} \rightarrow 12\mathrm{H_2} + 6\mathrm{CO_2} \tag{3.3.3}$$

Hydrogen is produced both by hydrogenase and nitrogenase enzymes and the production rate is comparable to hydrogenase-based production by green algae.

These methods seems to be the most cost effective however they present a low hydrogen production potential. Low H_2 production potential requires significant surface area to collect sufficient light. Furthermore as in the case of water electrolysis the requirement of having solar light in order to produce hydrogen is not compatible with the desired applications.

3.3.3 Dark fermentation

Dark fermentation is another process,that does not need oxygen, to obtain bio-hydrogen. Dark fermentation uses primarily anaerobic bacteria on carbohydrate rich substrate without oxygen presence. Glucose is the preferred source for this process and it can be obtained from agriculture wastes.

Bacteria catalyse the following reactions:

- Acetate fermentation:

$$C_6H_{12}O_6 + 2H_2O \longrightarrow 2CH_3COOH + 4H_2 + 2CO_2 \tag{3.3.4}$$

- Butyrate fermentation:

$$C_6H_{12}O_6 \longrightarrow CH_3CH_2CH_2COOH + 2H_2 + 2CO_2 \tag{3.3.5}$$

Glucose with the action of anaerobic bacteria produce acetic acid and hydrogen and CO_2 or butyrate acid hydrogen and CO_2.

With glucose the process cost can be expensive but it can be replaced by starch or cellulose allowing the process to become more low cost effective.

The amount of hydrogen produced by the process depends highly on the ph of the system that should be maintained between 5 and 6. As it can be seen in the reaction is necessary to remove the hydrogen and the carbon dioxide because the pressure of these gas increase in the reactors and these reduce the production of hydrogen according to the law of mass action.

Using dark fermentation light is not necessary, this means that the process can produce hydrogen day and night continuously and there isn't the need for large surfaces.

3.3.4 Photo-fermentation

Photo-fermentation use solar energy and organic acids. Photo-synthetic bacteria convert organic acids as acetic, lactic and butyric, into hydrogen and CO_2

$$\mathrm{CH_3COOH + 2H_2O + light\ energy\ \rightarrow 4H_2 + 2CO_2} \tag{3.3.6}$$

Higher H_2 production yields and reduced light energy demand can be obtained by using hybrid systems combining non-photosynthetic or anaerobic and photosynthetic bacteria.

It has also to be considered that photo-fermentation, dark fermentation and indirect bio-photolysis produce CO_2 besided hydrogen.

3.3.5 Inorganic chemical reactions that lead to hydrogen generation

$Al + 3H2O \longrightarrow Al(OH)_3 + \frac{3}{2}H_2$ is potentially an interesting solution but it needs to happen around $500 - 600°$ to reach a satisfying kinetic.

Aluminium hydrolysis is the mechanism behind $NaOH$ and KOH with aluminium reactions that lead to hydrogen generation. Al hydrolysis does not release carbon dioxide into the atmosphere or cause pollution. Additionally, the Al hydrolysis by-product is recyclable, has no toxicity, and can be employed directly as a flame retardant, alumina manufacturing feedstock and as water treatment agent. [8]

$$2Al + 6H_2O \longrightarrow 2Al(OH)_3 + 3H_2 \tag{3.3.7}$$

To solve the existing problem of the protective oxide layer on the aluminium surface and make it more feasible for quick hydrolytic hydrogen generation, normally NaH is added. After adding water, NaH reacts with water at first and forms NaOH, which further supports Al hydrolysis. This reaction can produce on-site hydrogen, and the hydrogen volume can be increased or decreased by controlling the water flow rate per requirement.[8]

$$2Al + 6H_2O + 2NaOH \longrightarrow 2NaAl(OH)_4 + 3H_2 \tag{3.3.8}$$

The aluminium metal is exposed when the hydroxide ions dissolve the coating of aluminium oxide. The newly exposed aluminium lacks the protective oxide coating and can easily react with water. Upon exposure, fresh aluminium react with water to produce aluminium hydroxide ($Al(OH)_3$) and hydrogen gas (H_2) in the presence of an adequate amount of self-generated heat and basic environment in the system.[8]

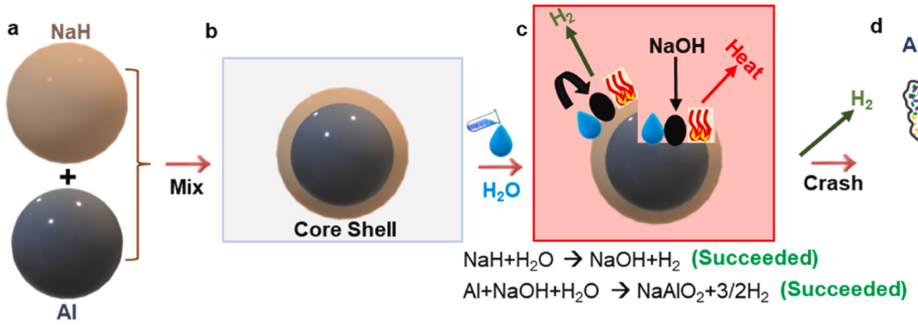


Figure 3.3: Preparation and H_2 generation process of Al-based NaH and solid fuel powders. (a) Al and NaH before mixing. (b) Al and NaH make a core shell after mixing, which protects Al from direct exposure to water. (c) Hydrogen generation reaction of Al-based NaH solid fuel powder produces NaOH and heat, which helps Al hydrolyse completely. (d) Al-based NaH solid fuel powder produces $Na_2Al_2O_4\breve{}6H_2O$ and $Al(OH)_3$ and crashes after the reaction. [8]

Studies have been conduced to understand which reactant gives the best yield in terms of hydrogen production and the results show that the reaction is strongly influenced by temperature, alkali concentration and metal shape. NaOH commonly promotes faster reactions and higher real yields than KOH. [7]

Sodium hydride is a suitable candidate not only for Al powder but also for aluminium foil of different sizes to react with water in an ambient environment.

3.4 Definition of performance targets

In order to make a data driven evaluation it is important to define clearly the variables impacting the functional performance of the system under development.

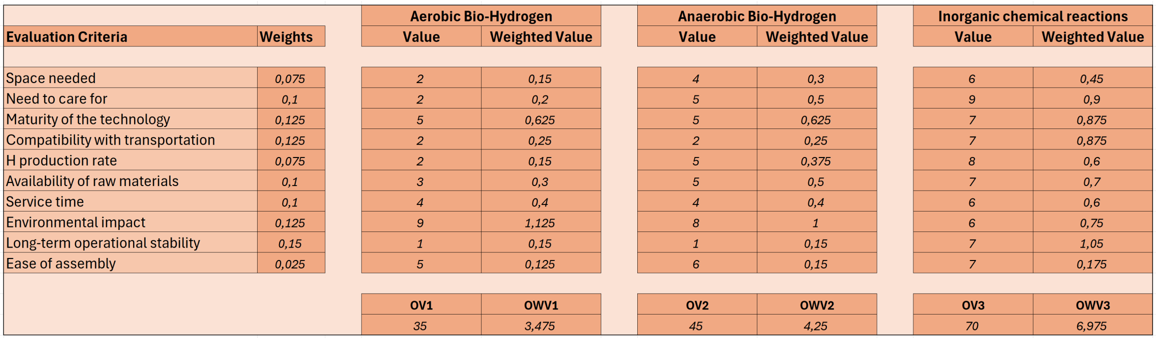
3.4.1 Functional requirements definition

The aspects that have to be monitored during the choice of the technology to be employed in the system are:

- **The space needed,** because a small system could fit better multiple purposes.
- **The need to care for,** since ideally a system that does not require many controls on the working environment fits a wider group of possible scenarios.
- **The safety of operators,** since it is important that the stocking phase doesn't put anybody in danger.
- **The maturity of the technology,** because the more a technology has been studied and the more it can be properly exploited.
- **The compatibility with transportation,** because some of the desired applications need the system to be easily transportable.
- **The hydrogen production rate,** due to the fact that to supply a fuel cell in order to guarantee the desired energy output it is necessary to to produce hydrogen with enough speed.
- **The availability of raw materials,** since a system without the possibility to be fed would be useless.
- **The service time,** because a frequent need to stop the system for service would be detrimental for its applications.
- **The environmental impact,** since one of the main advantages of using fuel cells is the opportunity to generate electricity without CO_2 emissions it would be a contradiction to pollute during the hydrogen production.
- **The long-term operational stability,** because once installed the system has to guarantee the desired life cycle.
- **The ease of assembly,** in order to keep the system as simple as possible.

3.4.2 Solutions comparison

In the following table (fig. 3.4) a comparison of the possible solutions previously described has been made. The solutions have been analysed based on the various keys factors described previously (sec. 3.4.1) weighted for the importance that they have in the context of the desired applications to perform a weak spot analysis.



		Aerobic Bio-Hydrogen		Anaerobic Bio-Hydrogen		Inorganic chemical reactions	
Evaluation Criteria	**Weights**	**Value**	**Weighted Value**	**Value**	**Weighted Value**	**Value**	**Weighted Value**
Space needed	*0,075*	*2*	*0,15*	*4*	*0,3*	*6*	*0,45*
Need to care for	*0,1*	*2*	*0,2*	*5*	*0,5*	*9*	*0,9*
Maturity of the technology	*0,125*	*5*	*0,625*	*5*	*0,625*	*7*	*0,875*
Compatibility with transportation	*0,125*	*2*	*0,25*	*2*	*0,25*	*7*	*0,875*
H production rate	*0,075*	*2*	*0,15*	*5*	*0,375*	*8*	*0,6*
Availability of raw materials	*0,1*	*3*	*0,3*	*5*	*0,5*	*7*	*0,7*
Service time	*0,1*	*4*	*0,4*	*4*	*0,4*	*6*	*0,6*
Environmental impact	*0,125*	*9*	*1,125*	*8*	*1*	*6*	*0,75*
Long-term operational stability	*0,15*	*1*	*0,15*	*1*	*0,15*	*7*	*1,05*
Ease of assembly	*0,025*	*5*	*0,125*	*6*	*0,15*	*7*	*0,175*
		OV1	**OWV1**	**OV2**	**OWV2**	**OV3**	**OWV3**
		35	*3,475*	*45*	*4,25*	*70*	*6,975*

Figure 3.4: Radar chart data

For example, long-term operational stability has the highest weight of 0.15 because the endurance of the system is considered crucial, while the ease of assembly has the lowest weight of 0.025 because although having a system easy to be assembled is important it is also true that the industry is nowadays able to pursue complex solutions without facing too many problems.

To obtain the score of the overall performance of all the studied solutions each one has received a score for every criterion, which has then been multiplied by the relative weight to obtain the weighted value. The final weighted scores show clear differences between the three options:

1. Inorganic Chemical Reactions: 6.975 (Net 70)
2. Anaerobic Bio-Hydrogen: 4.25 (Net 45)
3. Aerobic Bio-Hydrogen: 3.475 (Net 35)

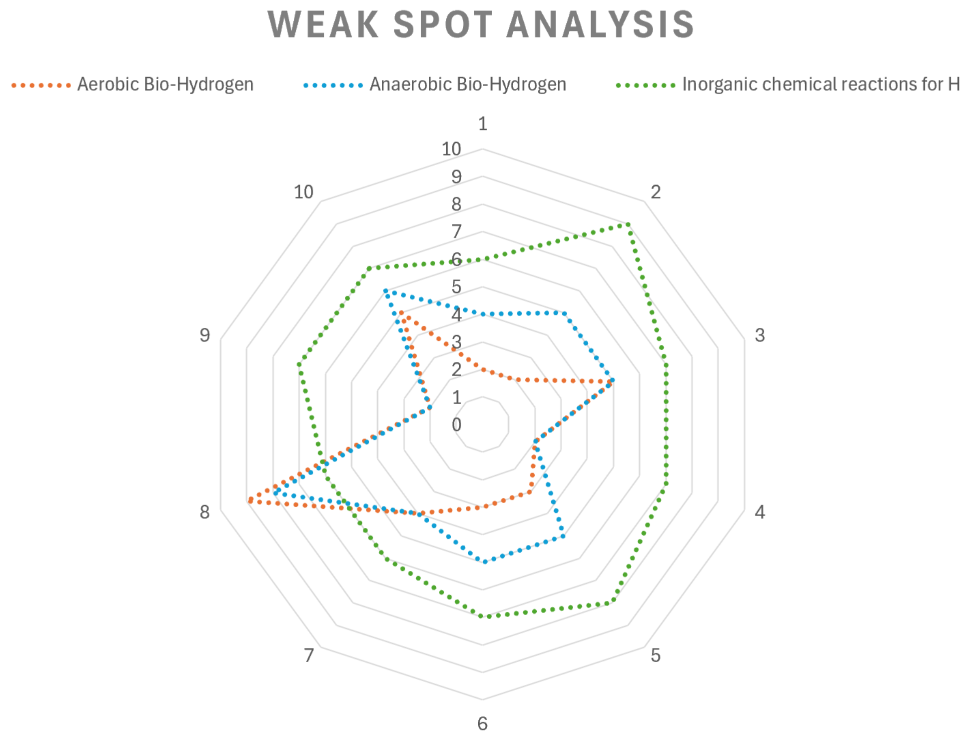


Figure 3.5: Radar chart

These results, as can be also seen in figure 3.5, indicate that inorganic chemical reactions achieve the highest overall score by a large margin. The anaerobic biological process performs moderately well, while the aerobic biological method scores the lowest.

Performance of Aerobic Bio-Hydrogen

The Aerobic Bio-Hydrogen (Direct bio-photolysis) generation method has its point of strength in the *environmental impact (9)* thanks to the nature of the reaction, producing the highest weighted value (1.125) among its criteria. However the overall performance is not satisfying due to several weaknesses in other criteria. It scores very low in *long-term operational stability (1)* and *hydrogen production rate (2)* due to the need of living bacteria to be employed, both of which are critical for practical industrial deployment. Additionally, the need for care and maintenance and relatively low compatibility with transportation systems limit its scalability.

As a result, despite its environmental advantages, the overall weighted score remains the lowest.

Performance of Anaerobic Bio-Hydrogen

As can be noticed the Anaerobic Bio-Hydrogen generation process performs better overall than the aerobic alternative so anaerobic systems are globally more suitable for the intended use. However, the method still faces limitations linked to the similar working principle of the aerobic approach. Its *long-term operational stability (1)* significantly reduces its total weighted score due to the high importance of that criterion.

While it performs well in several mid-weighted categories, it lacks the high scores in heavily weighted criteria necessary to compete with the inorganic chemical processes.

Performance of Inorganic Chemical Reactions

In can consequently clearly be understood that the Inorganic chemical reaction approach outperforms the two biological methods. It achieves consistently high scores across most criteria. In particular it excels in *need to care for (9)* thanks to the fact that once installed it does not require maintenance except for fuel refill, *technology maturity (7)* because these kind of reactions are well known and there are several studies available that investigated their optimisation to increase the hydrogen yeld and consequently the *hydrogen production rate (8).* Since these criteria carry moderate to high weights, they contribute significantly to the final weighted value.

Another major strength of inorganic chemical reaction approach is *long-term operational stability (7).* Although its *environmental impact score (6)* is lower than that of the biological alternatives, the difference is not large enough to offset its advantages in efficiency, reliability, and technological maturity.

Overall evaluation

While the biological methods offer environmental benefits, their lower stability and production efficiency significantly reduce their overall effectiveness thus considering the weighted scores and performance across all criteria of the weak spot analysis, Inorganic chemical reactions emerge as the best solution thanks to its positive characteristics for the most influential categories.

Chapter 4

Product proposal and requirement list

Summarising the analysis carried on in chapter 3 the following product proposal has been defined: **A versatile hydrogen production system, based on the reaction between NaOH and Al in presence of water, that can be installed wherever needed without specific system related constraints.**

4.1 System purpose

Following the previous analysis the objective is to design a system that is able to exploit the reactions between NaOH and Al in presence of water in equations 3.3.7 and 3.3.8 to generate hydrogen on board vehicles or where needed to directly supply fuel cells for electricity generation.

It has to be underlined that the system is not intended to compete with or replace other methods due to the impossibility to provide enough reactants (the aluminium in particular) for the general need of the transportation segment, but rather as a system that can be used in the specific contexts. For example for fuel cell vehicles, disaster relief vehicles, or auxiliary power units (APU).

It has been chosen the reaction involving NaOH over that involving KOH due to the fact that investigations found in literature showed that NaOH commonly promotes faster reactions and higher real yields than KOH. [7]

4.1.1 System applications

System use on moving vehicles

The system would be used on moving vehicles such as electrified bikes and cars (with different sizing based on the application) to feed the fuel cells installed on board to generate the desired energy to power the electric motors.

System use for stationary applications

Considered the desired modularity of the system it could be used to supply emergency fuel cell power generators, being deployed in areas that wouldn't be possible to reach with the conventional electrical network. The system is intended for a versatile use so with recurring switches on and off, consequently it is meant to be used coupled with a Polymer electrolyte membrane fuel cell (PEM) thus is neither intended or optimised for big energy plants using fuel cells like those based on Molten Carbonate Fuel Cells (MCFC) or Solid Oxide Fuel Cells (SOFC), for which the design would be completely different.

4.2 External constrains

Based on the intended use, different constrains have to be met for the system; the aim of a versatile design process is to find solutions that are complaint for all the possible scenarios.

4.2.1 External constrains for cars

Cars face moderate to high vibration levels thus a device that has to be installed on a car requires to not be affected by the presence of these vibrations in order to be able to work in all the scenarios.

The less space is needed by the system to be installed in a car to run and the more space is left for the users comfort thus a compact design is desirable. Serviceability and refuelling operations require accessible connections for maintenance. Furthermore a car has to face significative working temperature variance during the year.

The range of temperatures is significant, going from $-20C^{\circ}$ to $+100C^{\circ}$.

Safety in the eventuality of a crash is paramount. Any device mounted on a car must be safe in all the conditions, included after a crush and must not interfere with airbag deployment zones.

4.2.2 External constrains for 2 wheels vehicles

Although 4 and 2 wheels vehicles move on the same roads and face the same limitations there are some more specifically related to 2 wheels vehicles.

On motorcycles and bicycles vibration compatibility becomes even more important. Furthermore unlike cars, they offer minimal environmental protection thus a proper installation that ensures protection from weather and debris is crucial. It is also to be considered that devices installed on two wheels vehicles have to face also the roll of the vehicle during usage.

Weight distribution critically affects motorcycle handling. Varying the mass and its distribution affects the motorbike centre of gravity and inertia consequently alterating steering geometry and stability. Center of gravity considerations are pivotal also for safety. Motorcycles offer no crash protection. Falls and impacts are more likely to happen, thus a device to be installed on a motorbike has to be able to go through a crash ensuring that it won't cause injury during accidents.

But also, for bicycles, being human powered vehicles the weight sensitivity is even more crucial since each gram has to be carried by the user in the end. For this reason it must be considered also that the installation can not interfere with pedalling, steering, or braking. Additionally bicycle frames offer limited mounting points, the rear mounting case could be the ideal position despite it increases the height of the centre of gravity of the bicycle.

4.2.3 External constrains for stationary use

Unlike vehicular applications, stationary generators such those used in emergency situations have to run continuously for extended periods. The system service time must match generator usage intervals (typically hundreds of hours).

Being standing the system does not have to face vibrations in this application, neither the other problems related to being in movement. Service intervals require regular inspection and maintenance and so the hydrogen production system has to be positioned where technicians can access them without removing major components.

4.3 Functional requirements

The constrains exposed in section 4.2 can be translated into functional requirements for the desired system:

- Good hydrogen production capability.
- Possibility to have frequent switches on and off of the system without damages.
- Safe hydrogen production interruption in the event of a crash for vehicles applications (Failure mode and effect analysis (FMEA)).
- Service T: $-20C^{\circ}/+100C^{\circ}$.
- Desired weight: $\approx$ equivalent to the energy storage (batteries) weight of a commercial fuel cell vehicle.
- Compliance with road homologation requirements.
- Modularity of the mechanism for different sizes of vehicles (from bicycles to cars) applications and for stationary applications.
- Employment of commercial parts as far as possible to reduce the overall cost.

Failure Mode and Effect Analysis (FMEA) is a formalised analytical method for the systematic identification of possible failures and the estimation of the related risks (effects), that is the identification of the direct relationships between causes and consequences. For the case in study the possible failure could be an excessive hydrogen production when not needed and in particular in the event of a crash. In this case it is crucial to stop the production of hydrogen to avoid that the failure leads to the risk of accumulations that can cause additional problems in the crash site.

4.4 Requirements list

Based on the previous considerations of sections 4.2 and 4.3 it is possible to retrieve the requirement list. As can be seen in table 4.1 there are two types of requirements [10]:

- **Demands:** requirements that must be met under all circumstances or the solution is unacceptable. Usually a minimum performance and maximum performance range is defined.
- **Wishes:** requirements that should be taken into consideration during the design phase and implemented whenever possible.

List of Requirements for the H production system			
Wishes	***Demands***	***Requirements***	
	D	Length	< 100 cm
	D	Width	< 50 cm
	D	Height	< 85 cm
W		Mass	< 75 kg
	D	Range of service Temperature	$-20 < T < 100$ °C
	D	Hydrogen production emergency stop	(FMEA analysis)
W		Use of commercial components	
	D	Handles frequent cycling	
W		Modularity of the system	
	D	Interval between refuelling	> 200 km
W		Interval between maintenance	> 1 year
	D	Time to end of design	March 2026

Table 4.1: Requirements list

Chapter 5

Conceptual design

5.1 Identifying essential problems through abstraction

Starting from the requirement list previously defined in table 4.1 (chapter 4), an abstraction of the challenges has been carried on to identify essential problems and opportunities in order to enhance creativity. The main identified areas are:

- The energy demand response
- The mixing of the raw materials to obtain the solution of $NaOH$ and H_2O with the right proportion
- The actual reaction with aluminium to obtain Hydrogen

5.2 Establishing functional structures

Thought abstraction, the essential required functions of the system have been identified and they can be resumed in the general function structure in the following figure 5.1.

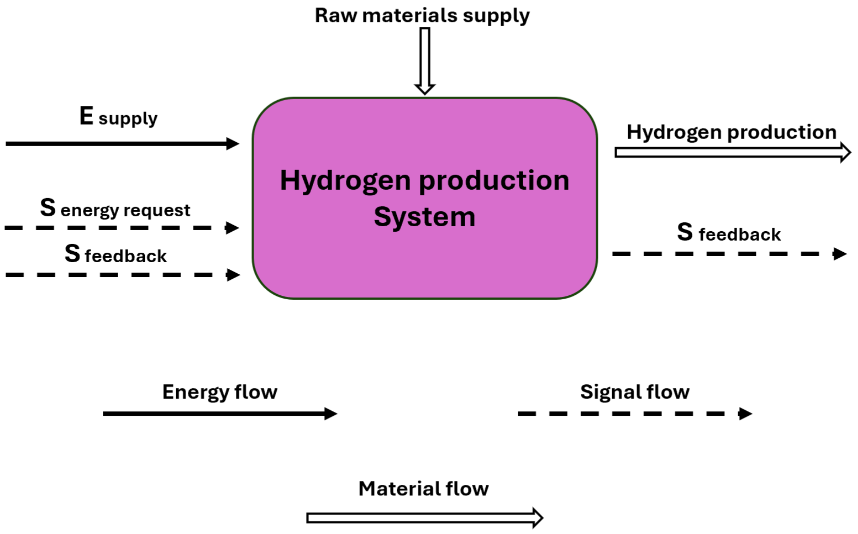


Figure 5.1: General function structure

On the left and on top there are the inputs:

- Energy flow from the supply
- Raw materials from the storage for the reaction
- A signal carrying the information about the energy request of the electric motors, that has to be translated into hydrogen request
- A signal giving information about the current state of the system (mixed solution and hydrogen avalability).

On the right there are the outputs:

- Hydrogen production, to be used in the fuel cell
- A feedback signal

It is possible to go deeper in the function structure definition obtaining the detailed function structure in the following figure 5.2.

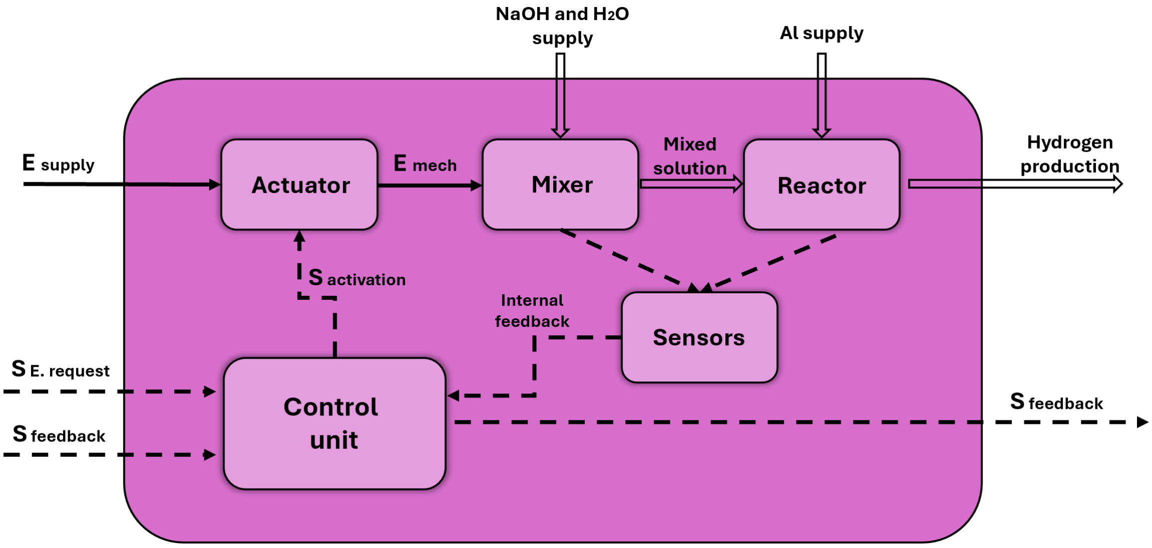


Figure 5.2: Detailed function structure

The two signals entering the system are received by a control unit, which based on the feedback information and the information coming from the sensors decides how and when activate the system.

The activation signal is then directed to the actuator, that transforms the input energy into mechanical energy which is then used by the system to properly mix the raw materials to obtain the desired solution that has to react with aluminium to generate hydrogen.

The idea here indeed is to study a way to stock separately $NaOH$ and H_2O and then mix them inside the system in order manage independently their supply and thus allowing to recycle the water coming from the reaction in the PEM fuel cell.

5.3 Working principle definition

Studying the literature on the reaction between $NaOH$ and Al exposed before (section 3.3.5) to exploit the aluminium hydrolysis a possible idea to be implemented is the development of a system that improves the concept behind the Kipps apparatus.

5.3.1 Introduction to Kipps apparatus

A Kipp's apparatus, also called a Kipp's generator, is an instrument designed for the preparation of small volumes of gases. The instrument was invented around 1844 by the Dutch pharmacist Petrus Jacobus Kipp (1808-1864).[18] As can be seen in figure 5.3 the glass apparatus consists of three vertically stacked chambers, roughly resembling a snowman. At the center of the top chamber is a tube that extends through its center into the bottom chamber. In figure 5.3a it is possible to see a photo of an authentic glass Kipp's apparatus while in figure 5.3b a CAD model of the system has been reproduced.

(a) Original Kipp's apparatus (b) Kipp's CAD model

Figure 5.3: Kipp's apparatus

The technical drawings of the CAD model parts can be found in appendix B.

A curiosity about the real Kipp's apparatus showed in figure 5.3a : Prior to 2012, this particular instrument had been displayed in a science classroom at Palisades High School, Kintnersville, Pennsylvania, as a historical piece of chemical equipment.

After concerns by the school administration about the connotations associated with the object's shape, the high school students added the label seen on the front of the apparatus which reads "This is not a bong."[18].

5.3.2 Kipp's apparatus working principle

The Kipp's apparatus is a very interesting device employed to take advantage of the reaction between $NaOH$ and Al in presence of water to produce H_2. As seen in section 5.3.1 the apparatus is composed by 3 elements:

- The first chamber with the inlet tube
- The base composed by two chambers divided by a restriction and a filter if needed
- The outlet that is linked to a stopcock

As can be seen in figure 5.4 the chamber of the first part of the apparatus is used as a tank for the solution of $NaOH$ and H_2O. In this case the solution has to be prepared previously separated and it is important to mix the elements in the right quantities to retrieve the desired concentration.

The base is made up of two divided chambers, the bottom one is used as a buffer tank, the top one is the place where the reaction takes place. Inside this chamber it is put the aluminium (can be in sheets or in pieces) that will start the reaction when in touch with the solution.

The chamber on top of the inlet, that works as solution tank, is put in connection to the rest of the apparatus through the inlet that crosses the other two chambers entering the second part (the base) from the bottom. This characteristic is very important and is the key element that makes the apparatus attractive for the desired use. In this way the solution will pass first trough the bottom chamber and then will rise to the second to start the reaction.

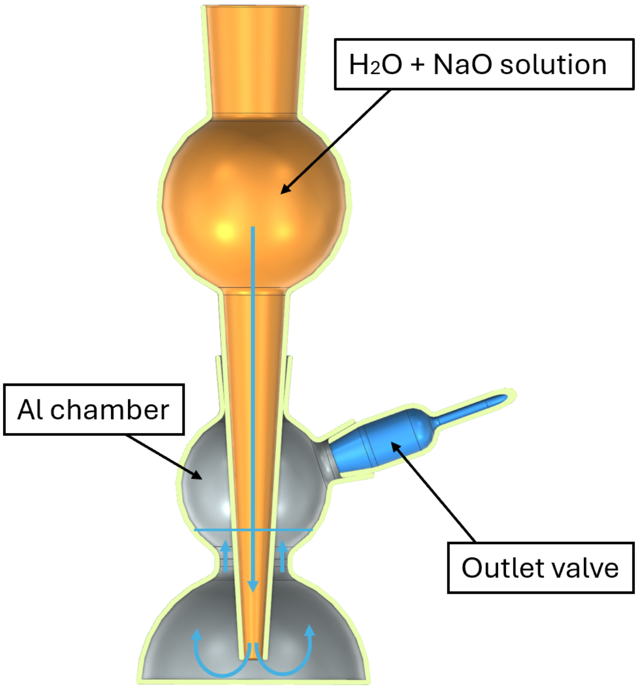


Figure 5.4: Kipp's solution inlet phase

Once in contact the reaction starts and hydrogen is produced. Thanks to its lower density (as seen in section 1.1) the produced hydrogen will start to flow trough the outlet when the stopcock is open. The production can go on as long as there are enough reactants.

However when the stopcock is closed it is not possible for the produced hydrogen to go away from the Kipp's apparatus and thus it starts to accumulate inside the reaction chamber. In this way the pressure inside the chamber starts to rise and when it reaches the head pressure due to the solution still present in the tank, it will start to push the solution to the bottom as can be seen in figure 5.5. In this way the solution is forced out of the reaction chamber impeding the encounter with the aluminium and consequently stopping the hydrogen production, avoiding in this way an undesired excessive stress on the chamber and the problems related to the accumulation of hydrogen.

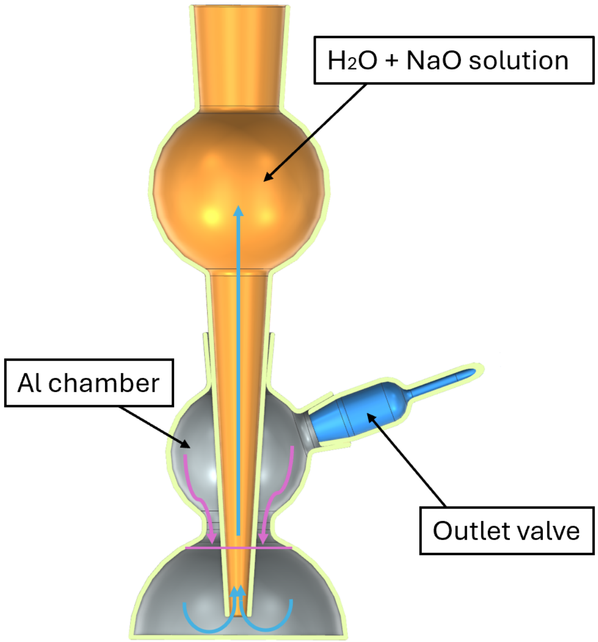


Figure 5.5: Kipp's hydrogen production interruption

This working principle is pivotal for the desired applications and the requirements expressed in chapter 4. As a matter of fact employing a solution like this one allows the system to have a safety control [compliant with the failure mode and effect analysis (FMEA)] that spontaneously avoids surplus of hydrogen production when the demand cease.

5.4 Combining working principles into working structures

Once the working principles have been defined and a reference system (the Kipp's apparatus) has been identified, the singular working principles and functional structures previously described (section 5.2) for each sub-function must be integrated into a coherent general working structure able to fulfil the overall system function. Each principle contributes to a specific aspect of the process, and their combination defines the working structure of the system.

5.4.1 Definition of an alternative solution for hydrogen fuel cell vehicles based on Kipps apparatus

Taking a cue from the Kipp's apparatus a system that satisfies the working structure necessary to achieve the system purpose (shown in figure 5.2) can be implemented.

First of all, contrary to the original system, it is necessary to store separately the reactants and mix them in the proper proportions when needed. This choice is beneficial for two reasons:

- Storing the $NaOH$ and H_2O separately it is possible to provide to their feeding separately thus isolating the two different supply chains.
- It is possible to take advantage of a virtuous circle: to create the solution needed for reaction that produces hydrogen water is needed $\longrightarrow$ hydrogen is produced in the reaction $\longrightarrow$ the hydrogen is used to supply a fuel cell to generate electricity $\longrightarrow$ the product of the reaction in the fuel cell is pure H_2O $\longrightarrow$ this water can then be used to be mixed with $NaOH$ to make the desired solution. Furthermore The resulting aluminium salt can be recycled to produce aluminium again. This completes the recycling cycle.

This virtuous circle is schematised also in figure 5.6. It is important to notice however that the reactions exploited here follow the mechanics expressed in equations 3.3.8 and 2.1.1 thus as can be understood analysing them it is not possible to satisfy the demand of water needed for the hydrogen production using only the water coming back from the fuel cell.

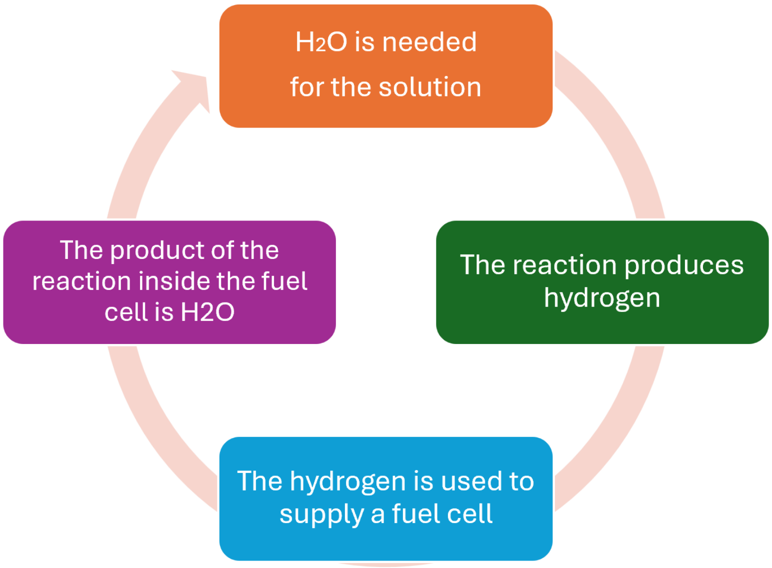


Figure 5.6: Water virtuous circle

Considering the reactions nature only half of the water needed can be retrieved from the PEM fuel cell products but still it is a significant benefit that allows to design a water tank sized to accommodate in the maximum loading case half of the water originally needed.

In this way all the advantages of the joint working principles of this chemical reactions and the fuel cell products are exploited and this wouldn't be possible loading directly a mixed solution of $NaOH$ and H_2O. The mixing of the reactants inside the system is for sure a challenge but it is worth to face it considered the great room for improvement that it offers.

Chapter 6

Embodiment design

6.1 System sizing

The first step to start the embodiment design of the system is to size it. Global dimension requirements have been defined in chapter 4 but clearly the space needed by the system varies significantly based on the desired application (cars, two wheels or stationary use). Nevertheless being the working principles general for all the scenarios the tools developed and presented in the following paragraphs can be used to size the system for each of the intended uses changing the data given as input. In the following paragraphs it will be taken as reference, to give an example, the sizing for the use on a car (FCV).

6.2 Codes analysis

In this section the codes developed to size the system for moving applications are analysed.

In order to size the system it has been needed to define the employment scenario and evaluate the factors influencing it. Thus starting from the requirement of a desired autonomy and the typical WLTP cycle that represents the average use of the cars during their daily use, a matlab script has been written to evaluate the energy needed to cover the distance. Once that the required energy has been identified it is possible to understand the amount of raw materials needed as reactants to obtain the amount of hydrogen necessary to produce that amount of energy with the fuel cell.

This matlab scripts models the energy consumption of fuel cell vehicle (FCV) powered by hydrogen generated through the aluminium–sodium hydroxide reaction. The objective of the model is to determine how many initial moles of reactants (Al and $NaOH$) are required by the vehicle to travel 200 km following a typical WLTP driving cycle.

Hydrogen is produced through the reaction in equation:

$$2Al + 6H_2O + 2NaOH \longrightarrow 2NaAl(OH)_4 + 3H_2 \tag{6.2.1}$$

Thanks to the virtuous circle described in section 5.4 and showed in figure 5.6 the water needed is assumed to be in part recovered from the fuel cell during the process. For the PEM fuel cell a global efficiency of $\eta = 0.6$ has been assumed.

The codes perform three main tasks:

- Define vehicle characteristics, cycle parameters and chemical informations.
- Compute the initial amount of reactants required using a root-finding algorithm.
- Simulate the full trip and plot the evolution of reactant moles, masses and total vehicle mass based on the results obtained in the previous step.

The program consists of three scripts:

1. A main script
2. A function computing the residual used in the root finding
3. A function performing the complete simulation and storing results

6.2.1 Main script

The main script retrieves the required data, performs the initialization, root-finding procedure and plotting of results. The vehicle used as reference is the last version of the Toyota Prius, one of the most diffused hybrid vehicles in the market. For this reason a comparison between the normal full hybrid version and an hypothetical fuel cell version supplied by the hydrogen produced using the system in study.

The choice of the Toyota Prius is related to its characteristics: the C_d measurement (drag coefficient) is just 0.24, the lowest achieved by any hatchback. Coupled with the car's lightweight aluminium and high tensile steel construction, this has a significant, positive impact on fuel economy and stability. [19]

Data definition

Based on the data declared by the constructor [19] the vehicle parameters considered are the following:

- Aerodynamic drag coefficient $c_d = 0.24$;
- Rolling resistance coefficien $c_r = 0.015$;
- Frontal area of the vehicle A = 2.2 m^2;
- Base vehicle mass excluding the components replaced by the hydrogen system m = 1545 - 131.5= 1413.5 Kg;

The data considered for the test environment sre the general ones:

- Gravitational acceleration g = 9.81 $\frac{m}{s^2}$;
- Air density $\rho = 1.225\ \frac{kg}{m^3}$;
- Average road inclination $\alpha = 5°$;

The WLTP cycle is characterised by four phases [20] as can be seen in table 6.1:

Phase	**Length (m)**	**Speed ($\frac{km}{h}$)**
Low	3100	18.9
Medium	4900	34.1
High	7200	54.4
Extra High	8300	94

Table 6.1: WLTP cycle characteristics

A parameter $r = \frac{200000}{d_{tot}}$ has been introduced to scale it to represent a 200 km trip.

A speed function has been defined using an interpolation:

$$v_fun = @(s)interp1(s_{break}, v_{vals}, s,' linear') \tag{6.2.2}$$

In this way it is possible to retrieve the vehicle speed at any position along the route based on the following inputs:

Inputs:

- s_{break} ⟶ known distances
- v_{vals} ⟶ speeds at those distances
- s ⟶ distance where speed is required
- 'linear' ⟶ linear interpolation between points.

Also the chemical data together with the system efficencies are introduced :

- Molar mass $PM_{Al} = 26.9815e^{-3}\ \frac{kg}{mol}$;
- Molar mass $PM_{NaOH} = 39.9971e^{-3}\ \frac{kg}{mol}$;
- Molar mass $PM_{prod} = 18.0016e^{-3}\ \frac{kg}{mol}$;
- Gibbs energy of hydrogen: $gibbs_{H2}$=$242e^{-3}\ \frac{J}{mol}$;
- η_{PEM}=0.6;
- $\eta_{reaction}$=0.98;

Thus the usable mechanical energy per mole of hydrogen produced is retrieved by the following:

$$G_{H_2} = gibbs_{H_2} \cdot \eta_{PEM} \cdot \eta_{reaction} \tag{6.2.3}$$

Then a residual function used for root finding is defined

$$fun = @(n_0)residuo_{finale}(n_0, s, v_{fun}, ...) \tag{6.2.4}$$

Where $n_0 = fzero(fun, [1e31e6])$ and fzero is a function that finds the value of n_0 for which:$fun(n_0) = 0$ [12]

The correct solution corresponds to the initial moles such that the aluminium supplied is exactly depleted at the end of the trip.

To simulate the whole path another function has been defined:

$$out = simula_{percorso\ moli}(...) \tag{6.2.5}$$

This function simulates the entire trip, storing the evolution of:

- reactant moles
- product moles
- total vehicle mass

The results are returned in a structure

6.2.2 Residual function

$$function\ res = residuo_{finale}(...) \tag{6.2.6}$$

This function evaluates the remaining aluminium at the end of the trip for a given initial amount and it is used by fzero to determine the correct initial moles. The vehicle is simulated step-by-step along the route.

The vehicle mass is determined as the sum of the base vehicle, the reactants and the products:

$$m = m_{car} + n_{Al} \cdot PM_{Al} + n_{NaOH} \cdot PM_{NaOH} + n_{prod} \cdot PM_{prod} \tag{6.2.7}$$

To evaluate the energy necessary to cover the desired path the forces acting on the vehicle have been considered:

- Aerodynamic drag: $F_d = \frac{1}{2}\rho C_d A v^2$
- Rolling resistance $F_r = c_r \cdot m \cdot g$
- Gravitational force due to slope $F_p = m \cdot g \cdot \sin\alpha$

Thus it is possible to calculate the energy required to ultimate the step with the following:

$$\Delta E = (F_d + F_r + F_p) \cdot (s(i+1) - s(i)) \tag{6.2.8}$$

Thus the moles of hydrogen needed can be directly retrieved: $\Delta n_{H_2} = \frac{\Delta E}{G_{H_2}}$
From the reaction stoichiometry it is possible to retrieve that:

$$3H_2 \leftrightarrow 2Al \Longrightarrow \Delta n_{reactants} = \frac{3}{2} \cdot \Delta n_{H_2} \tag{6.2.9}$$

So in each step reactants decrease, product increases and their quantity is updated as follows:

- $n_{Al} = n_{Al} - \Delta n$
- $n_{NaOH} = n_{NaOH} - \Delta n$
- $n_{prod} = n_{prod} + \Delta n$

If aluminium is exhausted before finishing the trip, the function stops.
A residual that equals the remaining aluminium at the end is defined but the root finding method ensures that $n_{Al\,final} = 0$

6.2.3 Simulation function

This function performs the complete path simulation and stores the results in a structure. The same physics as the residual function is applied, but in this case the quantities retrieved in the previous function are used and the values are stored at each step.

All the described codes can be found in appendix A.

6.2.4 Simulation graphs

As can be seen in the graph in figure 6.1 the codes have been able to calculate the exact amount of reactants needed to cover the desired distance, reaching the zero exactly at the end of the path.

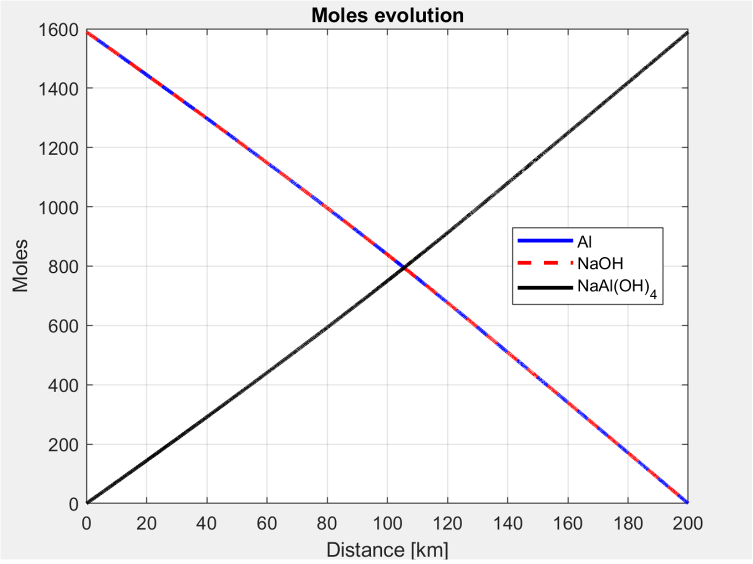
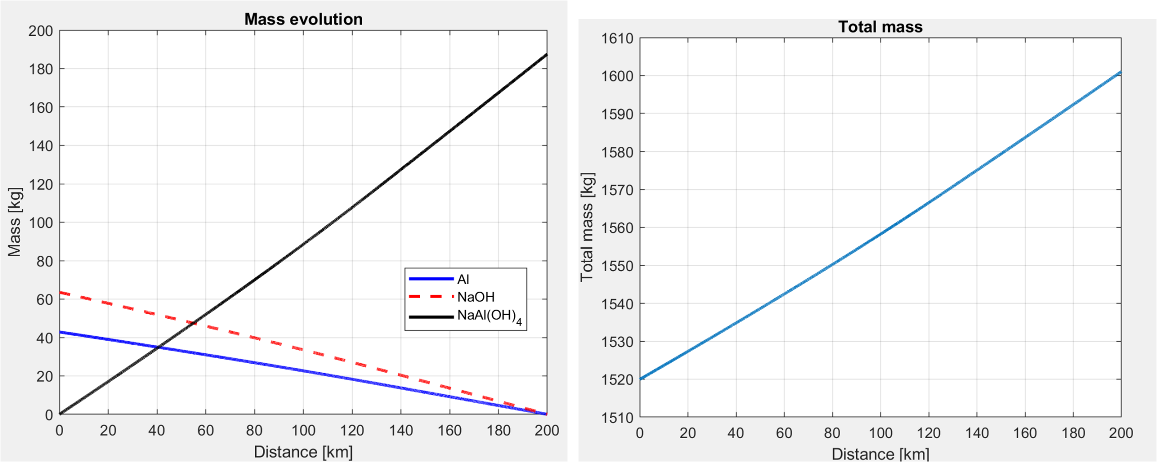


Figure 6.1: Moles evolution

Since as seen in the previous paragraphs, water is assumed to be partially recovered from the fuel cell during the process it is not represented in this graph because it is not a limiting reactant in this scenario.

However, this benefit doesn't come without side effects, indeed the water that comes from the fuel cell is being generated during its usage taking oxygen from the air. Thus globally, as can be seen in the graph in figure 6.2a the mass is increasing during the usage.



(a) Reactants and products mass evolution (b) Total car mass evolution

Figure 6.2: Mass evolution

This means that unfortunately the more one want to travel without refuelling using this system and the more it's gonna be inefficient because the mass is going to increase thus causing the vehicle to need even more energy to be moved.

Looking at this data it is important to remember however that tanks to the virtuous circle described in section 5.4 and showed in figure 5.6 the water needed is produced during the way by the fuel cell, but if it wasn't for this design choice is would be needed to carry all the water from the beginning thus the mass that can be seen at the end of the path would be the starting one. So considered this the water recycle solution is pivotal.

6.3 Architecture Overview

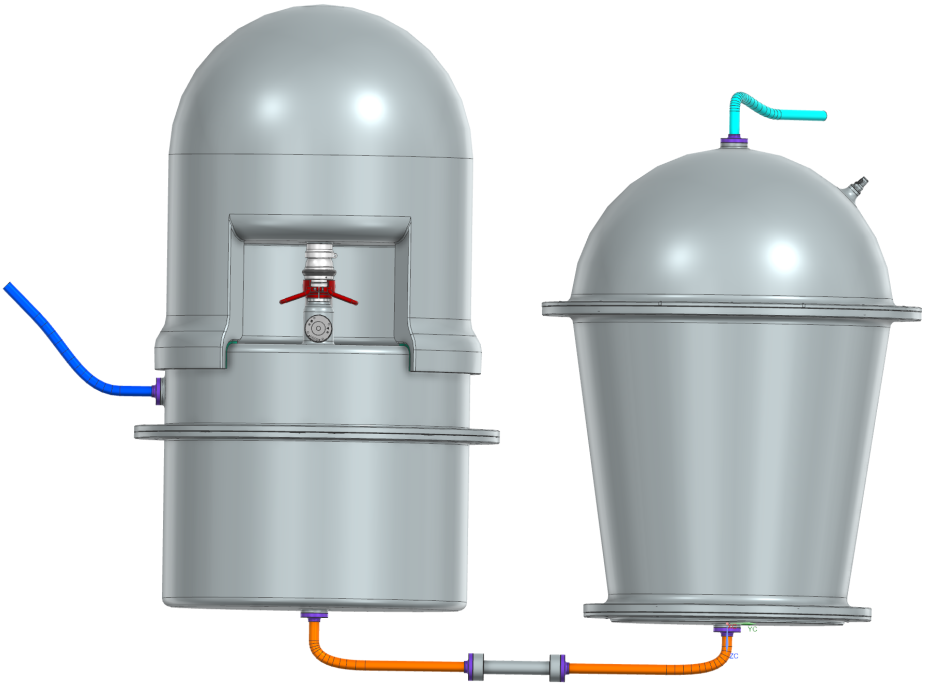


Figure 6.3: System assembly

In figure 6.3 the global architecture of the designed system is shown. This architecture is the result of the combination of all the requirements constraints and desired characteristics as exposed in chapter 4. This systems realise the intended working structure trough the combined work of the single components that frame the system.

In figure 6.4 a section view is shown to clearly identify the single elements. To ensure quality and reduce the overall price of the system commercial parts have been employed but when the CAD file of these was not available dedicated parts have been designed for reference only. For the technical data of the real commercial part to be employed refer to the dedicated paragraphs.

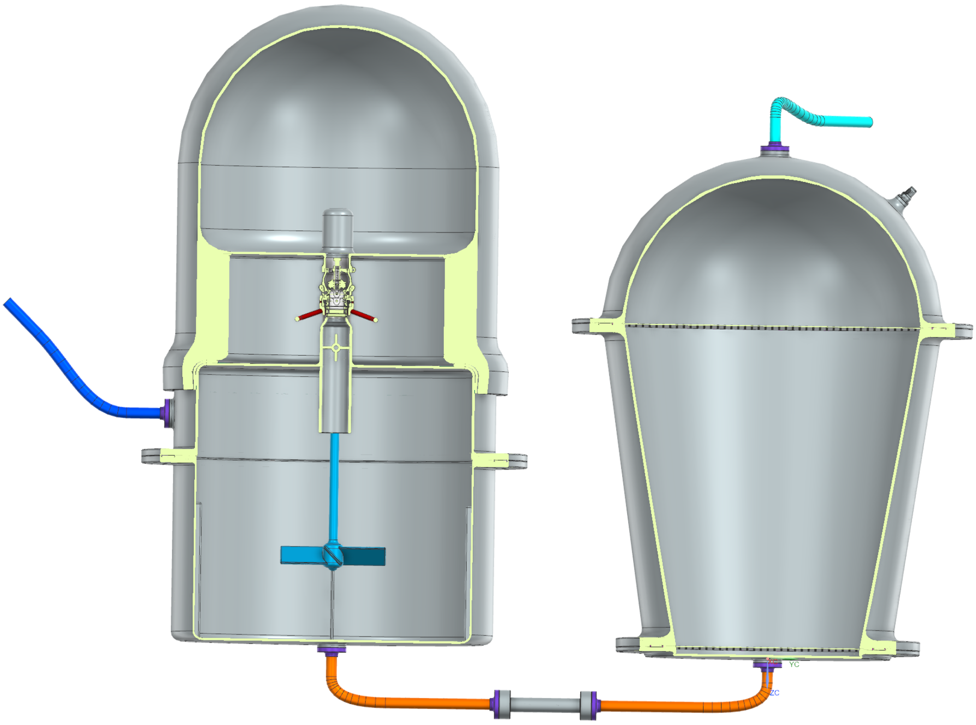


Figure 6.4: System section view

The system is composed by the following main assemblies:

- The NaOH tank
- The water and mixer tank
- A static mixer
- The reaction tower

- The connections

This architecture is meant to take the working principle behind the Kipp's apparatus and improve the working structure to satisfy all the requirements expressed in chapter 4.

The technical drawings of all the parts can be found in appendix B. The system satisfies the requirements for all the intended applications however here is displayed as reference the system sized for a car application.

6.3.1 NaOH tank

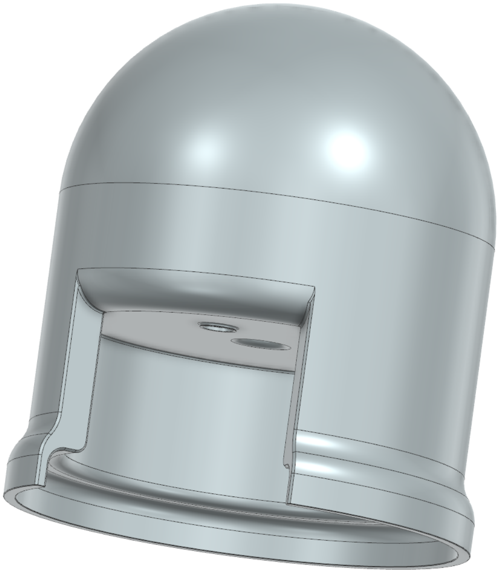


Figure 6.5: NaOH tank

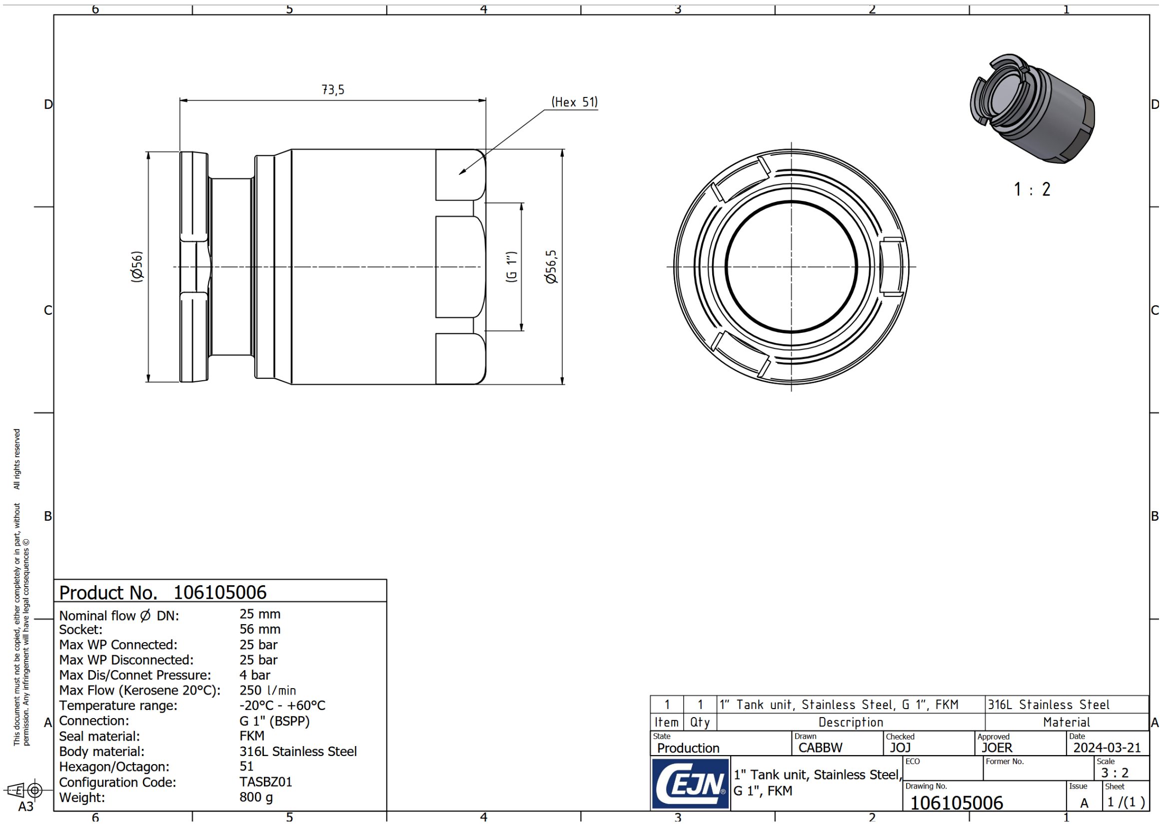
The first important thing needed for the correct running of the system is the availability of the raw materials, in this case the reactants. Since, as described in section 5.4.1, contrary to the original Kipp's apparatus, there are many benefits in storing separately the reactants and mix them in the proper proportions when needed, a dedicated tank only for NaOH has been designed.

As can be seen in figure 6.5 its shape has been adapted to be mounted on top of the mixer, where the NaOH it's gonna be mixed with water. These choice is beneficial for the following considerations:

- Being on top of the installation it is easy to remove an empty tank and replace it with a new one without having to remove any other component.
- In this way it is also possible to take advantage of the gravity to release the NaOH into the mixer.
- The space needed by the installation is optimised, avoiding the need for more space in the XY plane of the vehicle.

To ease the fitting of the tank on top of the mixer a viton pad has been introduced at the interface between the tank and the mixer. The bottom part of the tank is designed to invite the coupling with the mixer. Furthermore space has been left at the centre to give more space to the housing of the mixer electric motor.

In order to ease the replacement of the tank a quick release device has been installed. These solution allows for a fast replacement without needing to unscrew many components. As can be seen in the assembly CAD model in figure 6.7 a proposed solution is present for reference but many other commercial products, even smaller than that showed in the model, can be employed. A product reference is for example the product shown in figure 6.6



Product No. 106105006

Nominal flow ⌀ DN:	25 mm
Socket:	56 mm
Max WP Connected:	25 bar
Max WP Disconnected:	25 bar
Max Dis/Connet Pressure:	4 bar
Max Flow (Kerosene 20°C):	250 l/min
Temperature range:	-20°C - +60°C
Connection:	G 1" (BSPP)
Seal material:	FKM
Body material:	316L Stainless Steel
Hexagon/Octagon:	51
Configuration Code:	TASBZ01
Weight:	800 g

Item	Qty	Description	Material
1	1	1" Tank unit, Stainless Steel, G 1", FKM	316L Stainless Steel

State	Drawn	Checked	Approved	Date
Production	CABBW	JOJ	JOER	2024-03-21

1" Tank unit, Stainless Steel, G 1", FKM
ECO:
Former No.:
Scale: 3 : 2
Drawing No.: 106105006
Issue: A
Sheet: 1 /(1)

Figure 6.6: Commercial quick release drawing

6.3.2 Water and mixer tank

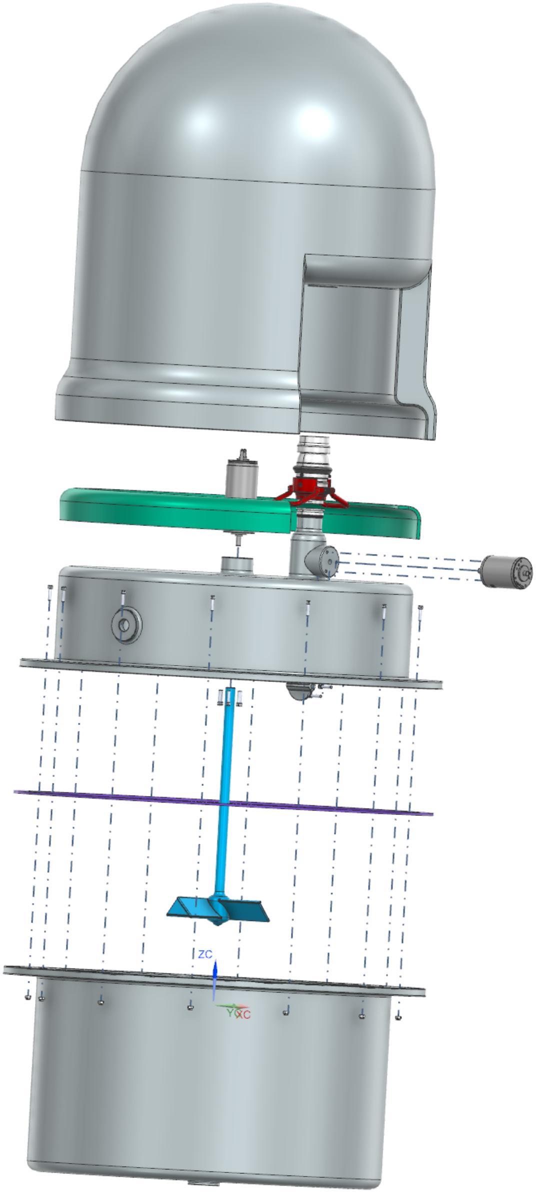


Figure 6.7: Mixer tower exploded view

In figure 6.7 an exploded view of the mixer and the NaOH tank is presented to show all the elements composing it. In green it's possible to see the viton pad previously described while between the tank and the mixer an example of quick release connection is shown for reference. As can be seen also in the section view in figure 6.8 when the NaOH leave the tank it encounters a doser before entering the tank.

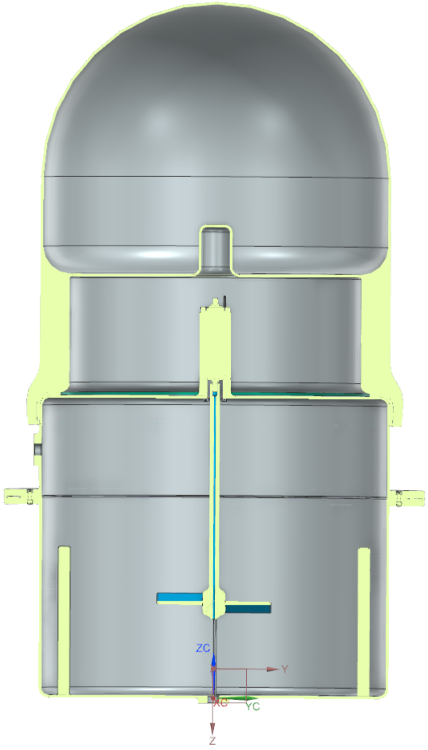


Figure 6.8: Mixer tower section view

Doser

The doser shown in figure 6.9 is a crucial part of the system. It's function is to control the amount of NaOH that is released into the tank and thus into the water.

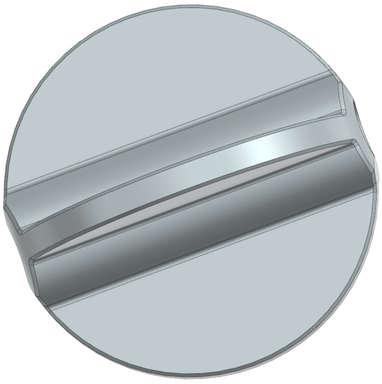


Figure 6.9: Doser

The amount of NaOH to be release is defined by the amount of water entering the mixer tank. Knowing the exact quantity of water present (a sensor is needed to retrieve this information) it is possible to retrieve the exact quantity of NaOH to be released as a multiple of the rotations of the doser. The doser is actuated by an electric motor, a model of the electric motor is shown in the exploded view (fig. 6.7). This is one suggested solution that has been found on the market but if not available any other similar solution could be fitted in the system to actuate the doser. In figure 6.10 the reference drawing from the produced is shown.

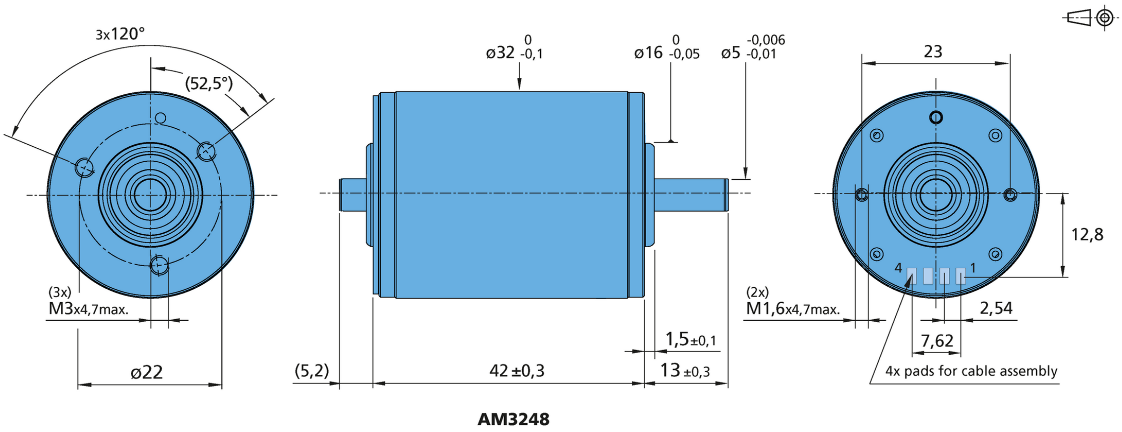


Figure 6.10: AM3248 motor from Faulaber drawing

Mixer

Since, as described in section 5.4.1, one of the desired characteristics of the system is to be able to mix in the proper proportions the reactants when needed, a mixer had to be designed.

Approaching the design of the mixer there were two possible paths to be followed:

- Add NaOH to the water
- Add water to the NaOH

However to decide with solution was the best to be implemented into the system some considerations regarding the heat generation mechanism during the dissolution had to be taken into account.

Indeed NaOH dissolution is highly exothermic, releasing about 44.5 $\frac{kJ}{mol}$ as hydration energy drives ions into solution, often raising temperatures up to $70°C - 100°C$ depending on concentration. When NaOH is added to water, the liquid immediately surrounds and dilutes small portions, absorbing and distributing heat across a larger volume via convection. This limits localized spikes that could exceed $150°C$.

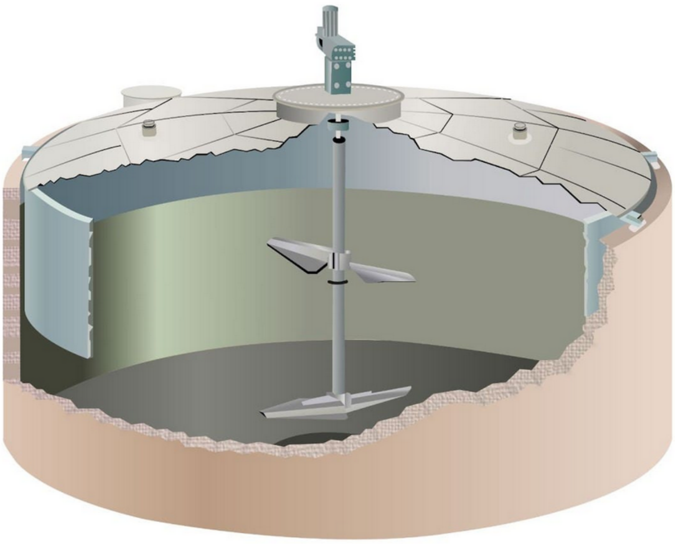


Figure 6.11: Standard industrial agitator

Reversing this process and so adding water to NaOH would concentrate heat in the dry powder mass first, causing rapid boiling, steam bursts, or splattering as water flashes to vapour on contact, since the NaOH lacks the initial heat sink capacity of water. Thus adding NaOH to water, rather than water to NaOH, better controls the exothermic dissolution heat by leveraging water's heat capacity and dilution dynamics and for this reason it has been preferred as dissolution method.

Starting taking as reference commonly used standard industrial agitator as the one shown in figure 6.11 the water tank has been designed not only to store the water but also to work as mixer element. Consequently it has been decided to introduce an impeller into the system.

Axial flow impellers cause the tank fluid to flow parallel to the impeller's axis of rotation while radial flow impellers cause the tank fluid to flow perpendicular to the impeller's axis of rotation [17]. The following figure 6.13 shows the different flow patterns achieved by using an axial flow impeller.

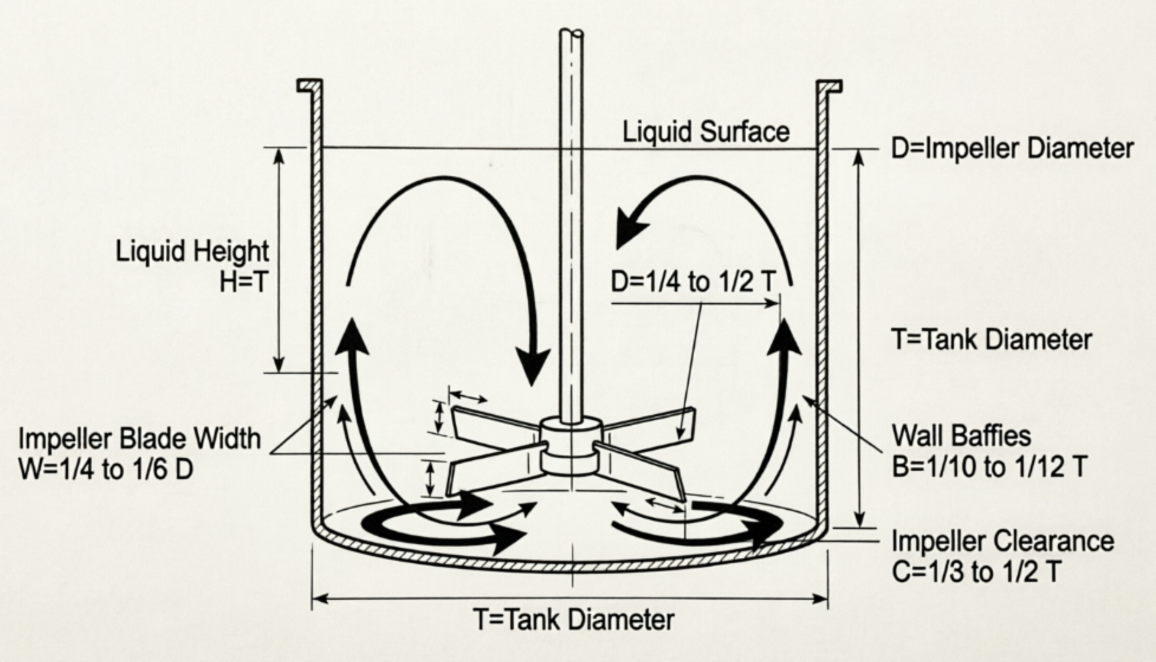


Figure 6.12: Axial impeller flow

Based on the theory [17] an axial flow impeller with 45° blades has been designed. In figure 6.13 the CAD model is shown.

Figure 6.13: Impeller

This solution has been preferred because axial flow impellers are very useful in mixing solid-liquid suspensions since they prevent the solid particles from settling at the bottom of the tank [17]. The sizing of the impeller has been implemented following the references found in literature [17]

The impeller shown in figure 6.13 is actuated by an electric motor, a model of the electric motor can be seen in the exploded view (fig. 6.7). This is one suggested solution that has been found on the market but if not available any other similar solution could be fitted in the system to actuate the doser. In figure 6.14 the reference drawing from the produced is shown.

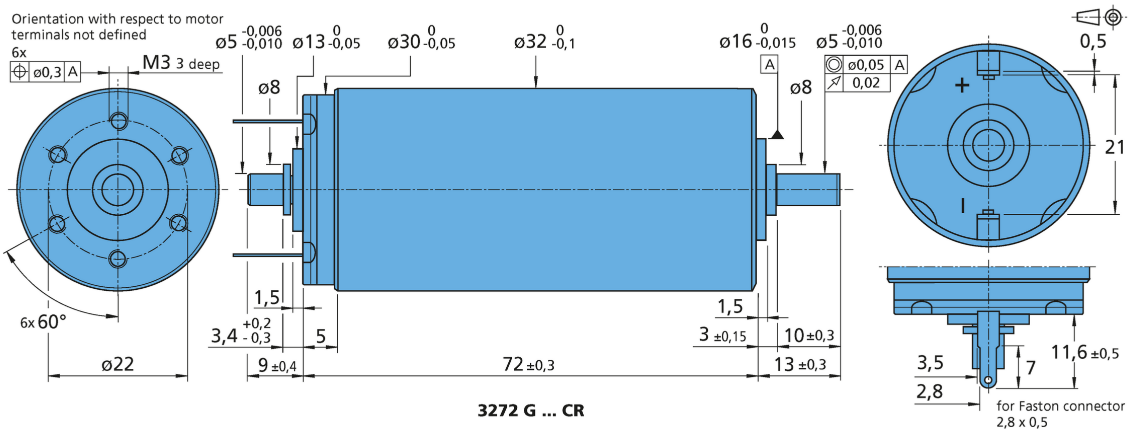


Figure 6.14: 3272 motor from Faulaber drawing

Baffles

Baffles are vertical plates positioned along the interior walls of mixing vessels. They can be seen both in figure 6.12 and in figure 6.15. The sizing of the baffles has been implemented following the references found in literature [17], as can be seen also in figure 6.12. Their implementation is important to achieve effective homogenization.

Baffles serve a critical hydrodynamic function by interrupting vortex formation and converting rotational energy into useful turbulence. Without baffles, liquid tends to rotate solidarily to the impeller, forming a central vortex that severely limits radial and vertical mixing.

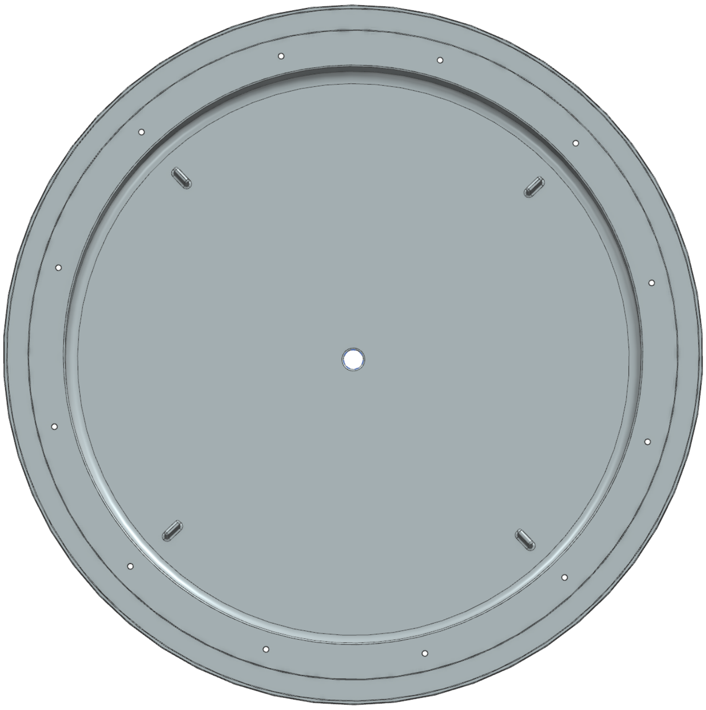


Figure 6.15: Mixer base with baffles

Industrial practice establishes four baffles arranged at 90° intervals as the optimal configuration. Baffle width typically ranges between $\frac{1}{10}$ and $\frac{1}{12}$ times the tank diameter (T) as can be seen in figure 6.12. Narrower baffles prove ineffective, while wider ones unnecessarily increase power requirements and create dead zones.

Two mounting approaches exist:

- Direct wall contact (simpler, widely adopted)
- Spaced installation respect to the wall

The latter reduces solid accumulation behind baffles and improves the effectiveness, thus it has been chosen for the positioning of the baffles in the tank.

6.3.3 Static mixer

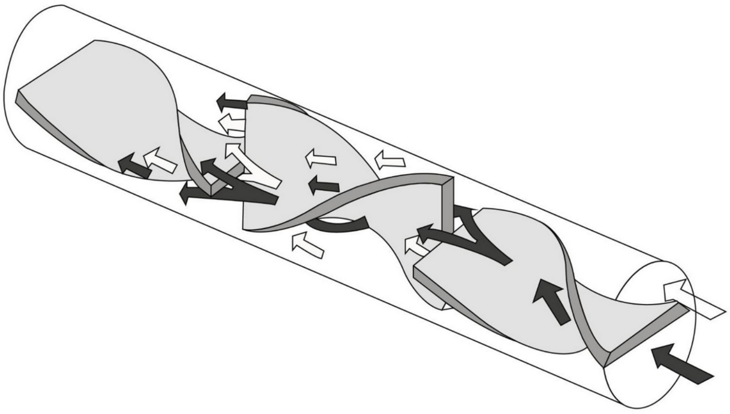


Figure 6.16: Static mixer working principle

To further improve the mixing of the reactants and ensure that the solution reaches the aluminium as desired to start the reaction a static mixer has been added along the connection between the mixer and the reactor tower.

As can be seen in figure 6.16 a static mixer is an element that does not contain moving parts but thanks to its geometry forces the flux to stir. The static mixer working principle is shown also in figure 6.17.

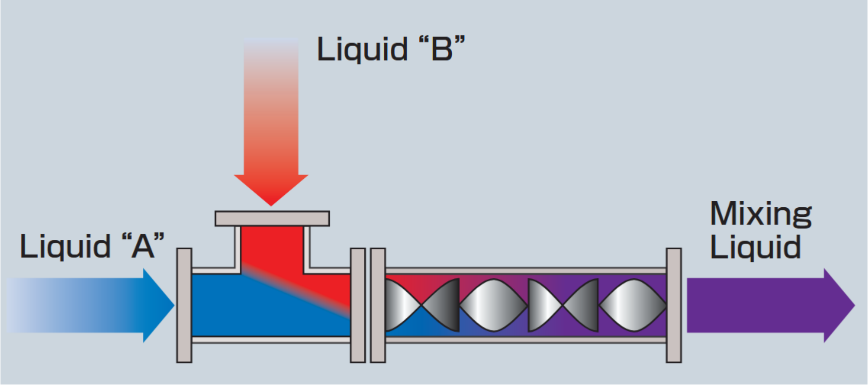
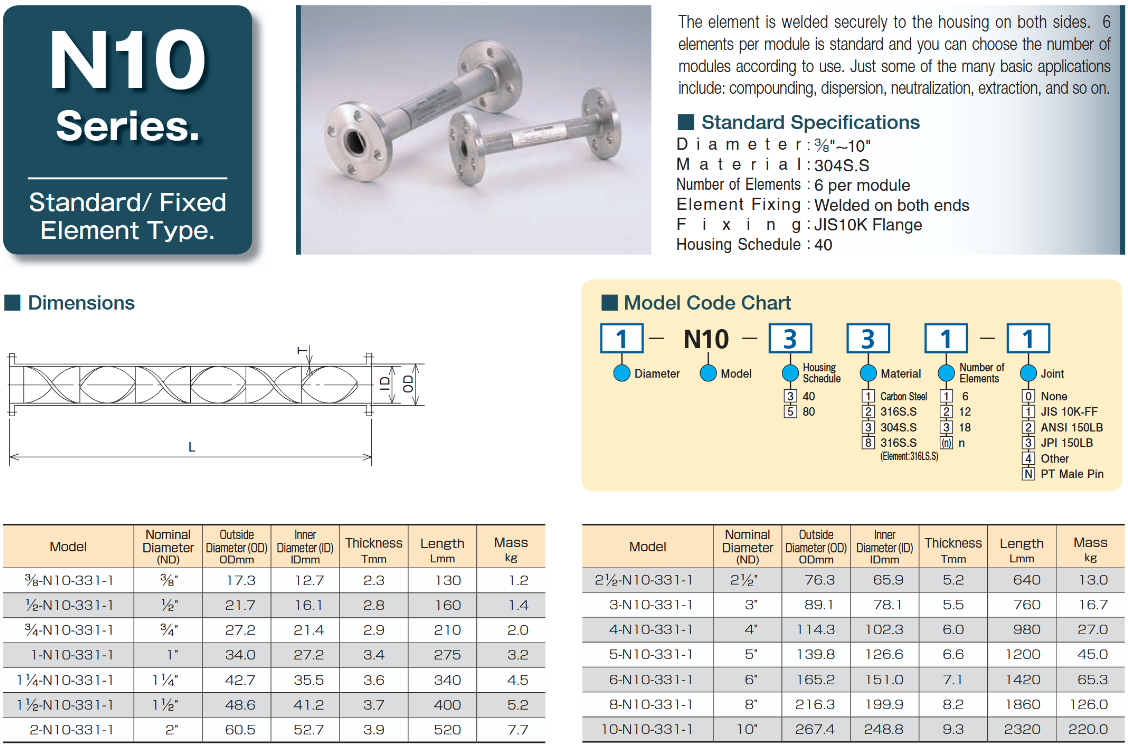


Figure 6.17: Noritake mixers scheme

Static mixers can be found on the market and different solutions are proposed based on the usage needed. In the following table in figure 6.18 an extract from a product catalogue is attached [4], this has been taken as reference for the static mixer model that is part of the assembly.



N10

Series.

Standard/ Fixed
Element Type.

The element is welded securely to the housing on both sides. 6 elements per module is standard and you can choose the number of modules according to use. Just some of the many basic applications include: compounding, dispersion, neutralization, extraction, and so on.

■ Standard Specifications

Diameter : ⅜"~10"
Material : 304S.S
Number of Elements : 6 per module
Element Fixing : Welded on both ends
Fixing : JIS10K Flange
Housing Schedule : 40

■ Dimensions

■ Model Code Chart

1 – N10 – 3 3 1 – 1

- Diameter
- Model
- Housing Schedule
  - 3 40
  - 5 80
- Material
  - 1 Carbon Steel
  - 2 316S.S
  - 3 304S.S
  - 8 316S.S (Element:316LS.S)
- Number of Elements
  - 1 6
  - 2 12
  - 3 18
  - (n) n
- Joint
  - 0 None
  - 1 JIS 10K-FF
  - 2 ANSI 150LB
  - 3 JPI 150LB
  - 4 Other
  - N PT Male Pin

Model	Nominal Diameter (ND)	Outside Diameter (OD) ODmm	Inner Diameter (ID) IDmm	Thickness Tmm	Length Lmm	Mass kg
⅜-N10-331-1	⅜"	17.3	12.7	2.3	130	1.2
½-N10-331-1	½"	21.7	16.1	2.8	160	1.4
¾-N10-331-1	¾"	27.2	21.4	2.9	210	2.0
1-N10-331-1	1"	34.0	27.2	3.4	275	3.2
1¼-N10-331-1	1¼"	42.7	35.5	3.6	340	4.5
1½-N10-331-1	1½"	48.6	41.2	3.7	400	5.2
2-N10-331-1	2"	60.5	52.7	3.9	520	7.7

Model	Nominal Diameter (ND)	Outside Diameter (OD) ODmm	Inner Diameter (ID) IDmm	Thickness Tmm	Length Lmm	Mass kg
2½-N10-331-1	2½"	76.3	65.9	5.2	640	13.0
3-N10-331-1	3"	89.1	78.1	5.5	760	16.7
4-N10-331-1	4"	114.3	102.3	6.0	980	27.0
5-N10-331-1	5"	139.8	126.6	6.6	1200	45.0
6-N10-331-1	6"	165.2	151.0	7.1	1420	65.3
8-N10-331-1	8"	216.3	199.9	8.2	1860	126.0
10-N10-331-1	10"	267.4	248.8	9.3	2320	220.0

Figure 6.18: Noritake catalogue extract [4]

6.3.4 Reaction tower

Figure 6.19: Reactor tower

After passing through the static mixer the solution of NaOH and water finally enters the reaction tower that can be seen in figure 6.19 and 6.20.

The solution is going to enter from the bottom and rise inside the main chamber where aluminium is present thanks to the piezometric head due to the solution present inside the mixer. Once that the mixed solution enters in contact with the aluminium the reaction starts and hydrogen and sodium aluminate ($NaAl(OH)_4$) are produced.

While the sodium aluminate produced remains inside the main core chamber of the reactor tower the hydrogen produced thanks to its lower density moves up to the top chamber.

Figure 6.20: Reactor tower section

The top chamber of the reactor acts not only as junction with the line that brings the hydrogen to the fuel cell but also as as hydrogen reservoir and as safety device.

Indeed here a working principle similar to that seen for the Kipp's apparatus in paragraph 5.3.1 is employed:

1. When the vehicle doesn't need energy generation the fuel cell is not going to need more hydrogen but the reaction goes on as long the reactants are in touch.
2. In this context the hydrogen start to accumulate in the top chamber.
3. When the pressure inside the top chamber overcomes the value of the piezometric head it is going to start pushing back the solution .
4. In this way the solution is going to be separated from the aluminium stopping the reaction and thus the hydrogen production.
5. When the fuel cell is going to consume enough hydrogen to lower the pressure inside the chamber under the value of the piezometric head the solution is going to enter again in touch with the aluminium starting again the production.

In order to be complaint with the FMEA analysis a backup solution is also installed, if for any reason the pressure inside the top chamber gets too high a pressure relief valve is installed to avoid problems, ensuring the fail safe principle. In this way one of the requirements of system is satisfied.

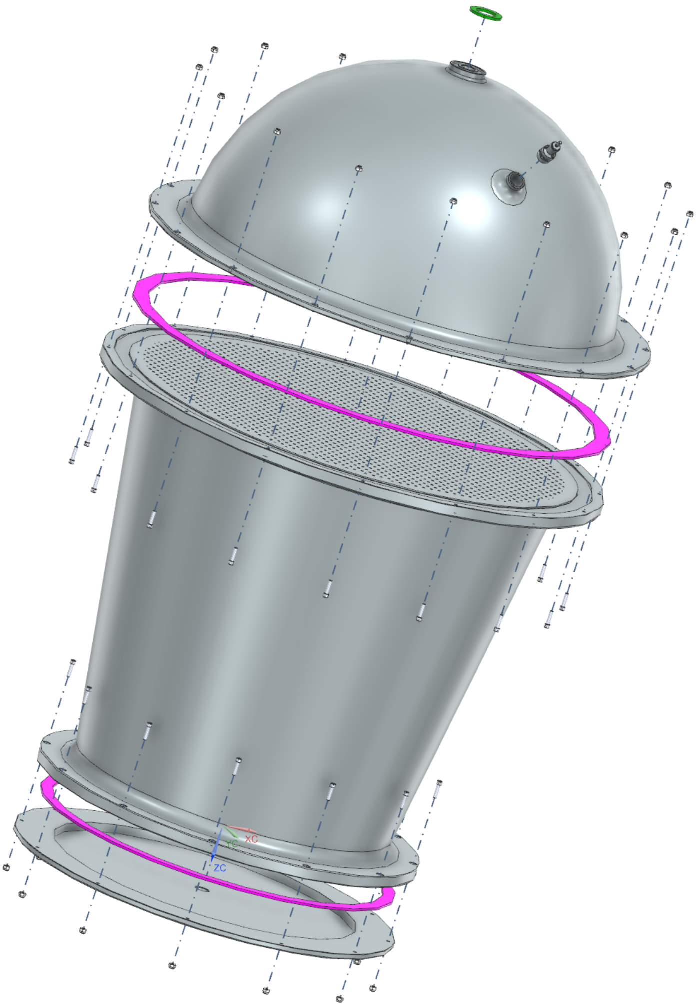


Figure 6.21: Reactor exploded view

The installation in the vehicle is a topic beyond the scope of this study but however it can be supposed that the top and bottom part of the reaction tower can be easily fixed to the vehicle with proper fairings. In this way the reactor core part can be removed easily with a slide after unscrewing the fixings. In this way, as for the NaOH tank it is easy to remove an empty part and replace it with a new one without having to remove any other component.

Unfortunately due to the compact design and the shape of the reactor differently to the NaOH tank it has not been possible to use a quick release device for this components.

6.3.5 Connections

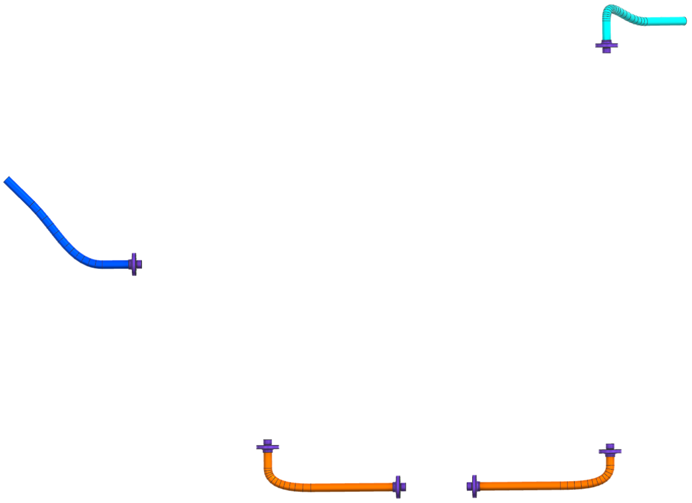


Figure 6.22: Connections assembly

In figure 6.22 it is possible to see the connections needed to link together all the components of the system.

In order to guarantee the proper functions of the system is important to consider that these connection have to ensure that the inner pressure is respected. For this reasons sealing have been employed. Many commercial products are available with standardised sizes [5] that guarantee that the connections work efficiently without any leakage. These sealing have been installed non only on the connections but also between the coupled parts of the single components of the system, as can be seen in the technical drawings in appendix B.

Furthermore it has to be considered that the pipes have to be in touch with the solution of NaOH and water, which purpose is to react with aluminium. Thus aluminium is not a viable choice for the pipes because it will be consumed by the solution itself. The pipes have to carry also the hydrogen produced from the reactor tower to the fuel cell with all the problems related to its transportation such as hydrogen embrittlement, as seen in paragraph 2.2. The industry is already prepared for this kind of challenges and for all the reasons taken into consideration "H_2 ready pipes" have been selected [3].

6.3.6 System working principle

Summing up the description of the previous paragraphs related to the single elements, in figure 6.23 is showed a section of the system with the working principle scheme. For the purpose of the desired applications the system is designed to be coupled with a PEM fuel cell. In figure 2.2 in 2.3.1 it can be seen a schematic representation of the PEM fuel cell together with the explanation of its working principle.

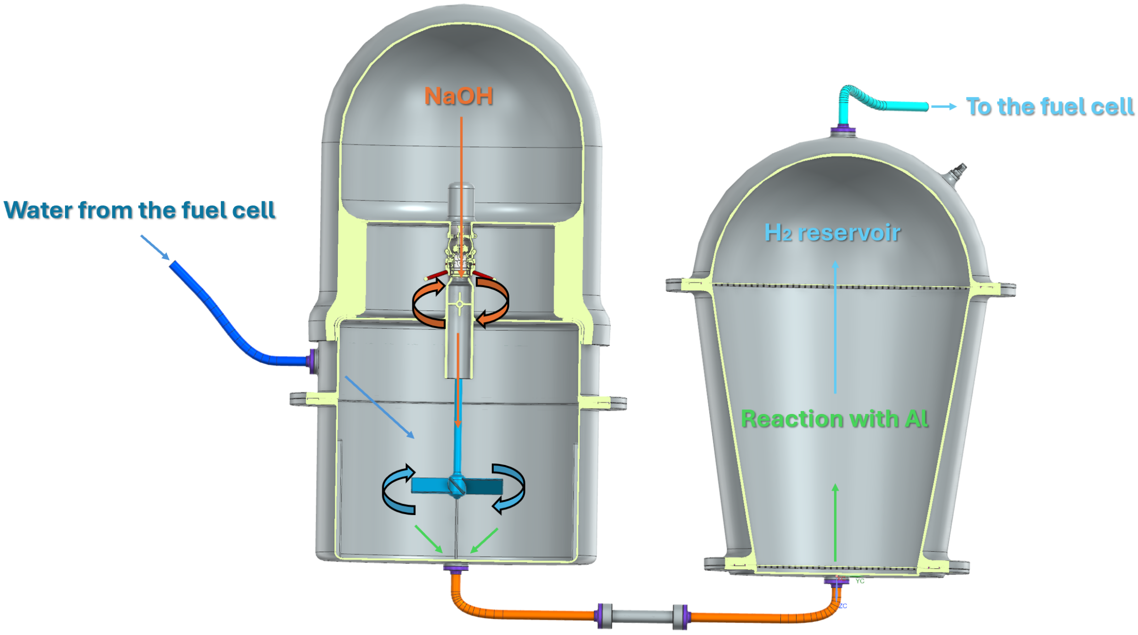


Figure 6.23: System working principle

Starting from the left of figure 6.23 the working principle is the following:

- As can be seen in blue thanks to the virtuous circle described in section 5.4 and showed in figure 5.6 water is recovered from the fuel cell during the process and is sent back to the mixer tank

- Once know the amount of water introduced into the tank the doser is actuated letting NaOH entering the mixer from the tank positioned on top of it.
- As described in paragraph 6.3.2 adding NaOH to water, rather than water to NaOH, better controls the exothermic dissolution. To ensure that the two reactants mix completely before entering in touch with the aluminium the propeller is activated.
- Exiting the mixer tank the solution is forced to pass trough the static mixer as additional element that helps completing the mixing.
- The solution then enters from the bottom of the reaction tower and rises inside the main chamber where aluminium is present. Once that the mixed solution enters in contact with the aluminium the reaction starts and hydrogen and $NaAl(OH)_4$ are produced. The production is regulated via the working principle described in section 6.3.4.
- The hydrogen produced is used to supply the PEM fuel cell.

6.4 Choice between Al powder and foils

It's important to consider that it's possible to introduce aluminium in the reactor in various forms. The main ones are as powder and as foils. Not only the powder is more appropriate when considering that can be retrieved directly from the products of aluminium scrap recycling process but it can increase the effectiveness of the reaction compared to aluminium foils.

The trends of hydrogen production as a function of time throughout the involved reaction are shown in Fig. 6.24 and Fig. 6.25 and for 1M NaOH/water solution reacting with aluminium powder and sheet, respectively. Hydrogen amount is presented as a volume over mass of aluminium used. In general, and particularly in Fig. 6.25 the profiles reveal three distinct phases throughout the reaction:

- an initial phase: the reaction has just started and the slope is rather low;
- an acceleration phase: rapid increase in produced hydrogen over time (i.e., steeper slope);

- a final phase: the curve grows at a slower rate, approaching stabilization before the end; reaction rate slows down even further slowed down as the reactants are depleted and the reaction approaches equilibrium (i.e., plateau).

Evidence of the complex nature of the process appears evident in the curves related to aluminium sheets Fig. 6.25, where the duration of each test is far more prolonged compared to that related to aluminium powder (Fig. 6.24). [24]

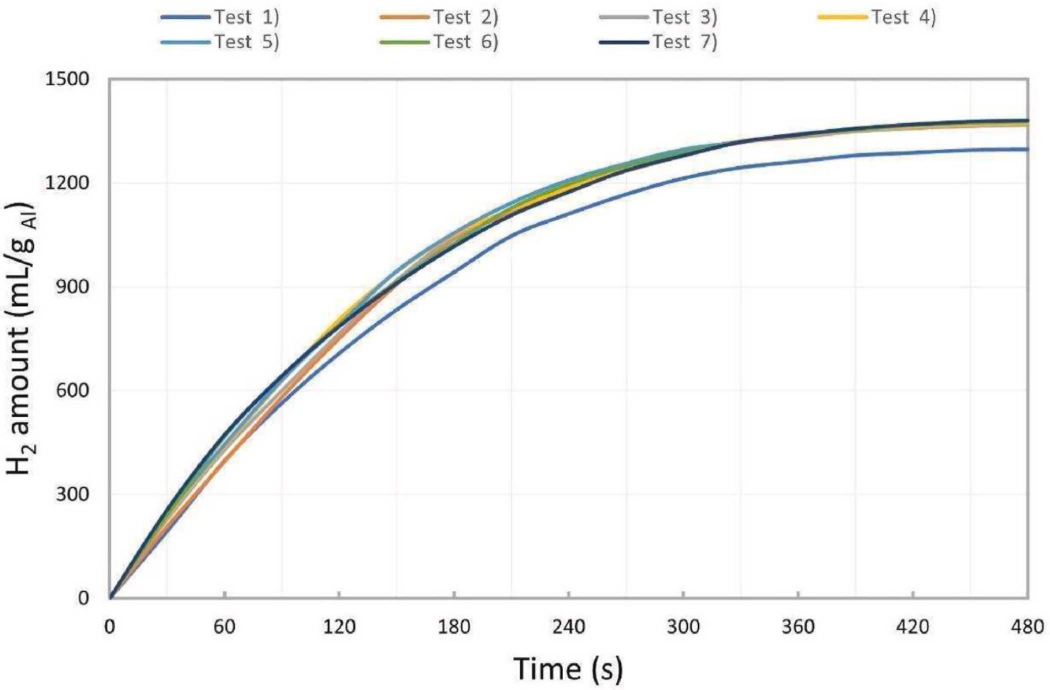


Figure 6.24: Aluminium powder reacting with 1 M NaOH aqueous solution: hydrogen produced at room temperature normalized by the amount of employed aluminium, as a function of time, seven repeats displayed.

This significant difference can be attributed to the higher specific surface area of aluminium powder which makes a larger surface available for interaction and reaction with water per unit mass.

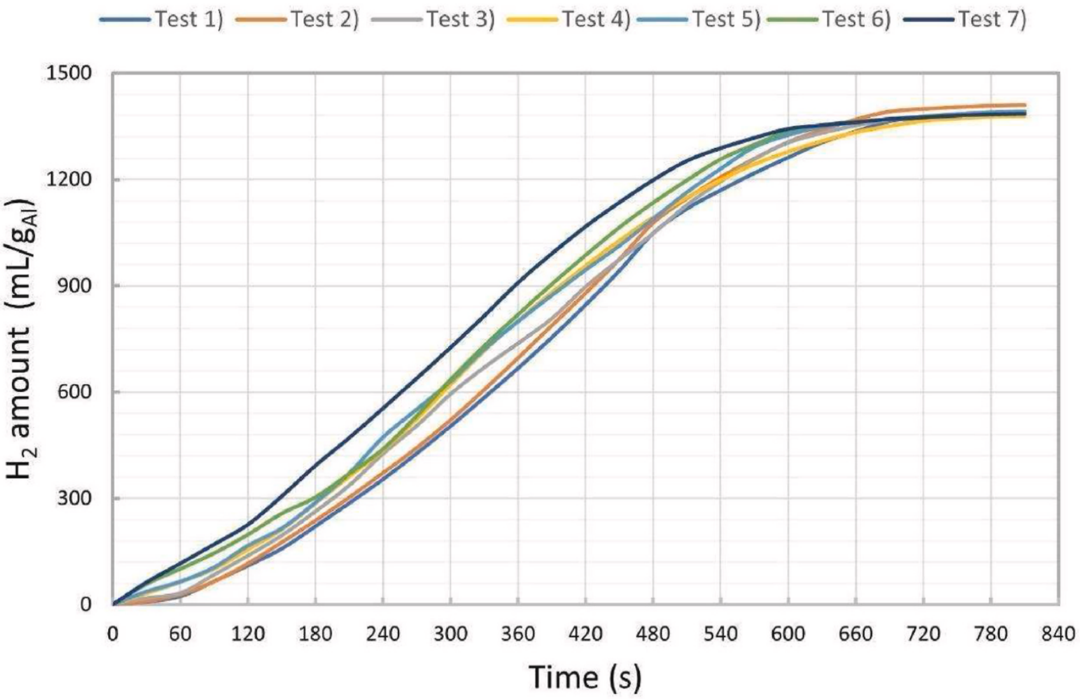


Figure 6.25: Aluminium sheets reacting with 1 M NaOH aqueous solution: hydrogen produced at room temperature normalized by the amount of employed aluminium, as a function of time, seven repeats displayed.

Furthermore not only the degree of fragmentation of aluminium samples but also molarity of the NaOH/water solution impact on the reaction kinetics. In the case of aluminium powder, the increase in NaOH concentration makes reaction rate increase by about six times, while a twofold increase occurs in the case of aluminium sheets [24]. For this reasons ensuring the proper concentration is pivotal for the system architecture.

Chapter 7

Environmental impact analysis

One of the key factors of the system usage is the possibility to use hydrogen to generate clean energy. For this reason is important to evaluate the overall environmental impact of the system, taking into consideration the raw materials supply and the products usages.

7.1 Al acquire from waste

For the intended use and the efficiency of the reaction what matters are not the mechanical characteristics but the purity of the aluminium. Thus it is possible to employ recycled aluminium instead of mining new one, consequently reducing significantly the the environmental impact of the aluminium supply chain.

Aluminium can be recycled indefinitely without losing its metallurgical quality; recycling uses about a 5% of the energy needed to make primary aluminium from bauxite. [1]

Not only recycling aluminium is beneficial for the use of a material widely diffused and available but also the environmental impact benefits from the parallel the energy savings. Primary aluminium production in 2022 generated approximately 15.1 tonnes of CO_2 equivalent per tonne of aluminium produced, while recycled aluminium production created only about 0.52 tonnes of CO_2 equivalent per tonne. This represents a carbon footprint reduction of nearly 97%. The environmental impact reduction is directly due to lower energy consumption and avoiding resource extraction activities.

[21]

The environmental benefits extend beyond emissions reduction. Recycling aluminium conserves water resources as well, with recycled production requiring much less water than primary production. This water conservation is increasingly important as many regions face growing water scarcity issues. Collectively, these environmental benefits make aluminium one of the most valuable materials to recycle. Its infinite recyclability without quality degradation means each recycling cycle delivers these environmental advantages repeatedly, creating a sustainable material cycle that helps protect the planet's resources for future generations.[21]

Furthermore the recycling process is being improved thanks to new technologies such as laser-induced breakdown spectroscopy (LIBS). This technology uses lasers to measure the unique light signature of materials, enabling more accurate sorting of aluminium alloys and resulting in higher-grade recycled materials.[21]. However, one of the benefits of this solution is that it can work with mixed aluminium alloys, which are difficult to separate, without affecting its working principle.

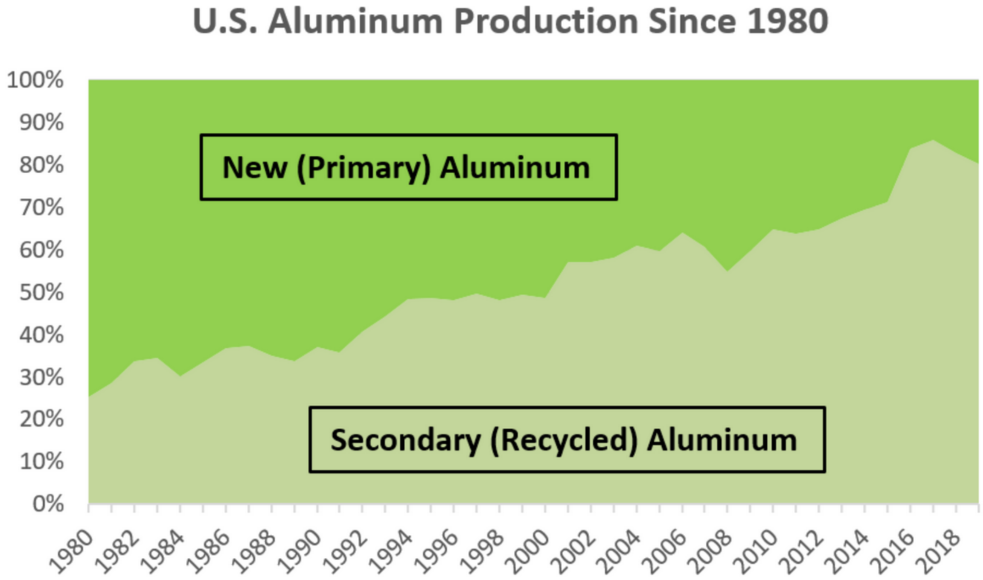


Figure 7.1: United states recycled aluminium growth

The generic industrial steps for aluminium recycling are: collection ⟶ sorting (often with eddy-current separators that "kick out" non-magnetic aluminium from mixed waste) ⟶ shredding/cleaning ⟶ melting ⟶ casting into ingots, sheet or billets.

Taking into consideration for example the united states of america more than 80% of U.S.A. production today is recycled (or secondary) aluminium. As can be seen in figure 7.1 this compares to 20% to 30% recycled production in the 1980s.[1]

It has to be taken into consideration also that recycling the aluminium already present is very helpful to reduce dependence on raw materials that aren't worldwide available.

7.2 Sodium aluminate ($NaAl(OH)_4$) usages

The product of the reaction sodium aluminate ($NaAl(OH)_4$) is an interesting material that can be used in many different applications. Thus after the usage in the vehicle , when the central part containing the product of the reaction is removed, it is possible to retrieve it and employ it in other industries.

Sodium aluminate primary usages

- Water treatment (Coagulation Aid)
- Construction (accelerator for concrete)
- Paper manufacturing (Retention aid)
- Precursor for aluminium hydroxide and alumina production

Thanks to these many usages the production of sodium aluminate ($NaAl(OH)_4$) during the production of hydrogen is not to be seen as the production of waste that has to be properly handled but instead as a very useful material that can be employed in many different industries. Using the sodium aluminate obtained as side product of the reaction will allow to avoid using other methods to retrieve $NaAl(OH)_4$ in these other industries.

7.2.1 Water Treatment

Sodium aluminate serves as a coagulant aid in both drinking water and wastewater treatment, promoting flocculation of suspended solids, removing phosphates, silica, and heavy metals while raising alkalinity without needing lime. [23]

Construction applications

In construction, sodium aluminate accelerates concrete solidification, especially in cold or frosty conditions, by acting as an additive that boosts early strength and durability. When added to cement or concrete mixes, sodium aluminate improves chemical resistance and reduces permeability. These factors extend the longevity of structures, especially in harsh environments. [23]

7.2.2 Paper manufacturing

Sodium aluminate enhances paper production by improving filler retention, sizing, and pitch control, leading to brighter, stronger sheets with less waste. [6]

7.2.3 Aluminium hydroxide production

The Bayer process is as a method for alumina recovery that involves digesting crushed bauxite in strong sodium hydroxide solutions at high temperatures, resulting in the dissolution of alumina and the formation of an insoluble residue known as "red mud." The process consists of two main stages: digestion and decomposition, ultimately producing alumina with varying forms and purities. [2]

Sodium aluminate serves as a critical intermediate in the Bayer process and other methods for producing high-purity aluminium compounds, specifically aluminium hydroxide ($Al(OH)_3$) and calcined alumina (Al_2O_3).

While the Bayer process typically starts with bauxite ore, sodium aluminate solutions are often generated during the digestion phase and then seeded to precipitate pure aluminium hydroxide. Aluminium hydroxide is precipitated from sodium aluminate solution bubbled with carbon dioxide, which is usually called carbonation decomposition process in alumina industry. [11]

Chapter 8

Conclusions

This thesis work has focused on the modelling of a reactor for H_2 production from aluminium in a NaOH solution for vehicle applications.

The work has covered all the design phases from the product planning to the final design, including the production of the technical drawings of the parts and the assembly. Starting from a very simple system such as of the Kipp's apparatus it has been possible to adapt the working principle to a more complicated system.

In this way it has been possible to develop a design that satisfies all the requirements expressed in table 4.1, ensuring that all the demands are met with a round design suitable for automotive integration.

The system's dimensions remain within the prescribed limits, resulting in a small packaging that ensures ease of installation on the desired vehicles. Furthermore the weight of the system is comparable to the weight of the devices that are not needed compared to a traditional ICE or hybrid vehicle, contributing to minimal impact on vehicle performance and efficiency. The system has been designed to effectively work within the required temperature range of -20°C to 100°C, ensuring functionality in diverse environment and driving conditions along all the seasons and the world. Safety has been rigorously addressed through the implementation of the hydrogen production stop working principle retrieved from the Kipp's apparatus.

The system has been designed to handle frequent cycling, having to stop only to replace products and reactants when they finish. In terms of operational performance, the system achieves a refuelling interval for an average car of 200 km, meeting the demand for practical driving range. This is possible also thanks to the choice of supplying separately the reactants and mixing them on board.

The system architecture has been thought with a modular design approach, enhancing flexibility of use at different scales based on the application desired. Maintenance requirements have been minimized, with service intervals extending beyond one year, aligning with user convenience and reduced lifecycle costs. Additionally it is to underline that the system produces pure hydrogen, perfectly suitable to be used in a fuel cell to produce electricity ensuring high efficiency.

In conclusion, the system brilliantly faces all the challenges encountered. Many aspects have still room for improvement but a good foundation has been layed down for further developments and exploration of this field.

Appendix A

Developed scripts

A.1 Main code

This is the main code.

```
clear; clc;

%% === CAR PARAMETERS ===
cd = 0.24;
cr = 0.015;
A  = 2.2;
m_auto = 1545 - 131.5;
g = 9.81;
rho = 1.225;
slope = 5;

%% === WLTP CYCLE ===
d = [3100 4900 7200 8300];
v = [18.9 34.1 54.4 94]/3.6;
d_tot = sum(d);

r = 200000/d_tot; %200 km var

s_break = [0 cumsum(d)*r];
v_vals = [v v(end)];
```

```
v_fun = @(s) interp1(s_break, v_vals, s, 'linear');

%% === CHEMICAL DATA ===
PM_Al   = 26.9815e-3; %Kg/mol Al
PM_NaOH = 39.9971e-3; %Kg/mol NaOH
PM_prod = 118.0016e-3; %Kg/mol NaAl(OH)4

gibbs_H2=242e3; %J/mol generated in the reaction

eff_PEM=0.6; % fuel cell efficiency
eff_reazione=0.98; %reaction efficiency

G_H2 = gibbs_H2 * eff_PEM * eff_reazione;

%% === DISCRETISATION ===
ds = 10;
s = 0:ds:(d_tot*r);

%% === SOLUTION ===
fun = @(n0) residuo_finale(n0, s, v_fun,m_auto, cd, cr, A,
    rho, g, slope, PM_Al, PM_NaOH, PM_prod, G_H2);

n0 = fzero(fun, [1e3 1e6]);

fprintf('\n=== RISULTATI FINALI ===\n');
fprintf('Moli iniziali reagenti: %.0f mol\n', n0);
fprintf('Alluminio iniziale: %.1f kg\n', n0*PM_Al);
fprintf('NaOH iniziale: %.1f kg\n', n0*PM_NaOH);

%% === COMPLETE PATH ===
out = simula_percorso_moli(n0, s, v_fun, ...
      m_auto, cd, cr, A, rho, g, slope, ...
      PM_Al, PM_NaOH, PM_prod, G_H2);

```

```
km = out.s / 1000;

%% === FIGURE 1: MOLES ===
figure;
plot(km, out.n_Al, 'b', ...
     km, out.n_NaOH, 'r--', ...
     km, out.n_prod, 'k', 'LineWidth', 2);
xlabel('Distance [km]');
ylabel('Moles');
legend('Al','NaOH','NaAl(OH)_4','Location','best');
grid on;
title('Moles evolution');

%% === FIGURE 2: MASS ===
figure;
plot(km, out.n_Al*PM_Al, 'b', ...
     km, out.n_NaOH*PM_NaOH, 'r--', ...
     km, out.n_prod*PM_prod, 'k', 'LineWidth', 2);
xlabel('Distance [km]');
ylabel('Mass [kg]');
legend('Al','NaOH','NaAl(OH)_4','Location','best');
grid on;
title('Mass evolution');

%% === FIGURE 3: TOTAL MASS ===
figure;
plot(km, out.m_tot, 'LineWidth', 2);
xlabel('Distance [km]');
ylabel('Total mass [kg]');
grid on;
title('Total mass');
```

A.2 Residual function

This is the code that evaluates the number necessary of moles.

```
function res = residuo_finale(n0, s, v_fun, m_auto, cd, cr, A
    , rho, g, slope, PM_Al, PM_NaOH, PM_prod, G_H2)

n_Al    = n0;
n_NaOH = n0;
n_prod = 0;

for i = 1:length(s)-1
    v = v_fun(s(i));

    m = m_auto ...
        + n_Al*PM_Al ...
        + n_NaOH*PM_NaOH ...
        + n_prod*PM_prod;

    Fd = 0.5*rho*cd*A*v^2;
    Fr = cr*m*g;
    Fp = m*g*sind(slope);

    dE = (Fd+Fr+Fp)*(s(i+1)-s(i)); %Energy needed in the
        single step

    dnH2 = dE/G_H2;

    dn = (2/3)*dnH2;

    n_Al    = n_Al    - dn;
    n_NaOH = n_NaOH - dn;
    n_prod = n_prod + dn;

    if n_Al < 0
```

```
            res = -1;
            return
        end
end

res = n_Al;
end
```

A.3 Path simulation

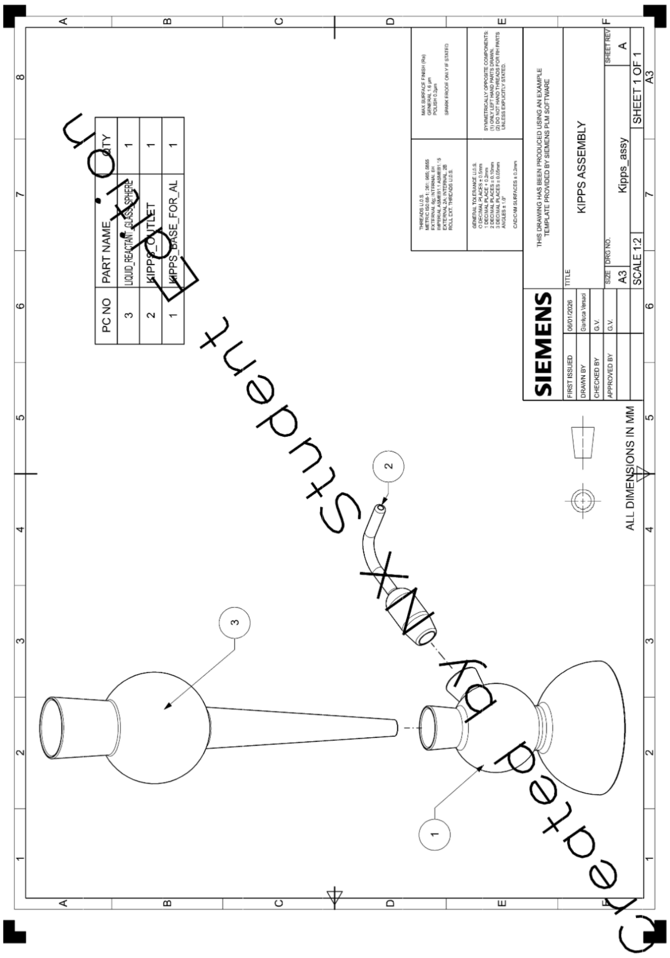
This is the code that simulates the whole path.

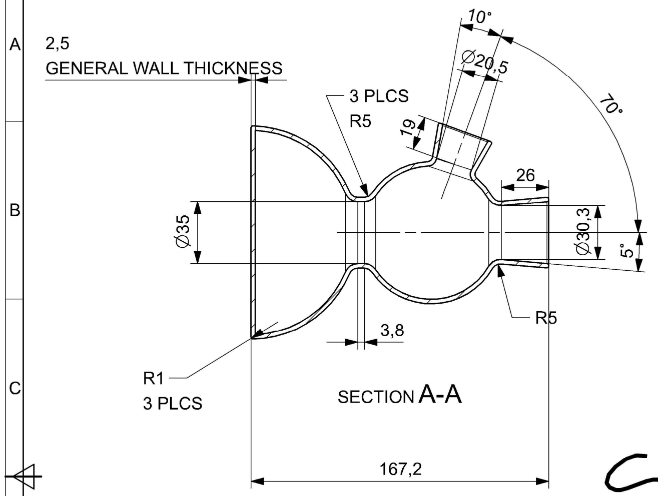
```
function out = simula_percorso_moli(n0, s, v_fun, ...
    m_auto, cd, cr, A, rho, g, slope, ...
    PM_Al, PM_NaOH, PM_prod, G_H2)

N = length(s);

% Pre allocation
n_Al    = zeros(1,N);
n_NaOH  = zeros(1,N);
n_prod  = zeros(1,N);
m_tot   = zeros(1,N);

% Initial conditions
n_Al(1)    = n0;
n_NaOH(1)  = n0;
n_prod(1)  = 0;

for i = 1:N-1
    v = v_fun(s(i));

    m_tot(i) = m_auto ...
        + n_Al(i)*PM_Al ...
        + n_NaOH(i)*PM_NaOH ...
        + n_prod(i)*PM_prod;

    Fd = 0.5*rho*cd*A*v^2;
    Fr = cr*m_tot(i)*g;
    Fp = m_tot(i)*g*sind(slope);

    dE = (Fd + Fr + Fp)*(s(i+1)-s(i));
    dnH2 = dE / G_H2;
```

```
    dn = (2/3)*dnH2;

    n_Al(i+1)   = n_Al(i)   - dn;
    n_NaOH(i+1) = n_NaOH(i) - dn;
    n_prod(i+1) = n_prod(i) + dn;
end

% final mass
m_tot(end) = m_auto ...
    + n_Al(end)*PM_Al ...
    + n_NaOH(end)*PM_NaOH ...
    + n_prod(end)*PM_prod;

% output
out.s = s;
out.n_Al = n_Al;
out.n_NaOH = n_NaOH;
out.n_prod = n_prod;
out.m_tot = m_tot;
end
```

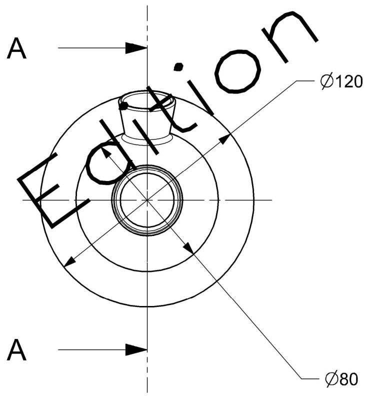
Appendix B

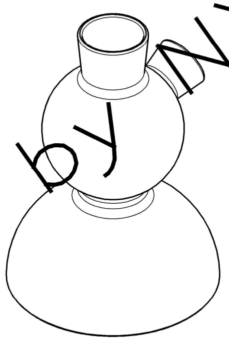
Technical drawings





SECTION A-A





NOTES:
- ISO VIEW FOR REFERENCE ONLY

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B
ROLL EXT. THREADS U.0.S.

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

SPARK ERODE ONLY IF STATED

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm
ANGLES ± 1.0°

CAD/CAM SURFACES ± 0.2mm

SYMMETRICALLY OPPOSITE COMPONENTS:
(1) ONLY LEFT HAND PARTS DRAWN.
(2) DO NOT HAND THREADS FOR RH PARTS
UNLESS EXPLICITLY STATED.

ALL DIMENSIONS IN MM

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FIRST ISSUED	06/01/2026
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CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE
KIPPS BASE FOR ALUMINUM

SIZE	DRG NO.	SHEET REV
A3	Kipps_base_for_Al	A
SCALE 1:2		SHEET 1 OF 1

A3

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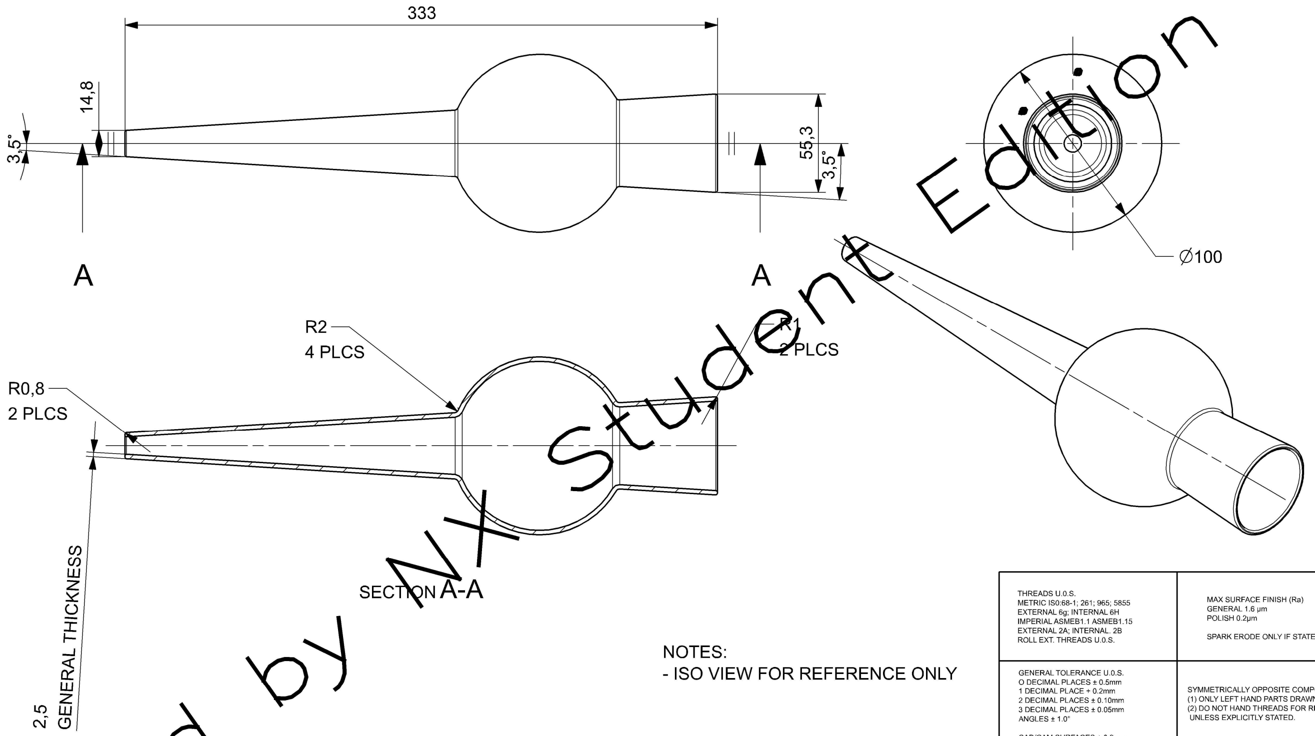

NOTES:
- ISO VIEW FOR REFERENCE ONLY

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B
ROLL EXT. THREADS U.0.S.

MAX SURFACE FINISH (Ra)
GENERAL 1.6 µm
POLISH 0.2µm

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GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
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2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm
ANGLES ± 1.0°

CAD/CAM SURFACES ± 0.2mm

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APPROVED BY	G.V.

TITLE
KIPPS LIQUID INLET

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SCALE 1:2
SHEET 1 OF 1
A3

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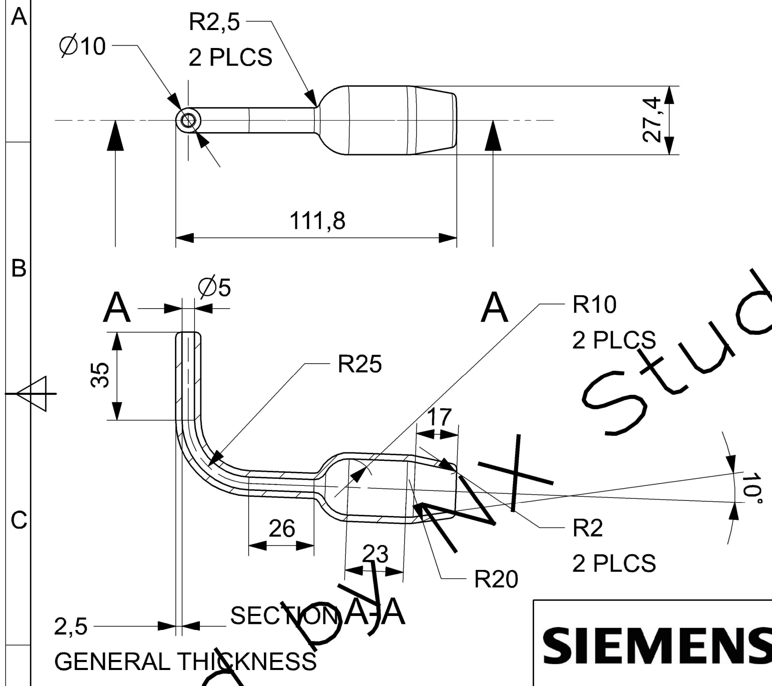

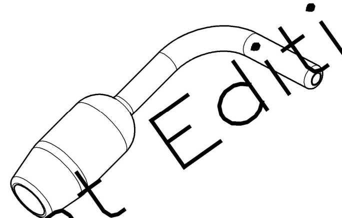

NOTES:
- ISO VIEW FOR REFERENCE ONLY

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GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0° CAD/CAM SURFACES ± 0.2mm	SYMMETRICALLY OPPOSITE COMPONENTS: (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.

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TITLE

KIPPS OUTLET

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SCALE 1:2		SHEET 1 OF 1

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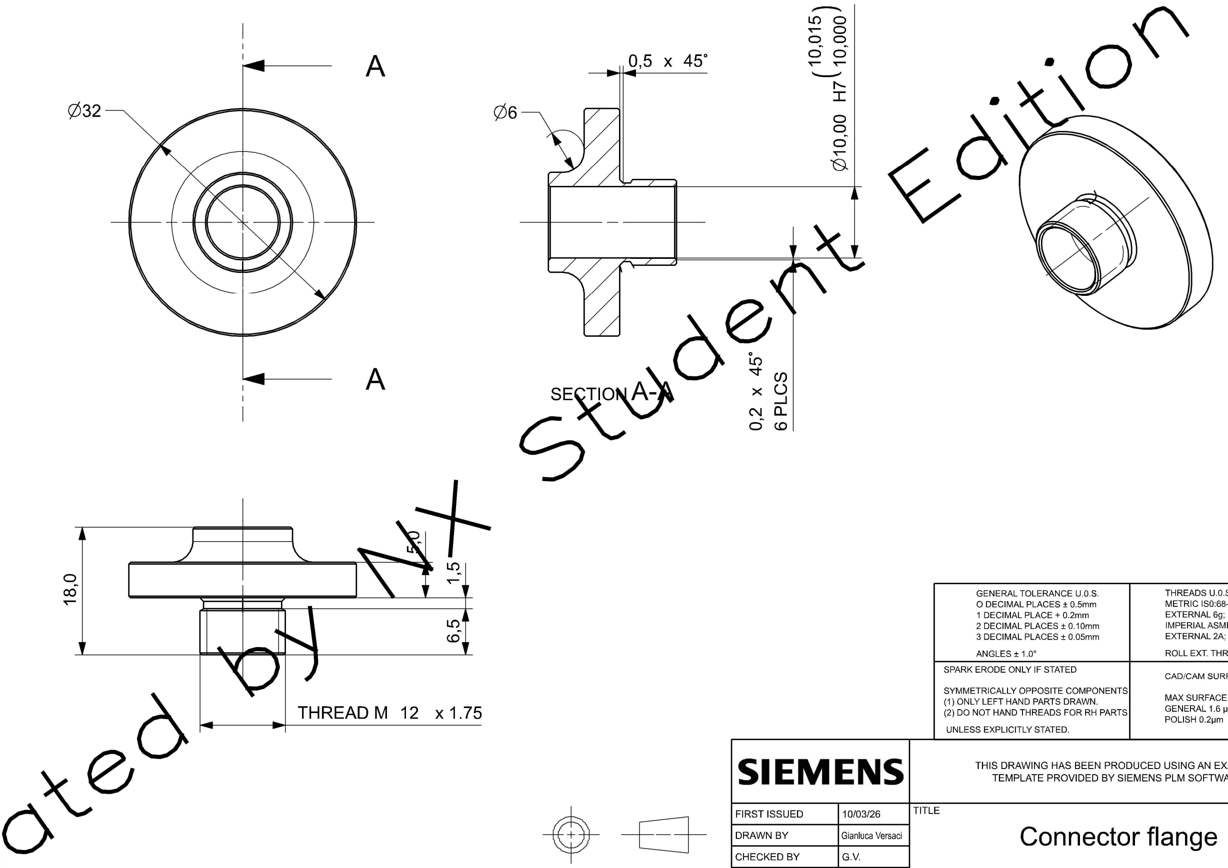

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S.
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1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

SPARK ERODE ONLY IF STATED

SYMMETRICALLY OPPOSITE COMPONENTS
(1) ONLY LEFT HAND PARTS DRAWN.
(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

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TITLE

Connector flange

SIZE	DRG NO.	SHEET REV
A3	Connectors_flange	A
SCALE 2:1	SHEET 1 OF 1	

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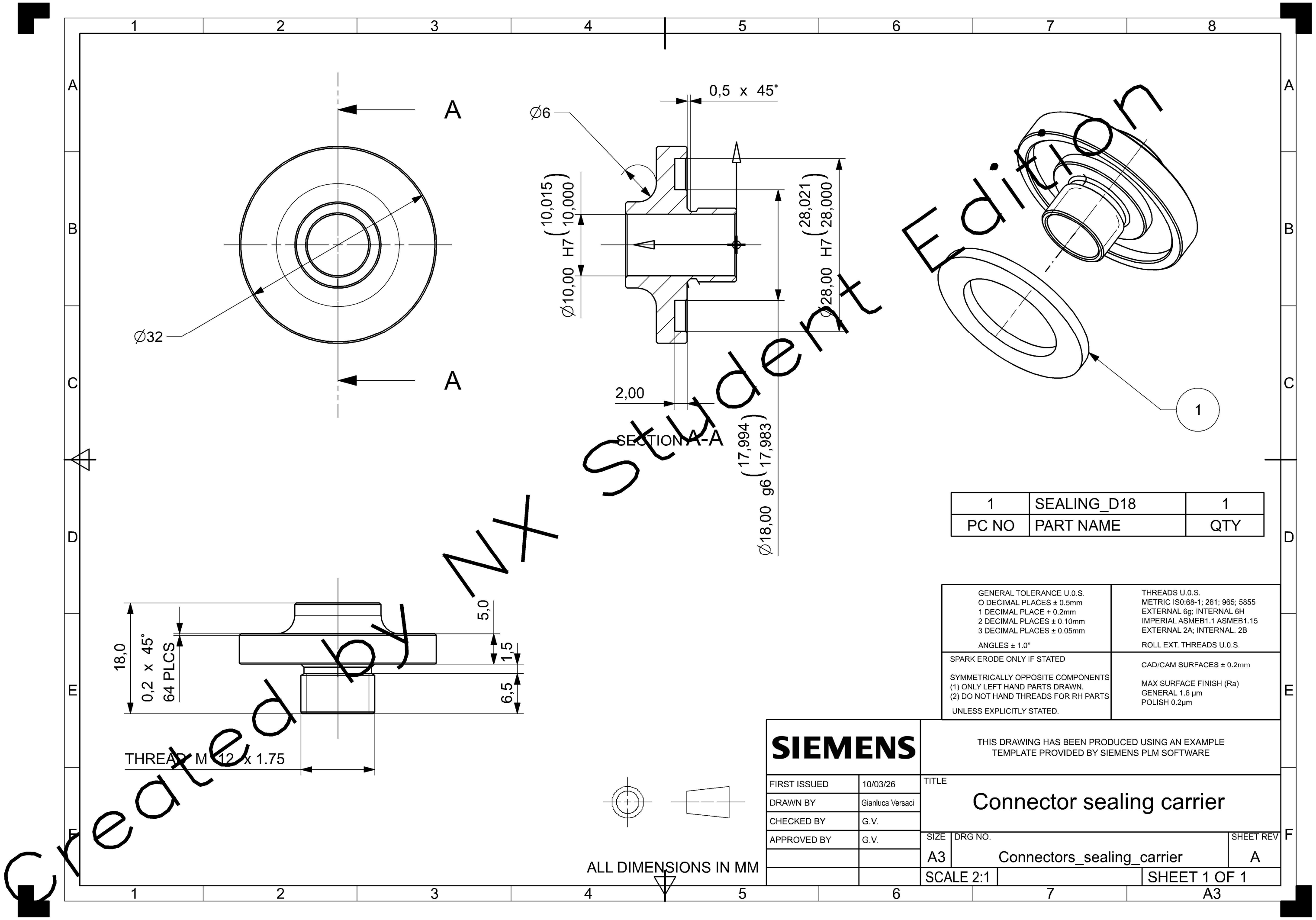

PC NO	PART NAME	QTY
1	SEALING_D18	1

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

SPARK ERODE ONLY IF STATED

SYMMETRICALLY OPPOSITE COMPONENTS
(1) ONLY LEFT HAND PARTS DRAWN.
(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

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DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE
Connector sealing carrier

SIZE	DRG NO.	SHEET REV
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SCALE 2:1
SHEET 1 OF 1
A3

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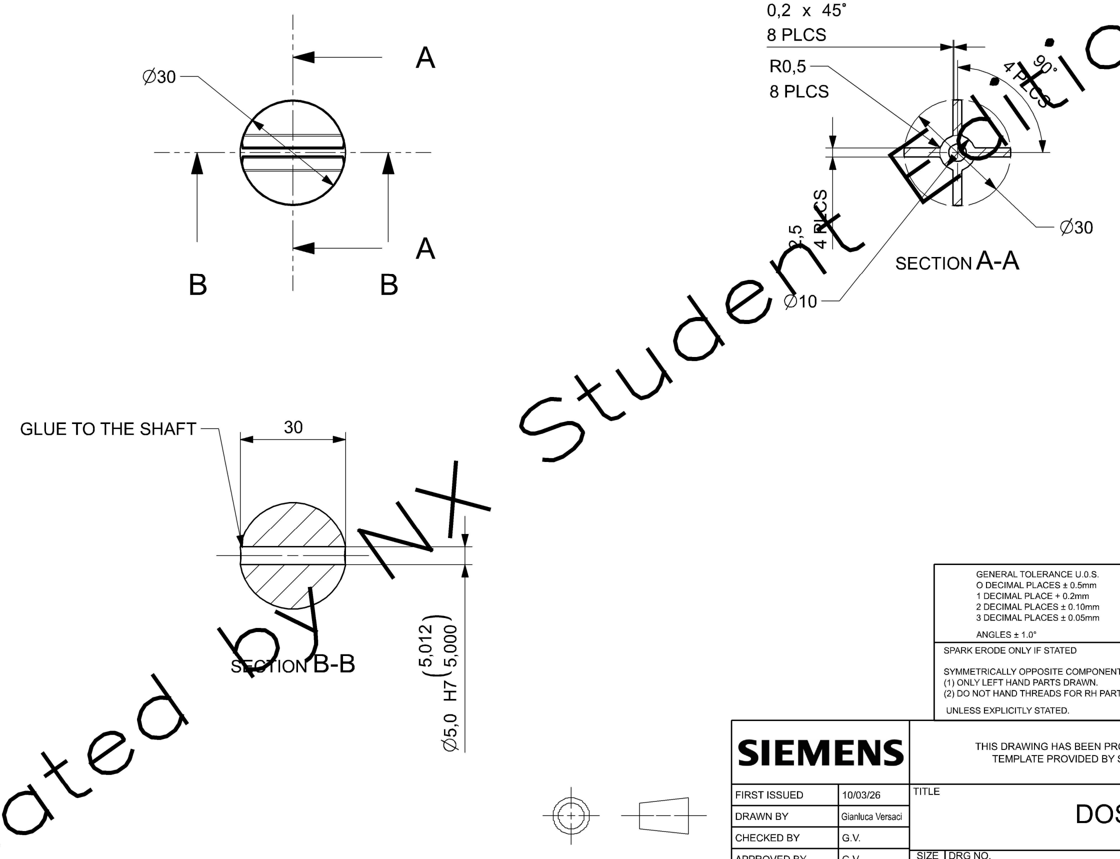

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.0.S. METRIC IS0:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL. 2B ROLL EXT. THREADS U.0.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 µm POLISH 0.2µm

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TITLE

DOSER

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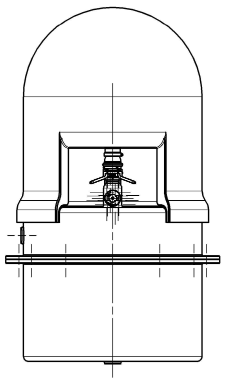
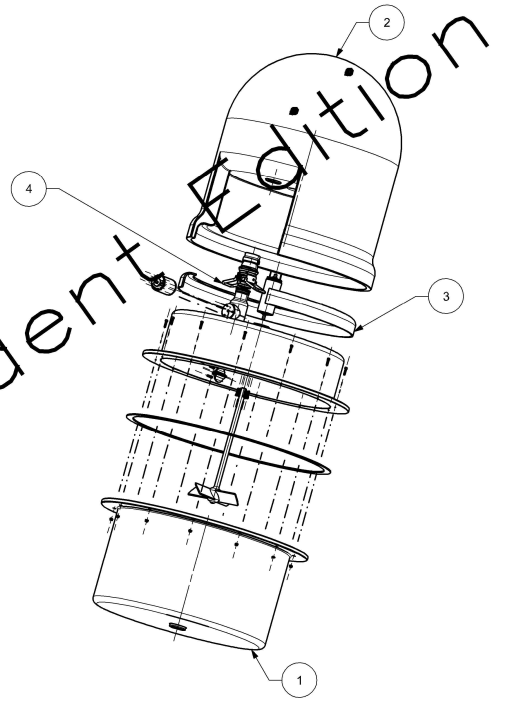
SCALE 1:1		SHEET 1 OF 1

A3

Created by NX Student Edition





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2	NAOH_CONTAINER	1
1	MIXER_ASSY	1

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

SPARK ERODE ONLY IF STATED

SYMMETRICALLY OPPOSITE COMPONENTS
(1) ONLY LEFT HAND PARTS DRAWN.
(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

SIEMENS

THIS DRAWING HAS BEEN PRODUCED USING AN EXAMPLE
TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

FIRST ISSUED	10/03/26
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

MIXER AND TANK ASSEMBLY

SIZE A2

DRG NO. N2O_NaOH_mixer_assy

SHEET REV A

SCALE 1:5

SHEET 1 OF 1

ALL DIMENSIONS IN MM

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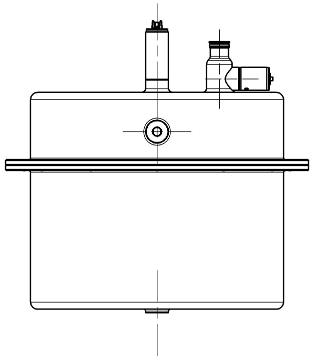

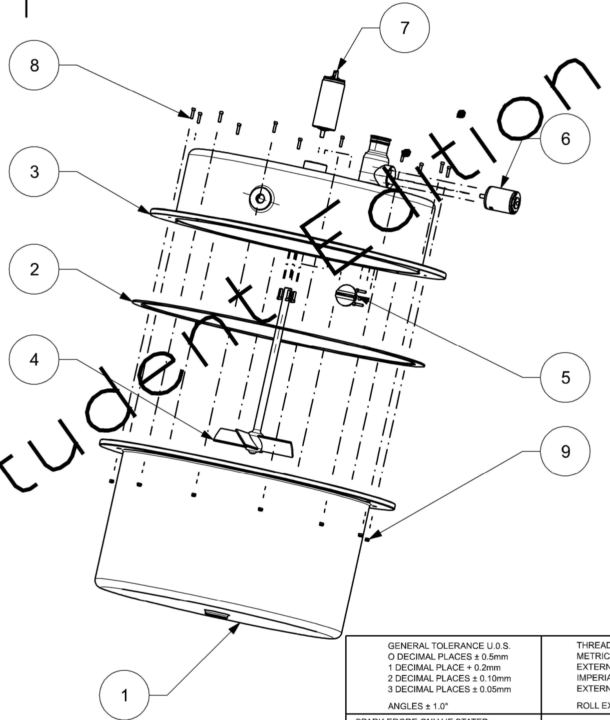

PC NO	PART NAME	QTY
9	NUT_M3	12
8	M3X12_STEP	21
7	3272G_CR_STP	1
6	AM3248_00+10_STP	1
5	NAOH_DOSER	1
4	MIXER	1
3	MIXER_TOP	1
2	MIXER_SEALING	1
1	MIXER_BASE	1

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

SPARK ERODE ONLY IF STATED

SYMMETRICALLY OPPOSITE COMPONENTS
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UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 µm
POLISH 0.2µm

ALL DIMENSIONS IN MM

SIEMENS

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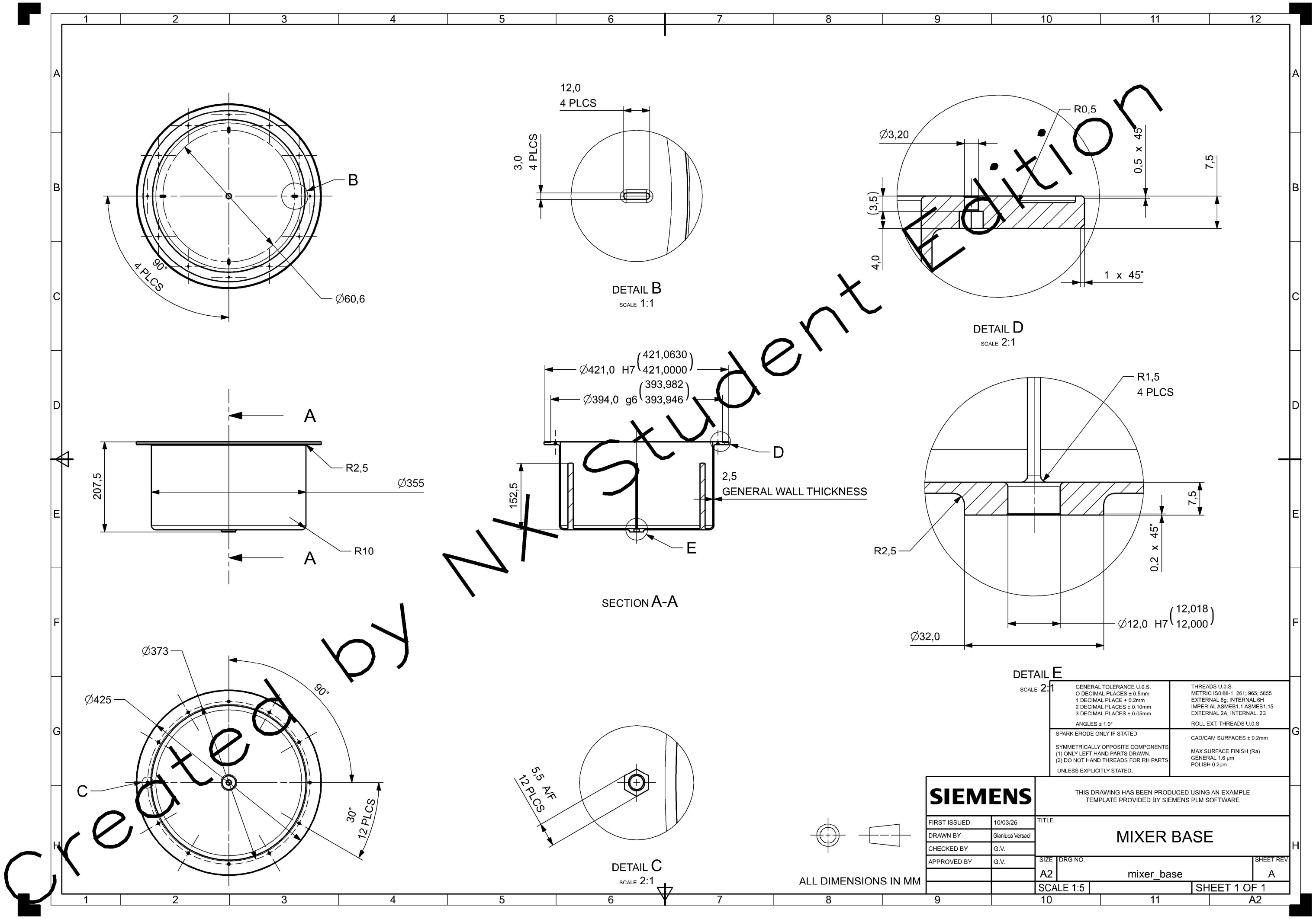
TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

FIRST ISSUED 10/03/26
DRAWN BY Gianluca Versaci
CHECKED BY G.V.
APPROVED BY G.V.

TITLE
MIXER ASSEMBLY

SIZE A3
DRG NO. mixer_assy
SHEET REV A
SCALE 1:5
SHEET 1 OF 1
A3

Created by NX Student Edition



GENERAL TOLERANCE U.O.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.O.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.O.S.

SPARK ERODE ONLY IF STATED

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(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

SIEMENS

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APPROVED BY	G.V.

TITLE

MIXER BASE

SIZE	DRG NO.	SHEET REV
A2	mixer_base	A
SCALE 1:5		SHEET 1 OF 1

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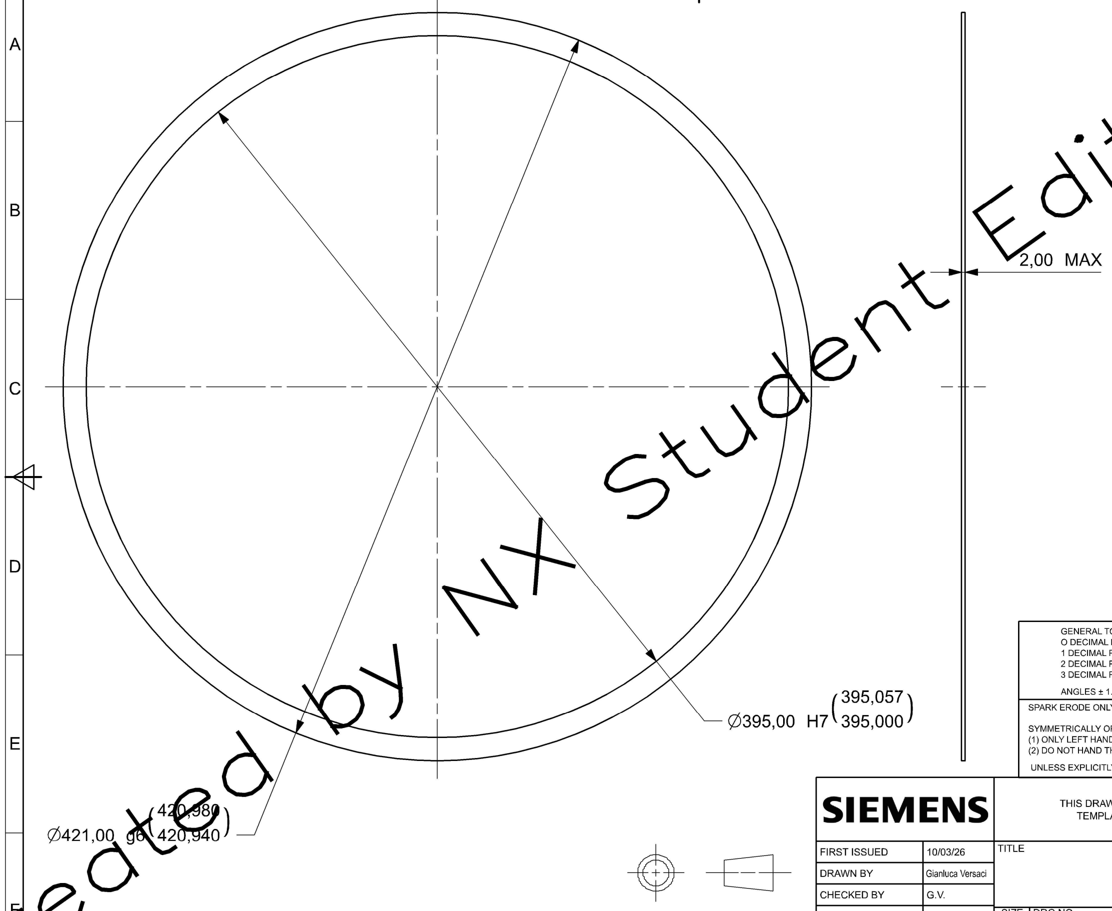

ALL DIMENSIONS IN MM

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GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.0.S. METRIC IS0:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL. 2B ROLL EXT. THREADS U.0.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 μm POLISH 0.2μm

SIEMENS

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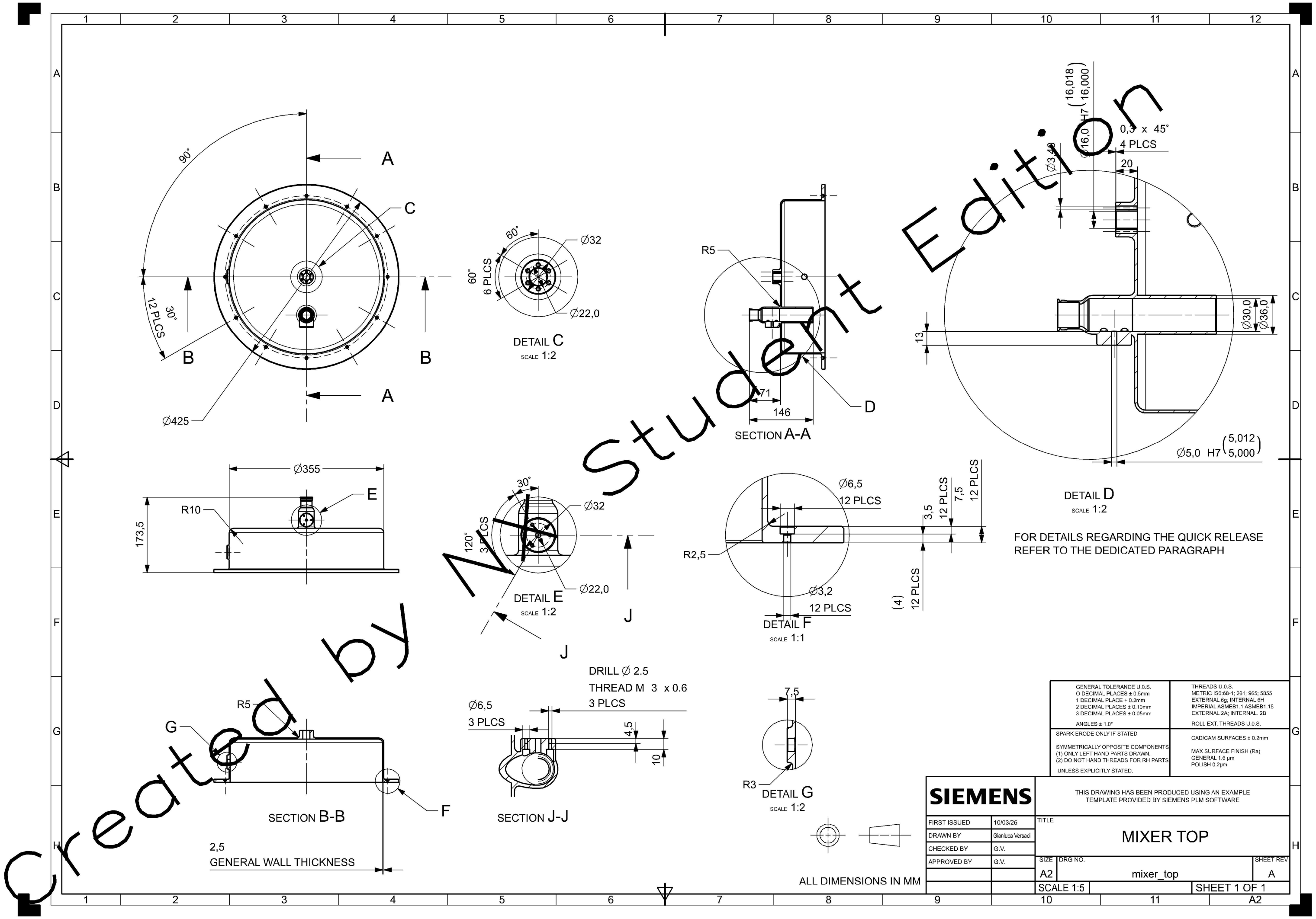
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

MIXER SEALING

SIZE	DRG NO.	SHEET REV
A3	mixer_sealing	A
SCALE 1:2		SHEET 1 OF 1



GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

SPARK ERODE ONLY IF STATED

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(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

SIEMENS

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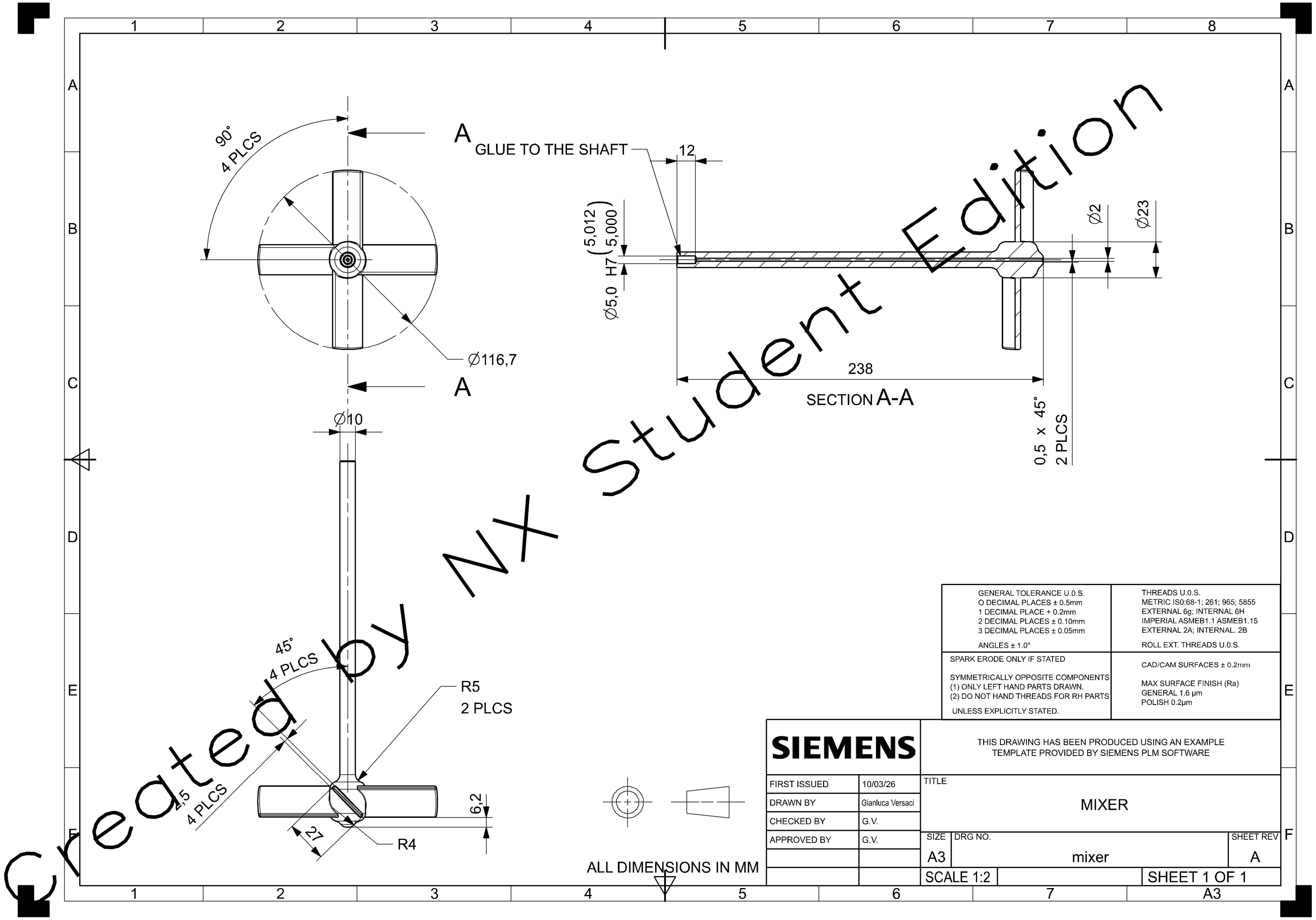
APPROVED BY	G.V.

TITLE
MIXER TOP

SIZE A2
DRG NO. mixer_top
SHEET REV A
SCALE 1:5
SHEET 1 OF 1
A2

Created by NX Student Edition



GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 µm
POLISH 0.2µm

SIEMENS

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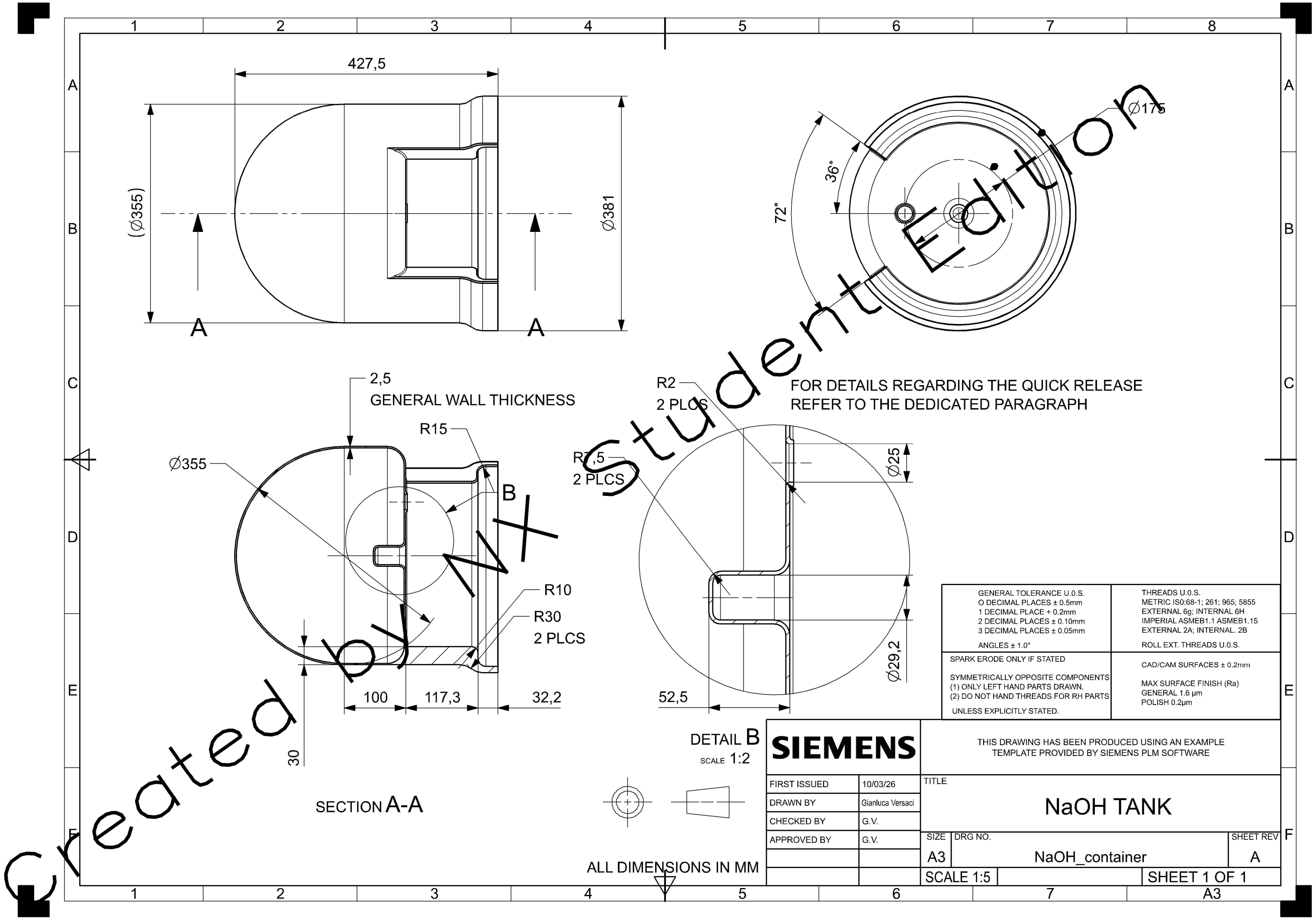
APPROVED BY	G.V.

TITLE
MIXER

SIZE	DRG NO.	SHEET REV
A3	mixer	A

SCALE 1:2
SHEET 1 OF 1

Created by NX Student Edition



FOR DETAILS REGARDING THE QUICK RELEASE
REFER TO THE DEDICATED PARAGRAPH

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
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POLISH 0.2μm

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CHECKED BY	G.V.
APPROVED BY	G.V.

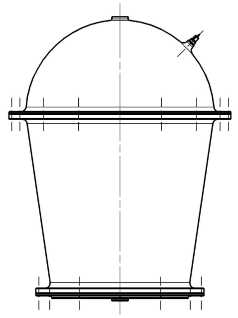
TITLE

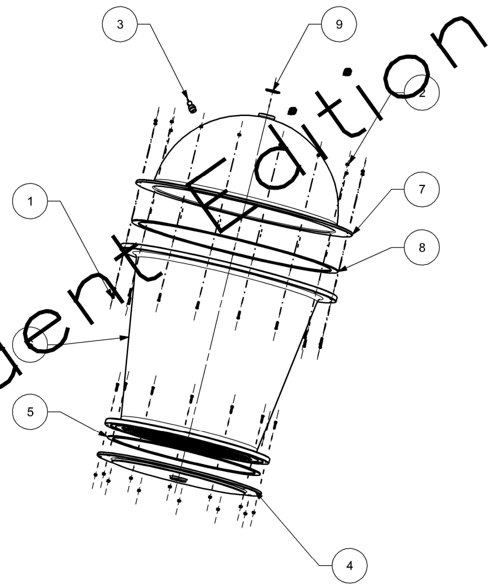
NaOH TANK

SIZE	DRG NO.	SHEET REV
A3	NaOH_container	A
SCALE 1:5		SHEET 1 OF 1

A3

Created by NX Student Edition





1	M3X12_STEP	28
2	NUT_M3	28
3	PRESSURE_RELIEF _VALVE	1
4	REACTOR_BASE	1
5	REACTOR_LOWER_ SEALING	1
6	REACTOR_MID	1
7	REACTOR_TOP	1
8	REACTOR_UPPER_ SEALING	1
9	SEALING_D18	1
PC NO	PART NAME	QTY

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

ALL DIMENSIONS IN MM

SIEMENS

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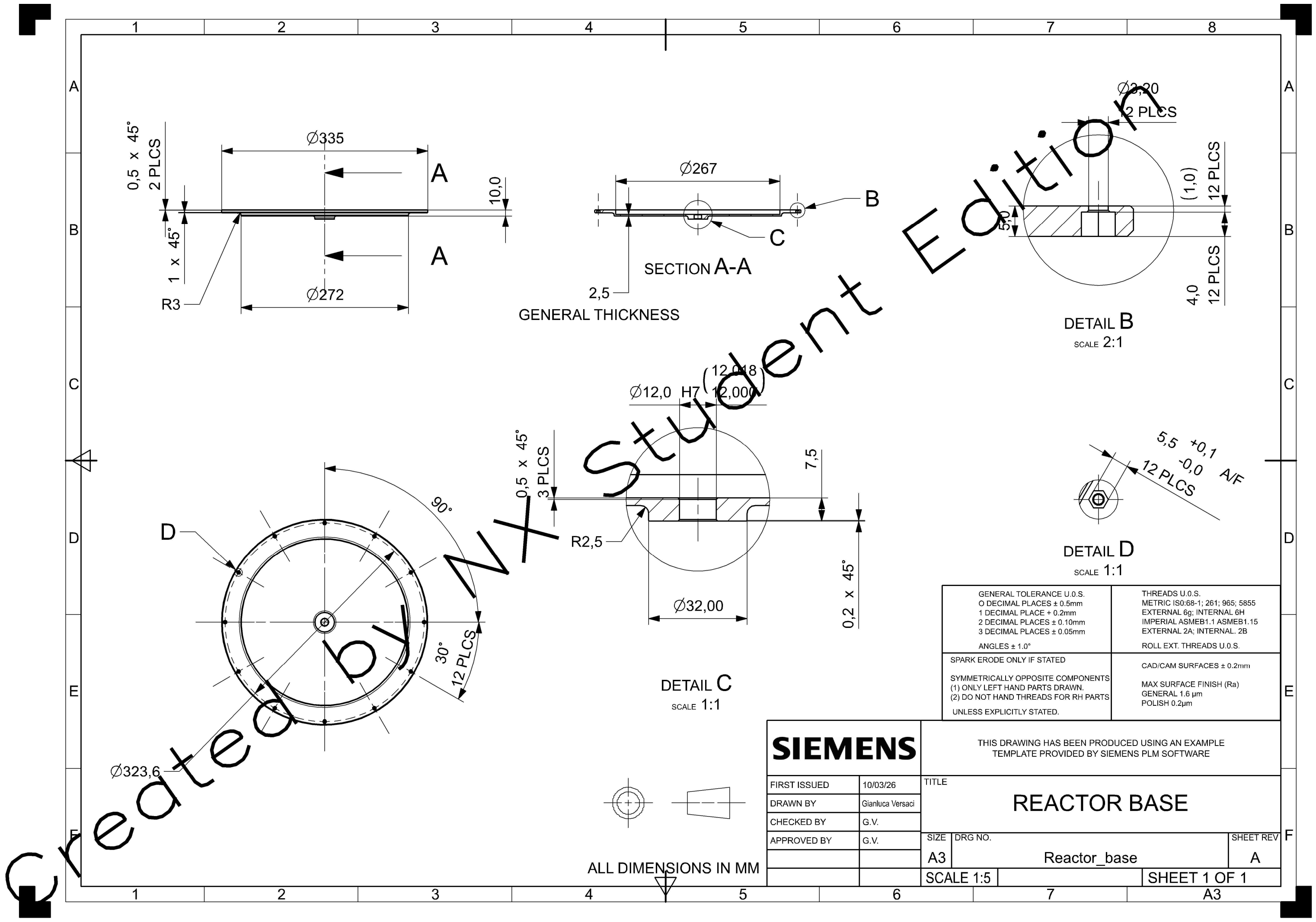
FIRST ISSUED	10/03/26
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE
REACTOR ASSEMBLY

SIZE A2
DRG NO. Reactor_assy
SHEET REV A
SCALE 1:5
SHEET 1 OF 1

Created by NX Student Edition



Created by NX Student Edition

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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(2) DO NOT HAND THREADS FOR RH PARTS

UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 µm
POLISH 0.2µm

SIEMENS

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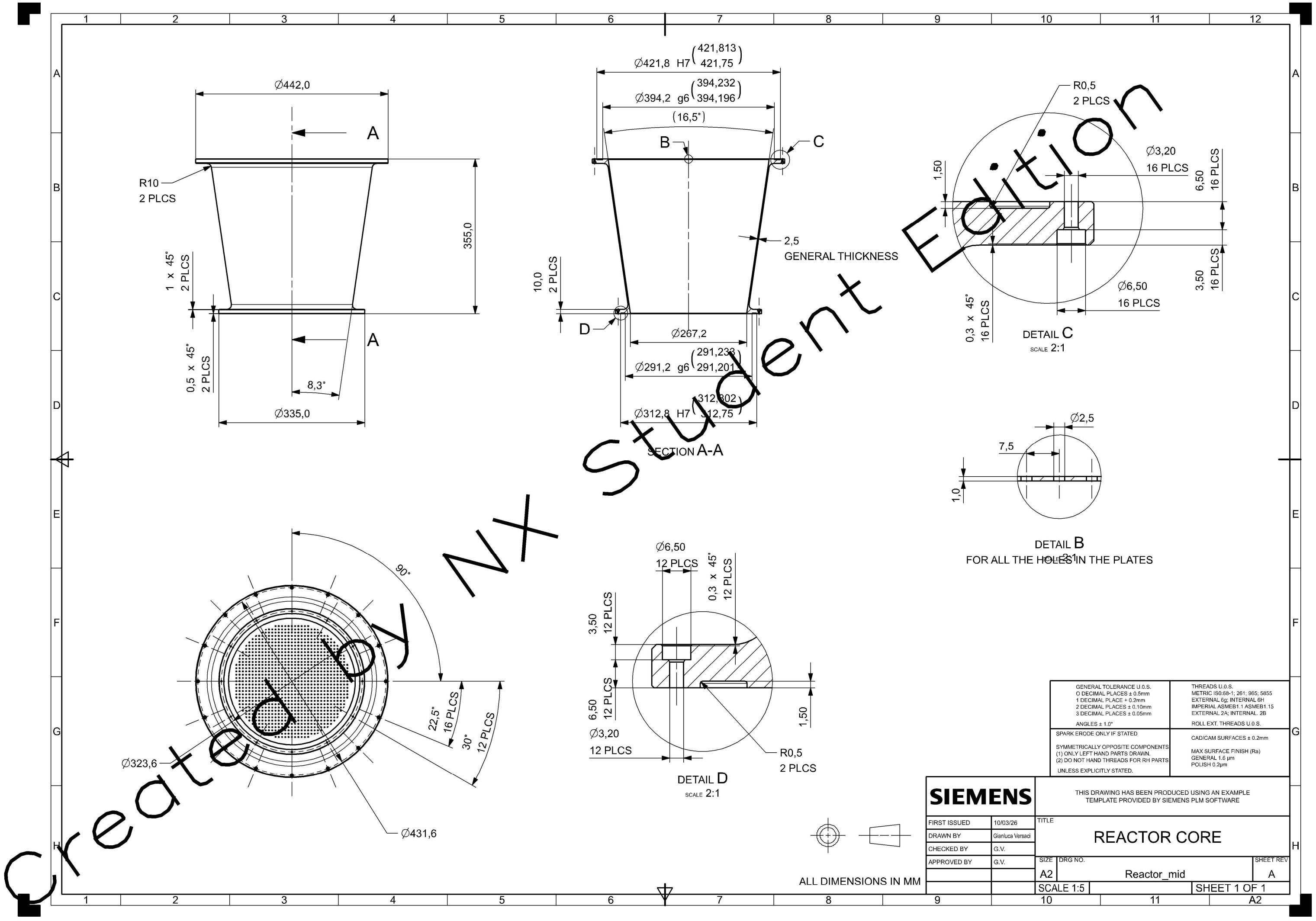
FIRST ISSUED	10/03/26
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE
REACTOR BASE

SIZE	DRG NO.	SHEET REV
A3	Reactor_base	A
SCALE 1:5		SHEET 1 OF 1



Created by NX Student Edition

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

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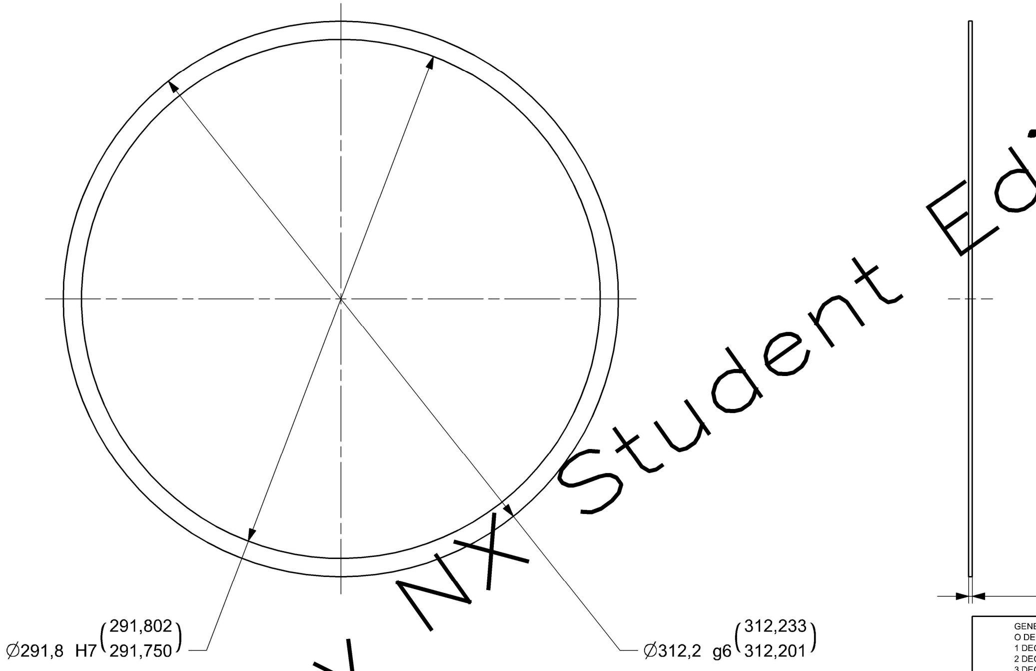
APPROVED BY	G.V.

TITLE
REACTOR CORE

SIZE	DRG NO.	SHEET REV
A2	Reactor_mid	A

SCALE 1:5
SHEET 1 OF 1
A2



GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

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CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

REACTOR LOWER SEALING

SIZE	DRG NO.	SHEET REV
A3	Reactor_lower_sealing	A
SCALE 1:2		SHEET 1 OF 1

ALL DIMENSIONS IN MM

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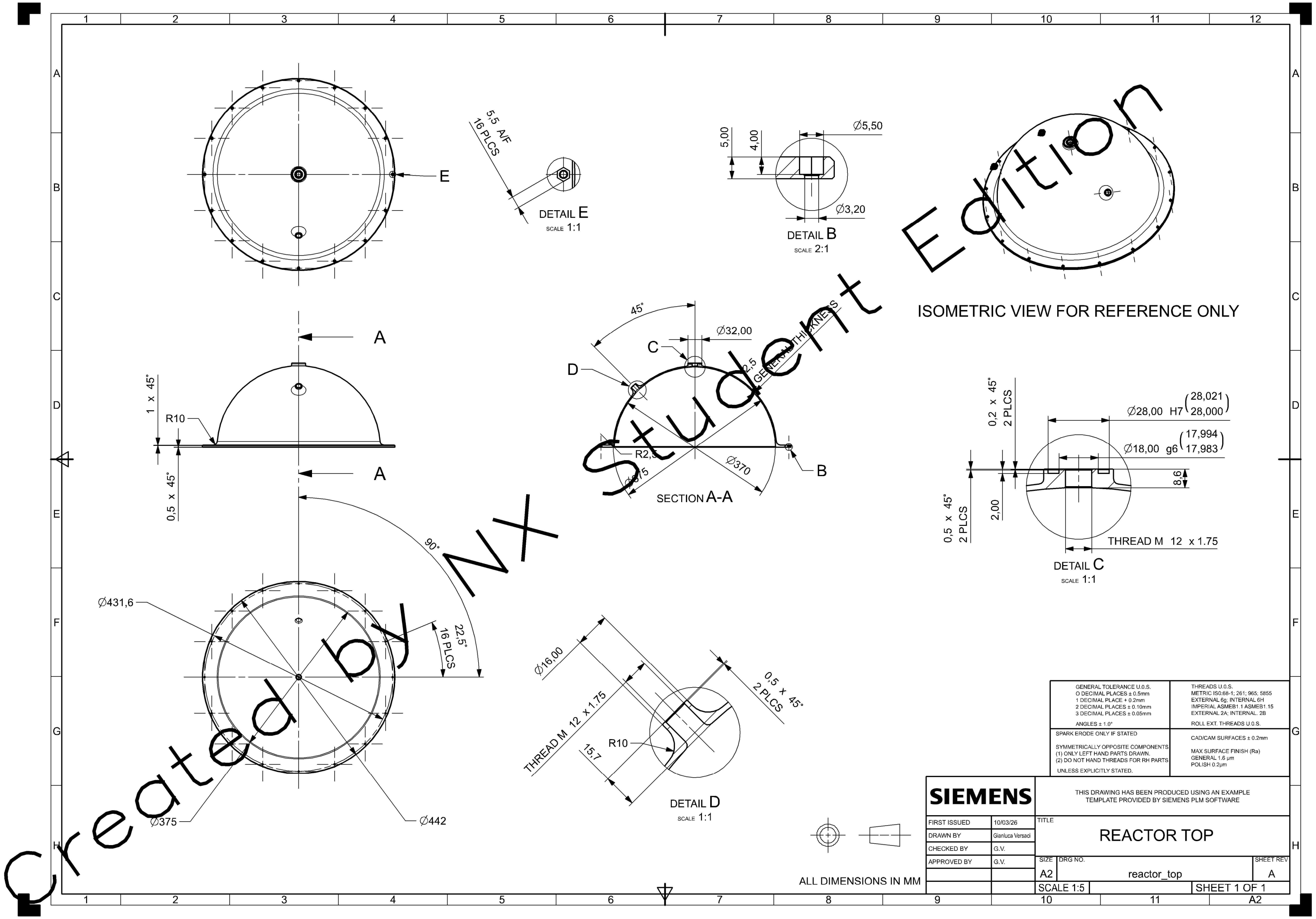

GENERAL TOLERANCE U.O.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.O.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.O.S.

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CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

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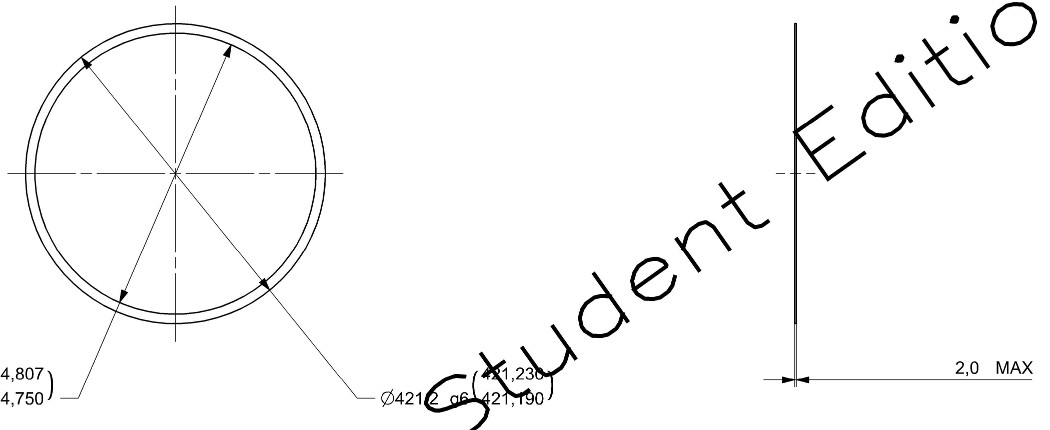
CHECKED BY	G.V.
APPROVED BY	G.V.

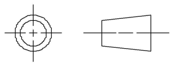
TITLE
REACTOR TOP

SIZE	DRG NO.	SHEET REV
A2	reactor_top	A

SCALE 1:5
SHEET 1 OF 1
A2

Created by NX Student Edition





ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S.
O DECIMAL PLACES ± 0.5mm
1 DECIMAL PLACE + 0.2mm
2 DECIMAL PLACES ± 0.10mm
3 DECIMAL PLACES ± 0.05mm

ANGLES ± 1.0°

THREADS U.0.S.
METRIC IS0:68-1; 261; 965; 5855
EXTERNAL 6g; INTERNAL 6H
IMPERIAL ASMEB1.1 ASMEB1.15
EXTERNAL 2A; INTERNAL. 2B

ROLL EXT. THREADS U.0.S.

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UNLESS EXPLICITLY STATED.

CAD/CAM SURFACES ± 0.2mm

MAX SURFACE FINISH (Ra)
GENERAL 1.6 μm
POLISH 0.2μm

SIEMENS

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CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

REACTOR UPPER SEALING

SIZE	DRG NO.	SHEET REV
A3	Reactor_upper_sealing	A

SCALE 1:5

SHEET 1 OF 1

A3

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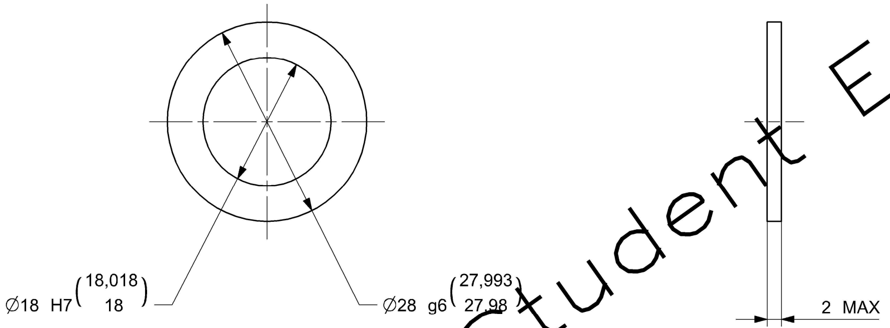

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.0.S. METRIC IS0:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL. 2B ROLL EXT. THREADS U.0.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 µm POLISH 0.2µm

SIEMENS

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TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

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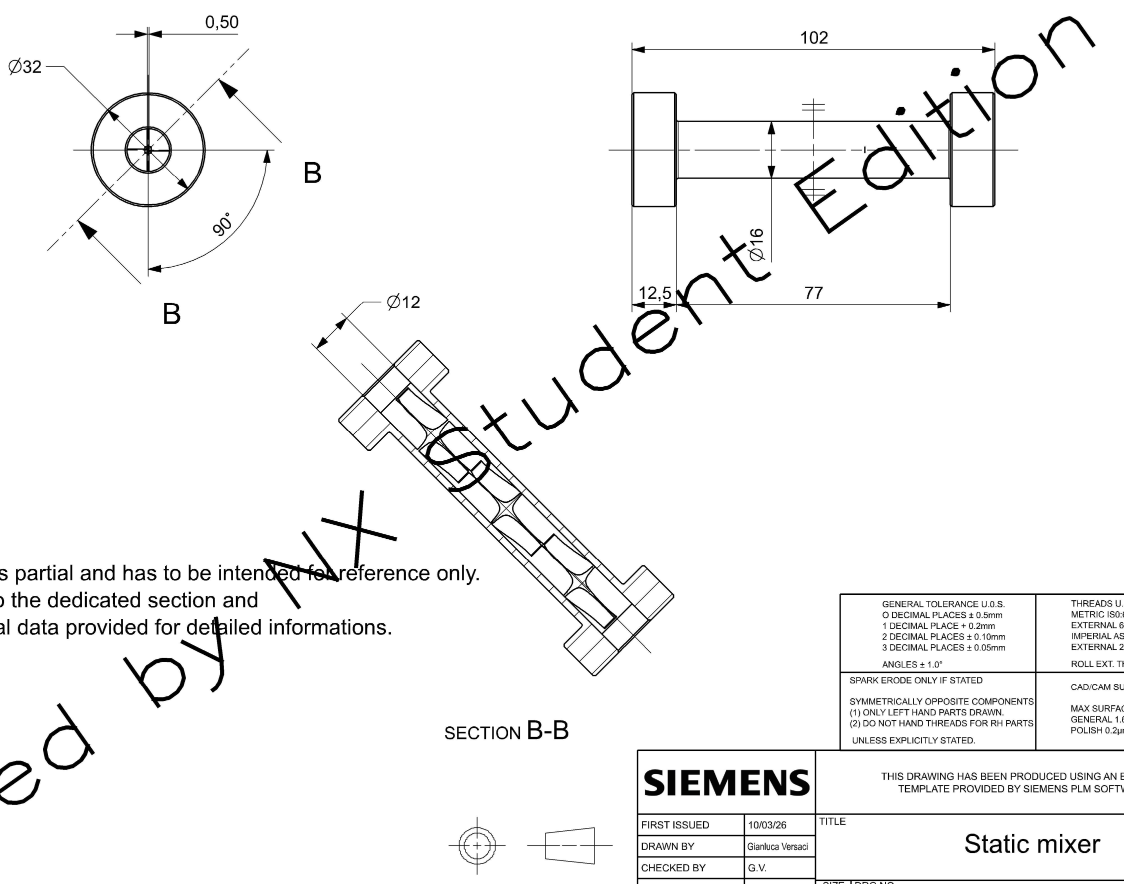
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

Sealing D18

SIZE	DRG NO.	SHEET REV
A3	Sealing_D18	A
SCALE 2:1		SHEET 1 OF 1

Created by NX Student Edition



This drawing is partial and has to be intended for reference only.
Please refer to the dedicated section and
the commercial data provided for detailed informations.

GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.0.S. METRIC IS0:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL. 2B ROLL EXT. THREADS U.0.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 μm POLISH 0.2μm

SIEMENS

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TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

FIRST ISSUED	10/03/26
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE
Static mixer

SIZE	DRG NO.	SHEET REV
A3	static_mixer	A
SCALE 1:1		SHEET 1 OF 1

ALL DIMENSIONS IN MM

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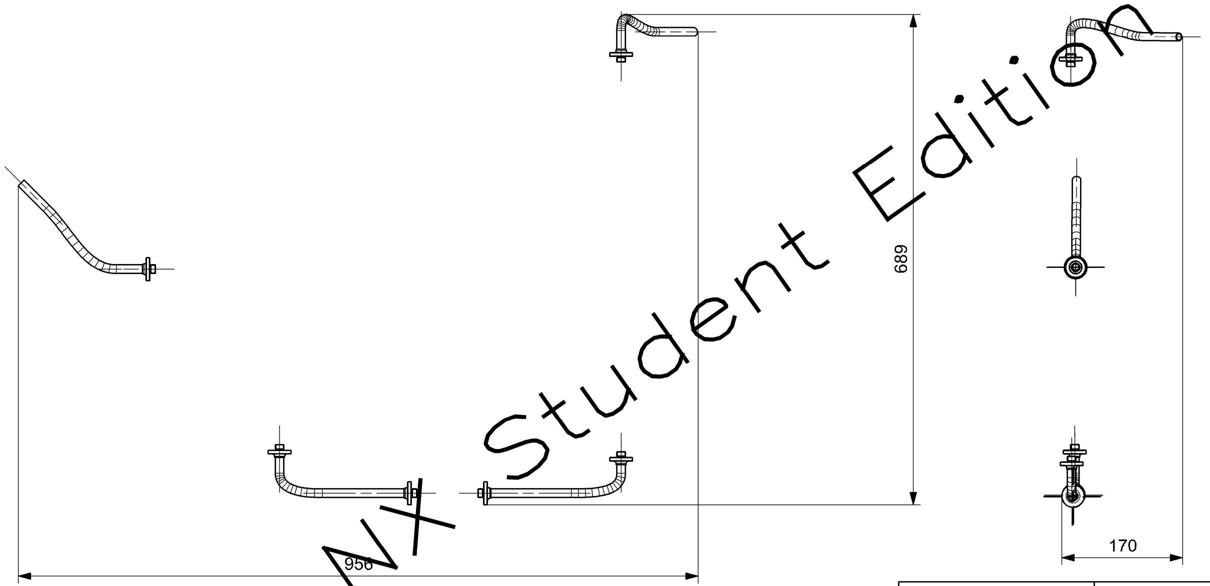

This view is partial and has to be intended for reference only.
Please refer to the commercial data provided for detailed informations

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.0.S. O DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE + 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.0.S. METRIC IS0:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL. 2B ROLL EXT. THREADS U.0.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 μm POLISH 0.2μm

SIEMENS

THIS DRAWING HAS BEEN PRODUCED USING AN EXAMPLE
TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

FIRST ISSUED	10/03/26
DRAWN BY	Gianluca Versaci
CHECKED BY	G.V.
APPROVED BY	G.V.

TITLE

Tubes assembly

SIZE	DRG NO.	SHEET REV
A3	tubes_assy	A
SCALE 1:5		SHEET 1 OF 1

A3

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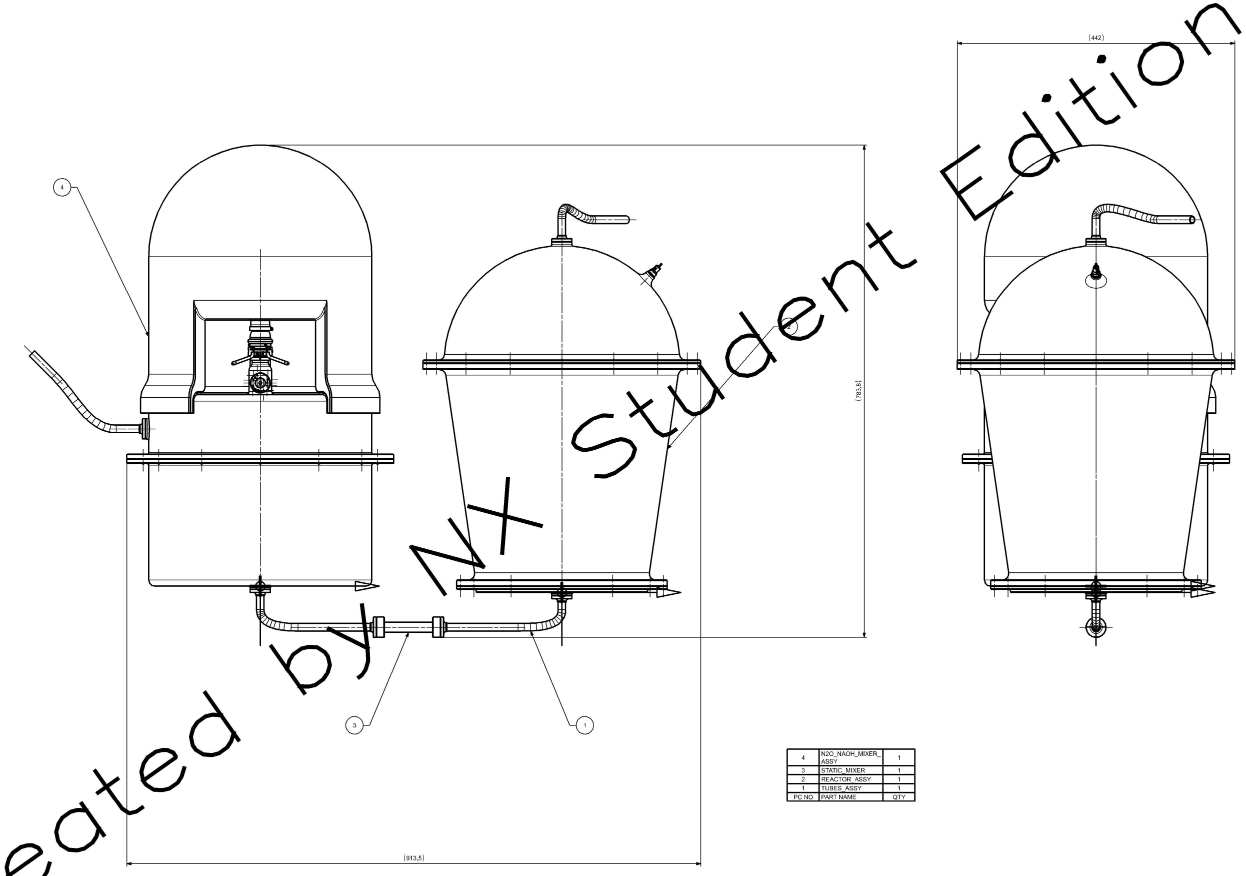

4	N2O_NAOH_MIXER_ASSY	1
3	STATIC_MIXER	1
2	REACTOR_ASSY	1
1	TUBES_ASSY	1
PC NO	PART NAME	QTY

ALL DIMENSIONS IN MM

GENERAL TOLERANCE U.O.S. 0 DECIMAL PLACES ± 0.5mm 1 DECIMAL PLACE ± 0.2mm 2 DECIMAL PLACES ± 0.10mm 3 DECIMAL PLACES ± 0.05mm ANGLES ± 1.0°	THREADS U.O.S. METRIC ISO:68-1; 261; 965; 5855 EXTERNAL 6g; INTERNAL 6H IMPERIAL ASMEB1.1 ASMEB1.15 EXTERNAL 2A; INTERNAL 2B ROLL EXT. THREADS U.O.S.
SPARK ERODE ONLY IF STATED SYMMETRICALLY OPPOSITE COMPONENTS (1) ONLY LEFT HAND PARTS DRAWN. (2) DO NOT HAND THREADS FOR RH PARTS UNLESS EXPLICITLY STATED.	CAD/CAM SURFACES ± 0.2mm MAX SURFACE FINISH (Ra) GENERAL 1.6 µm POLISH 0.2µm

SIEMENS

THIS DRAWING HAS BEEN PRODUCED USING AN EXAMPLE TEMPLATE PROVIDED BY SIEMENS PLM SOFTWARE

FIRST ISSUED	10/03/26	TITLE SYSTEM ASSEMBLY	
DRAWN BY	Gianluca Versaci		
CHECKED BY	G.V		
APPROVED BY	G.V	SIZE A0	DRG NO. system_assy
		SHEET REV A	
		SCALE 1:2	SHEET 1 OF 1

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