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-THEME-

Experimental Study and Desing of Hydrogen Surface Production and Exportation Unit using Typical model

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DEDICATION

DEDICATED TO OUR LOVING FAMILIES AND SUPPORTIVE FRIENDS, WHOSE UNWAVERING BELIEF IN OUR ABILITIES HAS BEEN THE DRIVING FORCE BEHIND OUR ACADEMIC JOURNEYS.

YOUR ENCOURAGEMENT, SACRIFICES, AND CONSTANT PRESENCE HAVE INSPIRED OUR ABILITIES TO REACH FOR THE STARS.

THIS THESIS IS A TRIBUTE TO THE COLLECTIVE LOVE AND SUPPORT OF OUR FAMILIES AND FRIENDS, WITHOUT WHOM THIS ACHIEVEMENT WOULD NOT HAVE BEEN POSSIBLE.

THANK YOU FOR BEING OUR PILLARS OF STRENGTH.

Résumé :

Cette mémoire vise à expérimenter la production d'hydrogène et à concevoir une installation HSPEU en étudiant l'électrolyse des eaux souterraines à l'aide du modèle ML-01 et en proposant des solutions innovantes. L'objectif de Ce travail est d'avoir l'efficacité de fonctionnement du modèle ML-01 (probablement un modèle pour prédire les performances de l'électrolyse), en réalisant des électrolyses sur deux échantillons d'eau différents dans diverses conditions. Il propose également une conception pour l'installation HSPEU qui combine l'électrolyse avec le craquage du méthane (probablement pour réduire la dépendance aux combustibles fossiles) et suggère des moyens de rendre le processus plus respectueux de l'environnement. Les résultats obtenus de cette expérience montrent que l'efficacité du modèle s'atteint à la température 42°C et d'un voltage de 18V. en fin ces résultats sont simulés par le software ASPEN PLUS

Mots-clés : Électrolyse, conception, hydrogène, échantillons d'eau

ملخص:

تهدف هذه الأطروحة إلى تجربة إنتاج الهيدروجين وتصميم تركيب HSPEU من خلال دراسة التحليل الكهربائي للمياه الجوفية باستخدام نموذج ML-01 واقتراح حلول مبتكرة. الهدف من هذا العمل هو الحصول على الكفاءة التشغيلية للنموذج ML-01 (ربما نموذج للتنبؤ بأداء التحليل الكهربائي)، من خلال إجراء التحليل الكهربائي على عينتين مختلفتين من المياه في ظل ظروف مختلفة. كما يقترح تصميمًا لمنشأة HSPEU التي تجمع بين التحليل الكهربائي وتشقق الميثان (ربما لتقليل الاعتماد على الوقود الأحفوري) ويقترح طرقًا لجعل العملية أكثر صداقة للبيئة. تظهر النتائج التي تم الحصول عليها من هذه التجربة أن كفاءة النموذج تصل إلى درجة حرارة 42 درجة مئوية وجهد 18 فولت. أخيرًا، تمت محاكاة هذه النتائج بواسطة برنامج ASPEN PLUS

الكلمات المفتاحية: التحليل الكهربائي، التصميم، الهيدروجين، عينات الماء

Abstract:

This thesis aims to experiment with hydrogen production and to design an HSPEU installation by studying groundwater electrolysis using the ML-01 model and proposing innovative solutions. The objective of this work is to have the operating efficiency of the ML-01 model (probably a model to predict electrolysis performance), by performing electrolysis on two different water samples under various conditions. It also proposes a design for the HSPEU facility that combines electrolysis with methane cracking (probably to reduce dependence on fossil fuels) and suggests ways to make the process more environmentally friendly. The results obtained from this experiment show that the efficiency of the model reaches a temperature of 42°C and a voltage of 18V. finally these results are simulated by the ASPEN PLUS software.

Keywords: Electrolysis, design, hydrogen, water samples.

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LIST OF ABBREVIATIONS

HER	Hydrogen Evolution Reaction
OER	Oxygen Evolution Reaction
PEM	Proton Exchange Membrane
AEM	Anion Exchange Membrane
SOEL	Solid Oxide electrolysis
HSPEU	Hydrogen Surface Production and Exportation Unit
MTU	main treatment unit
SCU	mechanical treatment
MSU	main separation unit
AHF	Adsorbed Hydrogen Fluid
HSF	Hydrogen Separation Factor
HDS	Hydrodesulfurization
HC-HV	Highly Complicated-Highly Variable
ESF	Electrolysis speed factor
DF	distribution factor
FVF	free volume factor
IHSPEU	integrated Hydrogen Surface Production and Exportation Unit
CFD	computational fluid dynamics
CCS	carbon capture and storage
EOR	enhanced oil recovery
WAG	water alternating gas

NOMENCLATURES

G	The Gibbs free energy.	J/mole
H	The enthalpy.	J/mole
T	Temperature.	K
Z	The moles electrons / moles substance	/
θ	The fractional coverage or the amount of gas adsorbed on the surface.	/
K	The Langmuir constant related to the affinity of the gas to the surface.	mol^{-1}
P	The pressure of the gas.	Pa
$\boldsymbol{\mu}$	Dynamic viscosity.	Pa*s
V	Voltage	V
Dp	Discharge pressure	Kpa
Fr	Flow rate	kmol/h

GENERAL INTRODUCTION:

Electrolysis, the process of using electrical energy to drive a non-spontaneous chemical reaction, has emerged as a pivotal technology in various industrial and environmental applications.

Electrolysis, fundamentally, entails the breakdown of electrolytes into their elemental components by applying an electric current. It operates by the migration of ions towards electrodes of opposite charge, triggering redox reactions that yield desired products. Widely utilized in hydrogen production, metal purification, wastewater management, and energy storage, electrolysis stands as a pivotal tool driving sustainability and technological advancement.

The pivotal importance of electrolysis lies in its ability to facilitate clean and efficient energy conversion, offering a pathway towards decarbonization and renewable resource utilization. By enabling the generation of hydrogen as a versatile energy carrier and facilitating the valorization of waste streams, electrolysis contributes to mitigating greenhouse gas emissions, enhancing energy security, and fostering a transition towards a circular economy.

In recent years, the development and application of mathematical and statistical models have emerged as invaluable tools for understanding, predicting, and optimizing electrolysis processes. The ML-01 model, introduced in 2023, exemplifies this paradigm shift by offering a sophisticated framework for elucidating the intricate interplay of parameters influencing water electrolysis under diverse operating conditions.

This dissertation explores using electrolysis for hydrogen production in a facility called HSPEU.

Chapter 1 provides a theoretical background on electrolysis and reviews previous work on the ML-01 model. Theoretical foundations elucidate the principles underlying electrolysis processes, while an overview of the ML-01 model sets the stage for subsequent experimentation and analysis.

Chapter 2 details experiments conducted on two distinct water samples, HTF-14 and OMN-223, under varying temperature (T°), pressure (P°), and voltage conditions. Through a series of electrolysis experiments, the behavior of these water samples is meticulously analyzed and compared, aiming to validate the efficacy of the ML-01 model in predicting electrolysis performance.

Chapter 3 presents the innovative solution of the HSPEU facility, integrating methane cracking with electrolysis using the Aspen Plus program. This integrated approach offers a sustainable pathway for hydrogen production while addressing challenges related to CO2 emissions. Furthermore, novel solutions are proposed to mitigate CO2 emissions and enhance the environmental sustainability of the facility

Overall, this dissertation investigates using electrolysis for sustainable hydrogen production.

Chapter I
Background to H2 production

Introduction:

Electrolysis technology stands as a cornerstone in the realm of industrial chemistry, offering a pivotal method for producing various chemicals and materials through the application of electrical current. Its significance spans from the production of essential substances like hydrogen and chlorine to the synthesis of specialized compounds used in diverse sectors such as pharmaceuticals, electronics, and renewable energy.

At the heart of electrolysis lies a complex interplay of physical and chemical phenomena, which necessitates a thorough understanding and precise control for optimal performance.

The ML-01 mathematical model, despite its name, does not rely on machine learning techniques. Instead, it represents a sophisticated mathematical framework meticulously crafted to capture the intricate dynamics of electrolytic processes. Developed through rigorous research and empirical validation, the ML-01 model leverages a combination of fundamental principles from electrochemistry, thermodynamics, and fluid dynamics to provide accurate predictions and insightful analysis. The model is indispensable in electrolysis technology, aiding in facility design, optimization, and troubleshooting. Despite lacking machine learning algorithms, it provides actionable insights for engineers and researchers, fostering continuous improvement. Its role is pivotal in advancing electrolysis towards sustainability and innovation.

History and chemistry of hydrogen:

In 1766, Henry Cavendish recognized hydrogen as a distinct substance, producing it through the reaction of metals with acids. Antoine Lavoisier later named it "hydrogen" in 1783, reflecting its role in water formation.

Initially seen as a curious, flammable gas, hydrogen found its first practical application in the late 18th century with experiments in balloons, notably by Jacques Charles and the Montgolfier brothers.

The Industrial Revolution revealed hydrogen's potential as a fuel, leading to its use in gas lighting and as a lift gas in airships and balloons.

The concept of a "hydrogen economy" emerged in the 20th century, envisioning hydrogen as a clean energy carrier for a sustainable future.

Hydrogen, with an atomic number of 1, consists of one proton and usually one electron. Despite belonging to Group 1 of the periodic table, its unique electron configuration sets it apart from other alkali metals, H2 has three isotopes: protium, deuterium, and tritium, each with distinct properties. (1)

Hydrogen readily reacts with oxygen to form water, releasing significant energy. This reaction is central to various industrial processes, including fuel cells, which produce electricity and water. H2 bonds play a crucial role in determining the properties of many substances, including water and DNA.

Understanding hydrogen's history and chemistry has paved the way for its widespread use in industries such as energy production and materials science, with ongoing research aimed at leveraging its potential for a sustainable future. (2)

I.1 Thermal cracking of CH4:

Thermal cracking, also known as pyrolysis, is a process in which organic compounds like methane (CH_4) are broken down into smaller molecules by exposing them to high temperatures in the absence of air or oxygen. In the case of methane, thermal cracking can be used to produce hydrogen (H_2) and carbon, following the chemical reaction:

CH_4 (methane) → C (carbon) + $2H_2$ (hydrogen)

This reaction typically occurs at temperatures ranging from 700°C to 1200°C, depending on the specific process conditions and desired products.

The thermal cracking of methane is an important industrial process, particularly in the production of hydrogen and carbon materials like carbon black (a reinforcing agent used in rubber products) and carbon nanotubes. It is also a significant reaction in the steam reforming process, which is one of the primary methods for producing hydrogen on an industrial scale.

During the thermal cracking process, the strong C-H bonds in methane molecules are broken due to the high temperatures, resulting in the formation of hydrogen gas and solid carbon, the reaction is endothermic, meaning it requires the input of heat energy to proceed several factors can influence the thermal cracking of methane, including temperature, pressure, residence time (the time the reactants spend in the high-temperature zone), and the presence of catalysts or additives. Optimizing these parameters is crucial for maximizing the desired product yield and minimizing undesirable side reactions or by-products.

It's worth noting that thermal cracking is a non-catalytic process, meaning it does not require the presence of a catalyst to initiate or accelerate the reaction. However, catalysts can be used in some cases to facilitate specific reactions or improve the selectivity towards desired products (3).

I.2 Electrolysis:

The primary components necessary to carry out an electrolysis operation include:

- **Two electrodes**

The cathode is the conductor in which the **Hydrogen Evolution Reaction (HER)** is affected and the anode that has the positive charge in which **Oxygen Evolution Reaction (OER)** is affected

- **A direct current (DC) supply**

It provides the energy necessary to create or discharge the ions in the electrolyte. Electric current is carried by electrons in the external circuit

- **An electrolyte**

It is a substance that contains free ions, which are the carriers of electric current in the electrolyte. If the ions are not mobile, as in a solid salt then electrolysis cannot occur. (4)

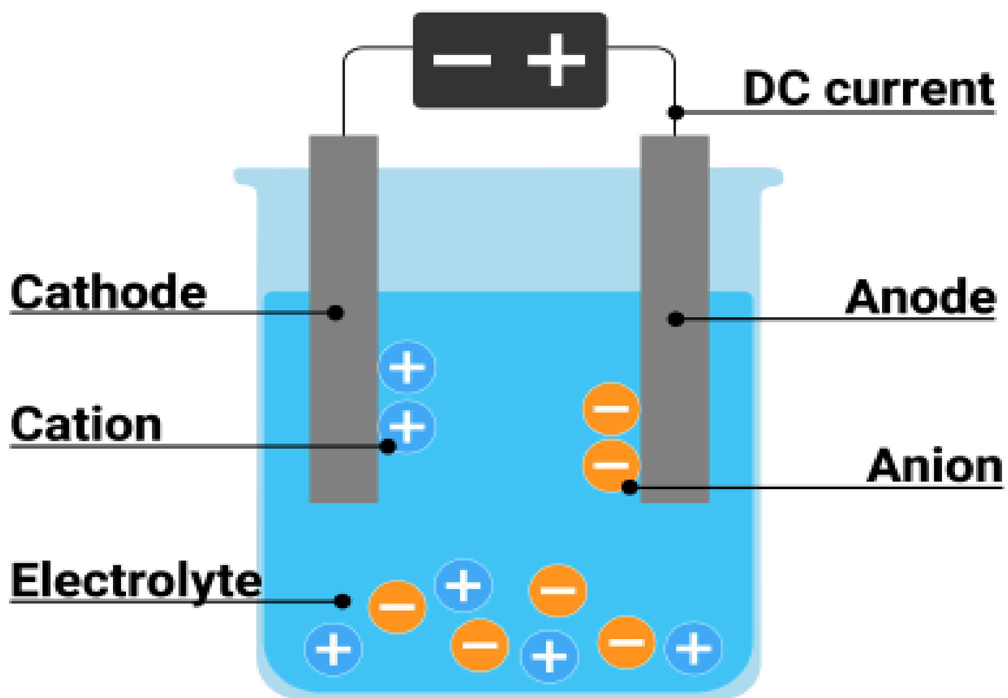

Figure I-1:Electrolyte. (5)

There are three principle main types of electrolysis: **Alkaline electrolysis**, **Proton Exchange Membrane (PEM) electrolysis** and **Solid Oxide electrolysis (SOEL)**.

- **Alkaline Electrolyzer:**

Alkaline electrolyzers operate via transport of hydroxide ions (OH^-) through the electrolyte from the cathode to the anode with hydrogen being generated on the cathode side. Electrolyzers using a liquid alkaline solution of sodium or potassium hydroxide as the electrolyte have been commercially available for many years. Newer approaches using solid alkaline exchange membranes (AEM) as the electrolyte are showing promise on the lab scale.

- **Polymer Electrolyte Membrane Electrolyzer:**

In a polymer electrolyte membrane (PEM), the electrolyte is a solid specialty plastic material.

- Water reacts at the anode to form oxygen and positively charged hydrogen ions (protons).
- The electrons flow through an external circuit and the hydrogen ions selectively moves across the PEM to the cathode.
- At the cathode, hydrogen ions combine with electrons from the external circuit to form hydrogen gas. Anode Reaction: $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ Cathode Reaction: $4H^+ + 4e^- \rightarrow 2H_2$.

- **Solid Oxide Electrolyzer:**

Solid oxide electrolyzers, which use a solid ceramic material as the electrolyte that selectively conducts negatively charged oxygen ions (O^{2-}) at elevated temperatures, generate hydrogen in a slightly different way.

Steam at the cathode combines with electrons from the external circuit to form hydrogen gas and negatively charged oxygen ions.

The oxygen ions pass through the solid ceramic membrane and react at the anode to form oxygen gas and generate electrons for the external circuit. (6)

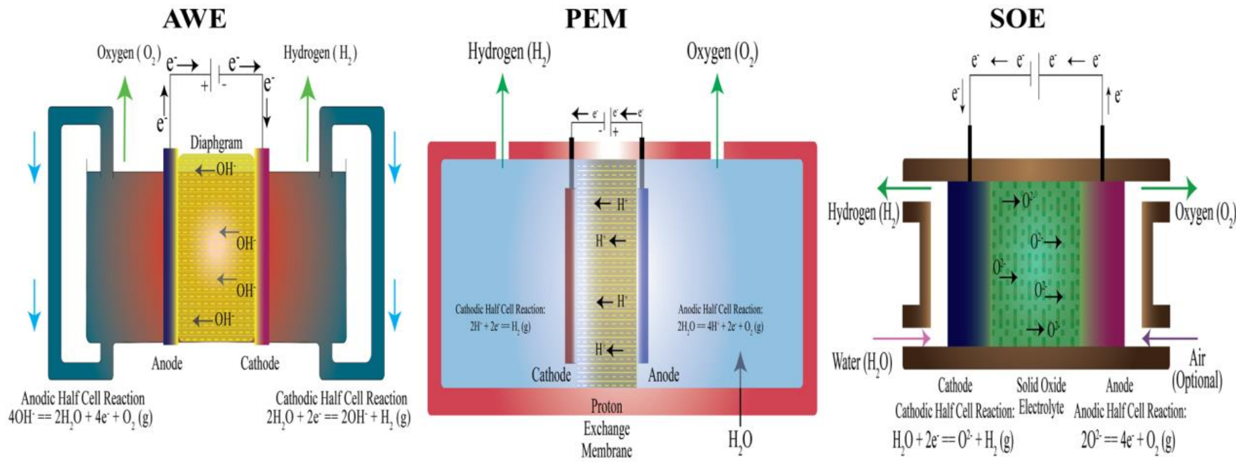

Figure I-2:Types of electrolyzers. (5)

I.3 Presentation of Hydrogen Surface Production and Exportation Unit (HSPEU)

Hydrogen gas production entails intricate procedures spanning from well extraction to industrial application, necessitating tailored handling and safety protocols. The HSPEU station streamlines the safe and effective generation of hydrogen from subterranean water sources, ensuring precise separation and electrolysis. Its goals encompass converting extracted water into H2 gas, upholding operational safety, enhancing electrolysis efficiency, and complying with environmental regulations.

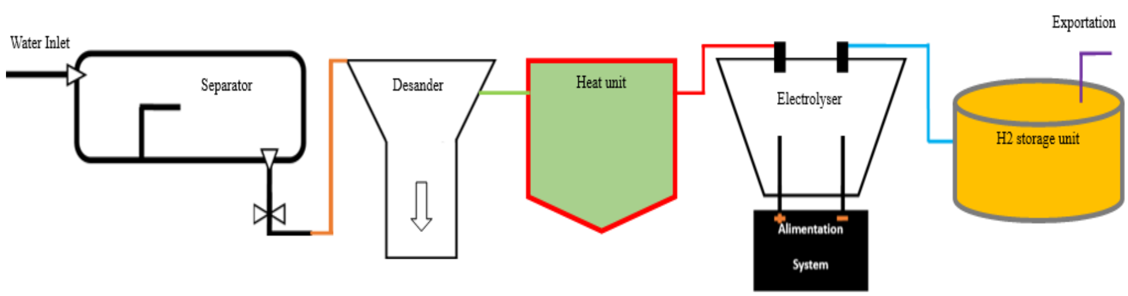

Figure I-3: HSPEU Different Units. (6)

I.3.1 Different HSPEU units:

The typical HSPEU stations comprise various units tailored to accommodate the diverse processes offered by the station:

- **Separator (active/abandoned wells).**
- **Desander**

- **Mixer/Heat unit.**
- **Electrolysis unit.**
- **Decantation unit.**
- **Storage unit.**
- **Delivery units.**
- **Exportation pipelines.**

I.3.1.1 Separator:

A separator is a vessel, either cylindrical or spherical, designed to segregate oil, gas, and water from the overall fluid stream produced by a well. These separators come in two primary orientations horizontal or vertical. They can be categorized into two and three-phase separators, the latter commonly referred to as free-water knockout separators. Two-phase separators manage oil and gas exclusively, whereas three-phase separators handle oil, water, and gas.

In various industrial processes, separators serve to segregate different constituents of a mixture. In the context of water separation, separators are typically employed to extract water from oil or gas streams, enabling each component to be utilized or processed individually. The separation of water from oil or gas holds significance across multiple industries, notably the oil and gas sector, where the presence of water can detrimentally affect equipment performance and the quality of the end product. (7)

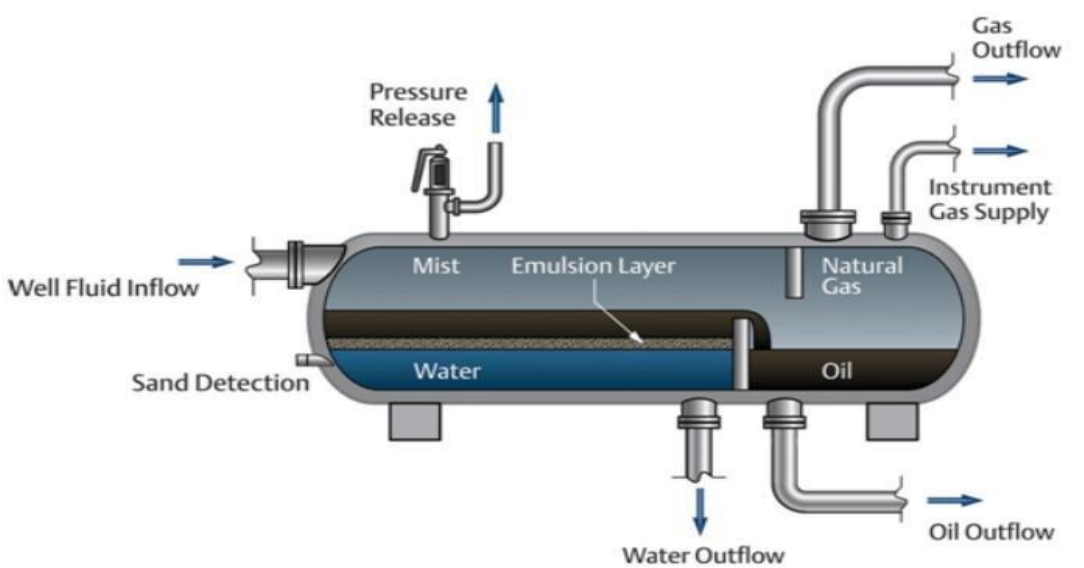

Figure I-4 : Three Phase separator (7).

Separators can be categorized based on several criteria:

- **Based on Function**
- **Based on Shape**
- **Based on Size** (7)

I.3.1.2 Main Treatment Unit (MTU):

The aim of the MTU is to prepare fluid for electrolysis through a combination of mechanical and chemical treatment. This is achieved by employing two integrated systems: the Solid Control Unit (SCU) and the Mixer/Heat Control Unit (MHCU). These systems work together to process the fluid, ensuring it is primed and ready for electrolysis (6).

I.3.1.3 Mechanical Treatment (SCU):

Desanders are essential solid control devices equipped with a series of hydro-cyclones designed to separate sand and silt from drilling fluids on drilling rigs, operating without any moving components. The efficacy of a desander is directly correlated with its internal diameter: the larger it is, the greater volume of drilling fluids it can process and the larger the solids it can remove.

Similarly, within an HSPEU station, desanders and desalters serve a crucial purpose in eliminating various solid particles. This is imperative to prevent the risk of precipitations on critical surfaces, posing serious dangers that must be mitigated. Despite these solid particles having no significant impact on the electrolysis process, and thus on the chemical composition of the electrolysis fluid, it remains imperative to address them thoroughly. (8)

Figure I-5: Desander from MLE 14S Well.

Furthermore, the presence of various valves and cross-overs, coupled with the inherent explosiveness of exported H2 gas, underscores the importance of the desanding and desalting process. Any precipitation can lead to alterations in section integrity and pose risks of clogging, underscoring the significance of these processes in ensuring the fluid is primed for electrolysis.

I.3.1.4 Chemical Treatment (MHCU):

In the realm of industrial process engineering, mixing stands as a pivotal unit operation aimed at manipulating heterogeneous physical systems to achieve greater homogeneity. Everyday scenarios, such as circulating water in a swimming pool to even out temperature or stirring pancake batter to eliminate lumps, exemplify this process (6).

Mixing serves to facilitate heat and/or mass transfer among various streams, components, or phases within a system. Virtually all modern industrial processes incorporate some form of mixing, with certain types of chemical reactors also doubling as mixers. With suitable equipment, it becomes feasible to blend solids, liquids, or gases into other solid, liquid, or gas mediums.

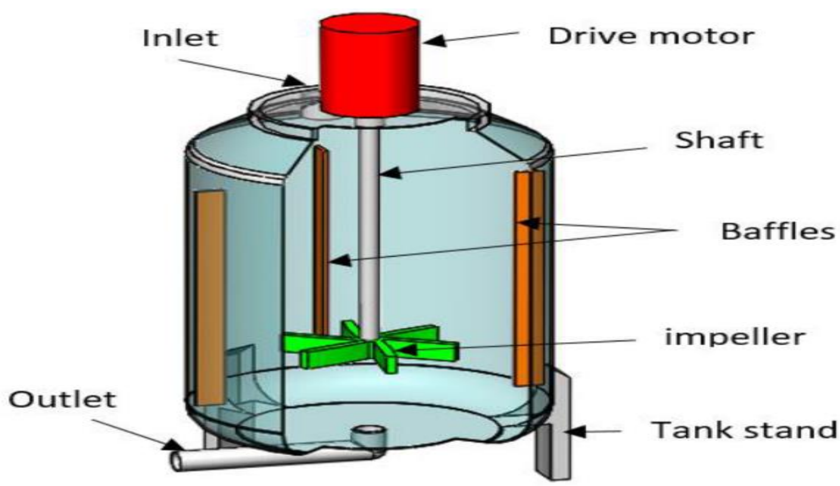

Figure I-6 :Typical Mixer (9)

The mathematics of mixing is highly abstract, and is a part of ergodic theory, itself a part of chaos theory.

- **Mixing classification**

The selection of mixing operation and equipment hinges on the state of the materials involved (liquid, semi-solid, or solid) and their miscibility. Within this framework, mixing can encompass stirring or kneading processes.

Various types of mixing units can thus be categorized:

- Turbines.
- Ribbon Blender.
- V Blender. (9)

I.3.1.5 Main Separation Unit (MSU):

The primary function of the Main Separation Unit (MSU) is to receive the fluid prepared for electrolysis or the electrolyte, directing it into the electrolysis process and ultimately converting it back into H2 gas.

The MSU in composed of:

- Electrolyser unit
- DC alimentation unit

A. Electrolyser:

An electrolyser is an electrical device that utilizes a DC power supply to provide the electrolyte with the required Gibbs free energy, enabling the separation of hydrogen ions from oxygen ions and the production of H2 gas.

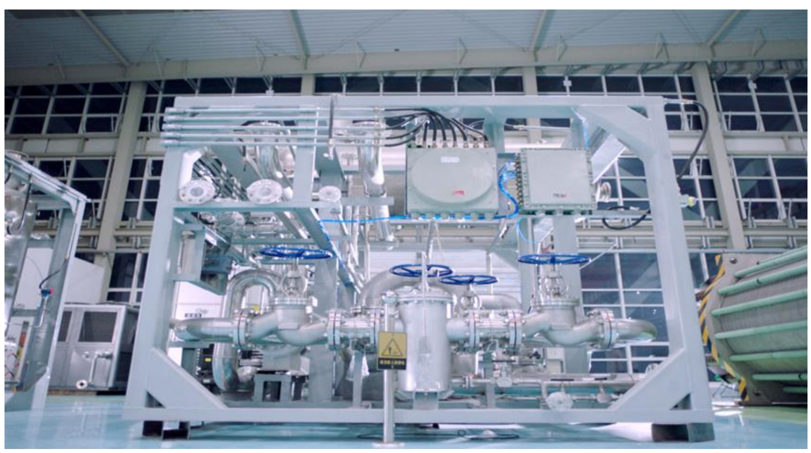

Figure I-7: Industrial-size Electrolyzer (Alkaline Water Electrolyser) (4).

A typical electrolyser unit is composed of:

a) A reservoir container is used to store the fluid ready for electrolysis.

b) Two conductors are employed, with one designated as the anode handling positive charge, and the other as the cathode handling negative charge. These conductors serve several key purposes:

- Facilitating efficient contact with electrolyte molecules.

- Transmitting DC current into the electrolyte.
- Generating the required voltage within the electrolyte between the two sides of the electrolyser.

c) Gas transportation pipes were manufactured to facilitate the evacuation of gas into storage containers. While the shape of the electrolyser does not directly affect electrolysis efficiency, factors such as construction model, size, and building materials are crucial considerations when constructing an electrolyser unit in an HSPEU station. Additionally, the influence of pressure and temperature on the volume of both electrolyte (liquid) and H2 (gas), alongside the electrolysis type (Alkaline/PEM /AEM), necessitates compatibility between the shape, inner construction, and other factors with the overall electrolysis modeling.

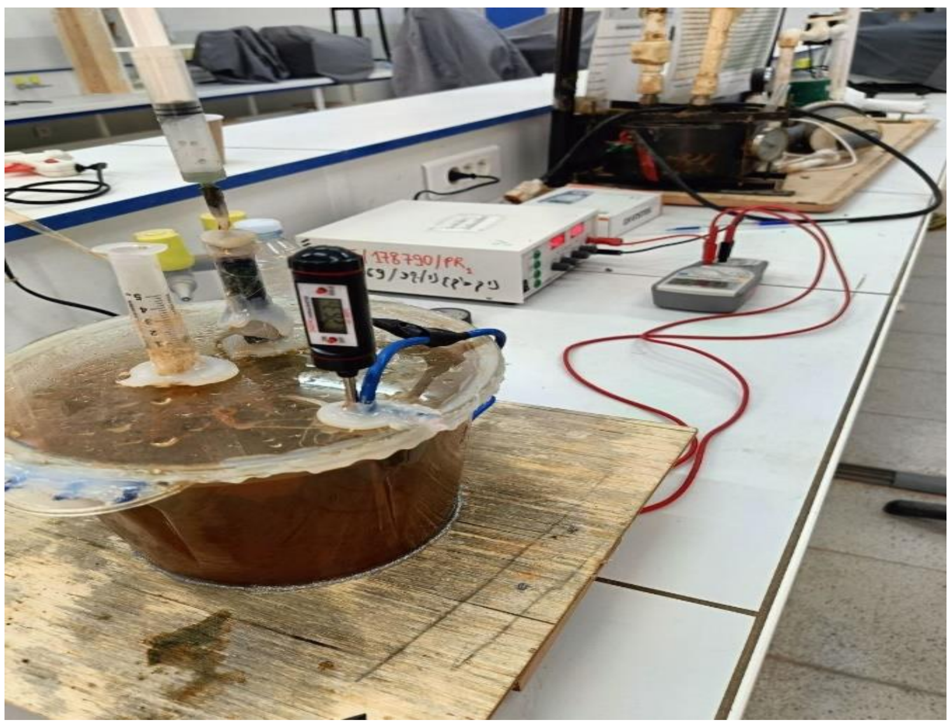

Figure I- 8: Typical electrolyser utilize in experiment.

d) DC current alimentation unit :

The power supply unit plays a crucial role in providing the required DC current to the electrolyser unit, facilitating the transmission of this current directly into the electrolyte through contact with conductors. Negative charges are conveyed by the cathode, while positive charges are carried by the anode. It's essential to maintain a specified voltage to ensure complete absorption of Gibbs free energy by the electrolyte.

In various applications, there are multiple options available for supplying the necessary DC current to our electrolyser:

1. Utilizing large-scale batteries designed for industrial use.
2. Employing a combination of generators and SCR (Silicon-Controlled Rectifier) systems, where the power source can be renewable energy or diesel-powered, similar to generators used in drilling operations).

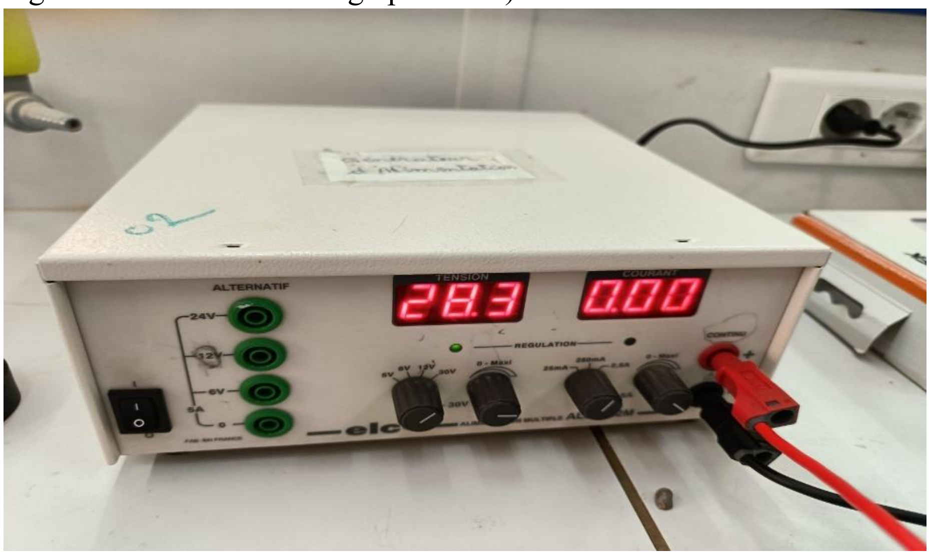

Figure I-9: DC Generator of our expriment.

I.3.1.6 Decantation/Storage unit:

The main role of this unit is to allow H_2 decantation and storage after arriving from the MSU unit. (7)

I.4 From separator to exportation pipelines:

After water being well extracted from mixed oil, it is directly pumped into the resting HSPEU units, in which a process of chemical and mechanical treatments followed by the electrolysis process are affected, ending with the final step of pumping H_2 gas in secured form.

The different HSPEU processes are:

I.4.1 Separation

Water separation marks the initial phase in the operational protocol of HSPEU stations. This step is paramount due to the significant volumes of water produced, whether sourced from free-flowing wells, emulsified with oil and gas phases in onshore oil wells, or obtained from offshore wells alongside seawater, known for its high salinity and diverse compositions.

In this study, with a specific emphasis on water extraction primarily from various wells, particularly abandoned ones, the process commences with water separation in separators. Subsequently, the separated water is directed into the electrolyser unit and then transported through exportation pipelines. (7)

I.4.2 Treatment

This crucial stage in the electrolysis process encompasses both mechanical and chemical treatments. Initially, mechanical treatments involve the use of desander/desalter machinery, followed by chemical treatment utilizing Mixer/Heater units. These processes prepare the electrolyte, transforming it into a fluid ready for electrolysis. (6)

I.4.3 Electrolysis

Once the water has been transformed into a fluid ready for electrolysis, it is then pumped into the electrolyser unit. Here, it enters the reservoir container and makes direct contact with the electrodes, which are supplied with the necessary Gibbs free energy in the form of a pre-defined DC electrical current from the DC power supply unit (such as SCR or batteries).

In configuring the electrolysis process within the HSPEU station, the choice of electrolysis method (Alkaline, PEM, AEM, etc.) and the design of the electrolyser are primarily determined by various factors. These include desired production outputs, hydrogen purity requirements, overall and additional costs, as well as technical, operational, and environmental considerations. (4)

I.4.4 Decantation/Storage

Once hydrogen (H2) has been generated, it undergoes a pumping process into a decantation unit where the hydrogen gas is separated from any impurities it may have acquired during transfer. The primary aim of this purification process is to remove as many impurities as possible, as they can affect transportation conditions, pose deposition risks, and hinder the overall energetic efficiency and economic value of hydrogen.

The standards for purification, in addition to the final purity and composition of the hydrogen, are established by the official contract between producers and consumers. (10)

I.4.5 Exportation

Following the purification process, hydrogen (H2) is now prepared for export to consumers via pipelines, boats, or other means. However, transporting H2 in its gaseous form is impractical due to the extreme temperatures required for liquefaction at atmospheric pressure (below or equal to -160 degrees Celsius), making it technically and operationally unfeasible. To address this challenge and ensure safe and efficient H2 transportation, a special fluid model known as Adsorbed Hydrogen Fluid (AHF) is employed.

AHF fluid offers a promising solution for secure and sufficient H2 transport by utilizing special materials capable of forming robust physical bonds. These bonds enable the adsorption of H2 molecules onto the surface of these materials. AHF fluid is essentially the outcome of an adsorption process between adsorbed molecules, preferably in liquid form, and H2 molecules in gaseous form. Specific temperature and pressure conditions are required to establish the necessary physical connections between the surface of the chosen adsorbent material and the hydrogen molecules). (10)

I.5 Optimization of H2 production through mechanical/chemical optimizations:

The value of H2 production under specific conditions can be influenced by two categories of parameters:

- Chemical Parameters:

- Undesired reactions occurring within the electrolyte.
- Interactions between electrodes and electrolyte.
- Various phenomena involving electrodes, electrode-electrolyte interfaces.
- Chemical composition of the electrolyte.

- Mechanical Parameters:

- Type of electrodes utilized.
- Configuration and design of electrodes.
- Electrode interface properties.

- Type of electrodes employed.
- Shape and design of electrodes.
- Interface characteristics of electrodes. (11)

I.6 Influence of water composition on production:

The chemical composition of water serves as a primary determinant affecting H2 production by influencing various phenomena encountered during electrolysis. Additionally, alongside mechanical properties like temperature and pressure, external factors such as rheological and intermolecular aspects are impacted by this parameter, playing crucial roles in the electrolysis process.

Through experimentation, the identification and elucidation of these influences on production enable engineers to predict, design, and execute the production of H2 gas from reservoir water with utmost safety and efficiency. Utilizing gain equations and considering a series of electrolysis laws, engineers can analyze the production process across micro and macroscopic intervals, facilitating a comprehensive understanding of electrolysis.

I.6.1 Ion's influence:

Various chemical elements exist in ionic form, and their interactions with other elements can lead to numerous reactions, each with its general and specific properties. Reservoir water, such as the sample extracted from HTF-14 used in this study, possesses a unique chemical composition that can significantly influence hydrogen (H2) production, both positively and negatively.

Throughout the life cycle of active wells, various operations are performed using techniques like Coiled Tubing Units (CTU) and Snubbing. These operations involve the use of operational and technical fluids, which, in some instances, may be injected into the reservoir rock. This can directly impact the reservoir properties, inducing changes in its chemical composition.

I.6.2 Density:

Density directly affects the molecular mobility of water. Additionally, molecular velocity, which governs flow rate, determines the extent of wave-like movement of water molecules within a given time frame.

I.6.3 Viscosity:

It's crucial to emphasize that viscosity holds greater importance than density. This conclusion is drawn from comparing the hydrogen (H2) yield of various systems with different compositions but identical densities, operating under different mechanical and environmental conditions where viscosity varies. Such comparisons distinctly illustrate that viscosity stands out as a primary parameter in the gain equation. (12)

I.6.4 Other rheological factors (Fick's first law):

Fick's first law describes the movement of molecules within a fluid system, typically liquids, where molecules flow in a wave-like manner across a defined surface, moving from regions of high concentration to regions of lower concentration in a spontaneous process.

$$\mathbf{J} = -\boldsymbol{D_{iff}} * \left(\frac{dc}{dx}\right) \quad \text{......(I-1)}$$

Where:

J: the flow-wave in (mol/ $(m^2 * s)$).

$\boldsymbol{D_{iff}}$ **:** the diffusion constant in (m^2/s).

$\left(\frac{dc}{dx}\right)$**:** the concentration gradient in (mol/m^4).

Fick's first law is essential as it assists in comprehending the behavior of water molecules under particular conditions and optimizing their alignment within conductors. (13)

I.6.5 Hydrogen Separation Factor (HSF):

A wide array of water models exists across different scales, each characterized by distinct properties including chemical composition, origin, rheological attributes such as density and viscosity, and additional factors like Yield Point and Bubble Point. Consequently, the behavior of water molecules within the electrolyte utilized for hydrogen (H2) production is unique, leading to the emergence of various phenomena during this electrochemical process.

$$\text{HSF} = \frac{V_{H2}}{V_{total\ H2O}} \quad \text{....... (I-2)}$$

I.6.6 Influence of Temperature and Pressure on H2 production:

Temperature and pressure are mechanical parameters that play a crucial role in the design, operation, and technical processes of electrolysis, as well as in environmental considerations.

Temperature has a significant influence on electrolysis, primarily affecting the movement of molecules within the electrolyte volume. Previous studies have highlighted the importance of temperature in electrolysis; however, these studies have often failed to quantify or demonstrate the direct impact of temperature on gain, and the specific relationship between temperature and gain remains unclear.

- ✓ **Distribution Factor (DF)**

$$\mathbf{DF} = \frac{N_{water\ to\ be\ electrolysed}}{N_{total\ H2O}}$$

$$\mathbf{J' = DF*J}$$

$$\mathbf{J' = -\ DF*}D_{iff}*\ \left(\frac{dc}{dx}\right)\text{......}\mathbf{(I\text{-}3)}$$

In which DF can be defined as follow:

$$\mathbf{DF} = -\ \frac{J'}{D_{iff}*\ \left(\frac{dc}{dx}\right)}\ \text{......}\mathbf{(I\text{-}4)}$$

- ✓ **Electrolysis Speed Factor (ESF)**

$$\mathbf{C\ =\ I*t\ =\ N\ *\ }Q^{*}_{ele}\text{......}\mathbf{(I\text{-}5)}$$

$$\mathbb{C}_{ele} = \frac{N}{S} = \frac{I*t}{S*\ Q^{*}_{ele}}\text{......}\mathbf{(I\text{-}6)}$$

$$\mathbf{ESF} = \frac{t_{th}}{t_r} = \frac{I_r}{I_{th}} = \frac{I_r - \sum I\ loss}{I_{th}}\text{......}\mathbf{(I\text{-}7)}$$

- ✓ **Non-desired Reactions Factor (NRF)**

$$\mathbf{NRF} = \frac{V_{NRF}}{V_{total\ H2O}} = \mathbf{(1\text{-}DF)\ *\ (1\text{-}a*HSF) - FVF\text{......}(I\text{-}8)}$$

- **Influence of Pressure**

$$G_{H2} = \frac{V_{H2\ real}}{V_{H2\ th}}\text{......}\mathbf{(I\text{-}9)}$$

$$= a_0 * \left(\frac{J'*L*\mu}{T}\right)^2 - b_0 * \left(\frac{J'*L*\mu}{T}\right)\ \text{......}\mathbf{(I\text{-}19)}$$

I.7 Uses of Hydrogen Gas in Petroleum Industrial Applications:

Hydrogen gas (H2) finds various applications in the petroleum industry due to its unique properties and reactivity. Here are some key uses of hydrogen gas in petroleum industrial applications:

I.7.1 Hydrodesulfurization (HDS):

Hydrogen is used in the hydrodesulfurization process to remove sulfur compounds from petroleum fractions, such as gasoline, diesel, and jet fuel. Sulfur compounds are undesirable as they contribute to air pollution and can cause corrosion in engines and equipment. Hydrogen reacts with sulfur compounds in the presence of a catalyst, converting them into hydrogen sulfide (H2S), which can be removed.

I.7.2 Hydrotreating:

Hydrotreating is a process that uses hydrogen to remove contaminants like sulfur, nitrogen, and metals from petroleum fractions. It improves the quality and stability of fuels by reducing the risk of corrosion and enhancing combustion properties. Hydrogen reacts with the contaminants, converting them into more easily removable forms.

I.7.3 Hydrocracking:

Hydrocracking is a catalytic process that uses hydrogen to break down large, complex hydrocarbon molecules into smaller, more valuable products like gasoline, jet fuel, and diesel. Hydrogen plays a crucial role in this process by facilitating the cracking of long-chain hydrocarbons into shorter, more desirable molecules.

I.7.4 Hydrogenation:

Hydrogen is used in hydrogenation processes to add hydrogen atoms to unsaturated hydrocarbon molecules, thereby increasing their degree of saturation. This process is important for producing products like lubricating oils, waxes, and specialty chemicals.

I.7.5 Fuel cell applications:

Hydrogen gas is a potential future energy carrier and can be used in fuel cells to generate electricity through an electrochemical reaction with oxygen. Petroleum companies are exploring the use of hydrogen in fuel cell technologies for transportation and power generation applications.

I.7.6 Hydrogen production:

The petroleum industry is a significant producer of hydrogen gas through processes like steam reforming of natural gas or catalytic reforming of naphtha (a petroleum fraction). The produced hydrogen is used in various refining processes or can be purified and sold as a product.

I.7.7 Ammonia synthesis:

Hydrogen is a key component in the production of ammonia (NH3), which is an important feedstock for the production of fertilizers and other chemicals. Ammonia synthesis involves the reaction of hydrogen with nitrogen under high temperature and pressure conditions.

Overall, the use of hydrogen gas in the petroleum industry is crucial for improving fuel quality, facilitating various refining processes, and exploring new energy technologies. The petroleum industry's expertise in handling and producing hydrogen gas makes it a significant player in the development of a potential hydrogen-based economy (14).

Conclusion:

In conclusion, advancing electrolysis technology is paramount in achieving greater energy efficiency and sustainability in various industrial processes. By harnessing renewable energy sources and optimizing operational parameters, electrolysis holds the potential to revolutionize the production of essential chemicals and materials while reducing reliance on fossil fuels and minimizing environmental impact.

At the forefront of this endeavor stands the ML-01 mathematical model, offering a profound understanding of electrolysis phenomena and enabling precise control and optimization of electrolysis facilities. Through its comprehensive description of the underlying physical and chemical processes, the ML-01 model empowers engineers and researchers to unlock new frontiers in efficiency, selectivity, and scalability.

By leveraging the insights provided by the ML-01 model, practitioners can fine-tune electrolysis processes, minimize energy consumption, and enhance product quality, thereby maximizing the economic and environmental benefits of electrolysis technology. As we continue to innovate and refine our understanding of electrolytic processes, the integration of advanced mathematical models like ML-01 will play a pivotal role in realizing the full potential of electrolysis as a cornerstone of sustainable chemical synthesis and industrial production.

Chapter II

Comparison between different HC-HV water systems

Introduction:

In this chapter, we embark on a journey delving into the intricacies of electrolysis phenomena through a series of diverse experiments conducted on multiple underground water samples. Our objective is twofold: to elucidate the fundamental principles underlying electrolysis and to refine the predictive capabilities of the ML-01 model through empirical validation and continuous improvement.

We conduct controlled electrolysis experiments on underground water samples to uncover factors impacting chemical transformation efficiency and selectivity. Through rigorous analysis, we aim to enhance understanding of electrolytic processes for industrial use. Additionally, we utilize findings to refine the ML-01 model, integrating empirical data for improved predictive accuracy and reliability in simulating electrolysis phenomena across varied operational scenarios.

Ultimately, this chapter serves as a testament to the symbiotic relationship between experimental investigation and mathematical modeling in advancing our understanding of electrolysis technology. Through the synergy of empirical data and theoretical insights, we aim to pave the way for more efficient, sustainable, and economically viable electrolysis processes, underpinned by the rigorous scientific foundation provided by the ML-01 model.

II.1 Improve of ML-01 model:

In our experience we going to confirm our gain low specifically use temperature and voltage.

II.2 Presentation of the gain low and gain Experiment:

Hydrogen gain is defined mathematically as the relation between produced hydrogen in real conditions versus the same produced in theoretical or reference conditions (T° = 298,15 K, P° = 1 atm), which also can be defined -by definition of HSF- as the relation of both real and theoretical Hydrogen Separation Factor (HSF).

$$\boldsymbol{G_{H2} = \frac{V_{H2\,real}}{V_{H2\,th}}} \text{......(II-1)}$$

In physics, Hydrogen gain is the factor that represents what limit of production that we can produce over a specified electrolyte model characterized by its special HSF value (15).

Is defined by the following formula:

$$\boldsymbol{= a_0 * \left(\frac{J' * L * \mu}{T}\right)^2 - b_0 * \left(\frac{J' * L * \mu}{T}\right)} \text{ ......(II-2)}$$

Where:

a_0 = descending production factor = ESF * (1 – a*HSF) = $\left(\frac{I_r - \sum I\ loss}{I_{th}}\right)$*(1 – a*HSF)

b_0 = ascending production factor = ESF * (a*HSF – FVF) = $\left(\frac{I_r - \sum I\ loss}{I_{th}}\right)$* (a*HSF – FVF)

II.3 Data generation using MATLAB program:

Using MATLAB simulation of electrolysis with consideration of all possible values of different electrolysis parameters and for an HSF range of 100 to 500, we obtain the following results:

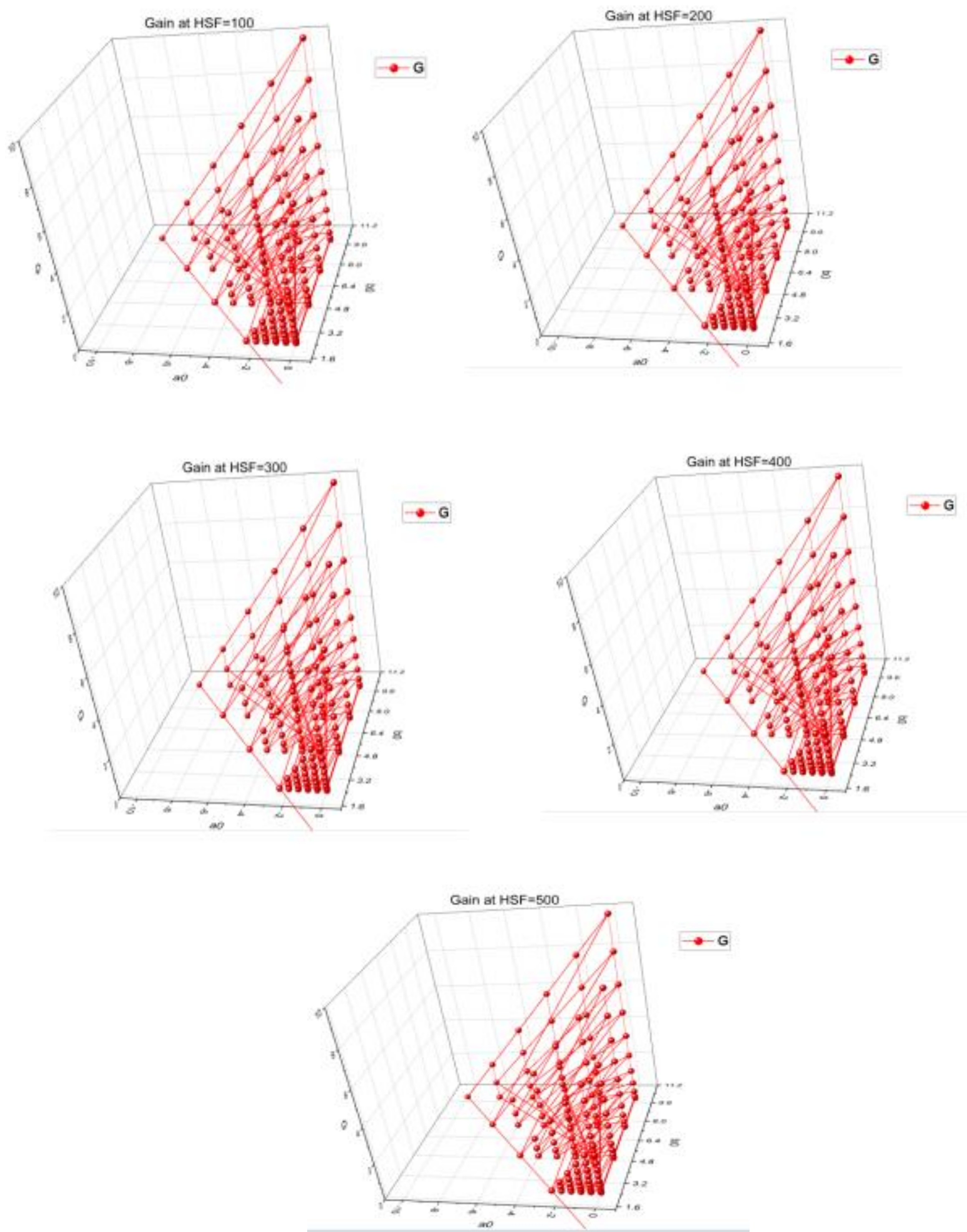

Figure II-1: MATLAB Gain results ***(15)*****.**

II.4 Analyses and interpretations:

a) Analyze of results:

As shown in the figures up, which represent the H2 Gain Cloud, we observe the following:

- The gain clouds are similar in different HSF values.
- The cloud has a 3D **Peak-Shaped** form with a range of 0.0 to 8.1 of gain.

b) Interpretation of results:

We can Elucidate the reason why all those curves were identic even HSF value is not the same (which represents different electrolyte model) as following:

- First, -even if HSF is not the same but the other factors were the same for all the cases- the similarity means that for different electrolyte models, the general behavior is identic, which means that the type of the electrolyte is not a decisive factor for obtaining the targeting gain.
- Second, we conclude that Gain or HSF are not also decisive parameters, in other terms, we can obtain the same results for reservoir or sea water, lac or even water evaporated in air in condition of having the same DF, ESF and FVF factors.
- Third, in specific conditions, Gain has an upper-peak that called **Peak Point (PP)**, which represents the maximum reachable gain, can be obtained by electrolysis in determined conditions (15).

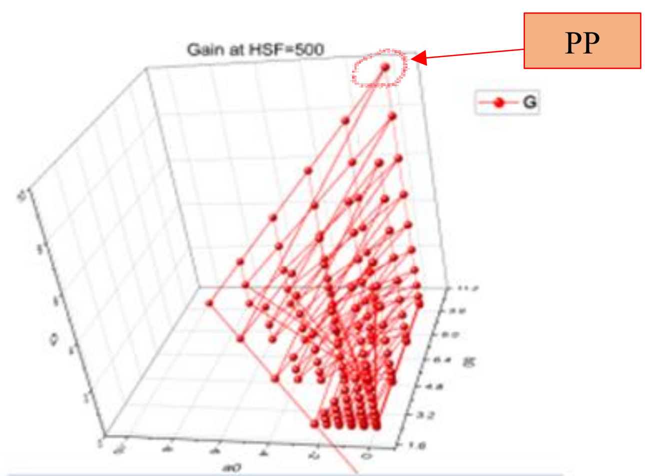

Figure II-2: PEAK Point (15).

II.5 influence off temperature and voltage in different tow water:

Temperature and voltage those tow parameter that we can control them and influence quickly and directly in our water to improve the ML01 model:

II.5.1 temperature:

For temperature it influences in molecule movement and ions in our water for higher T the molecules and ions movement his growth quickly and we're going to improve watch for specific value is going to be the best temperature (gain T) and if it's higher than this volume or lower it's going to be this desirable value.

II.5.2 Voltage:

For voltage if we increase it the conductivity of our anode it's become the best value because of our surface of Anode Become full if we raised voltage for more we're going to desirable reaction and our gain became lower.

II.6 Experiment:

II.6.1 Material:

a) **Voltmeter:**

A voltmeter is an electrical measuring instrument that is used to measure the difference in electrical potential, expressed in volts (V), between two points in an electrical circuit. Electrical voltage is a fundamental quantity in electricity that represents the driving force that allows electric charges to flow in a circuit. In our experiment, we used:

Digital voltmeters: These voltmeters use an analog-to-digital converter (ADC) to convert the electrical voltage into a digital signal that is then displayed on a screen. Digital voltmeters are more accurate and easier to use than analog voltmeters (16).

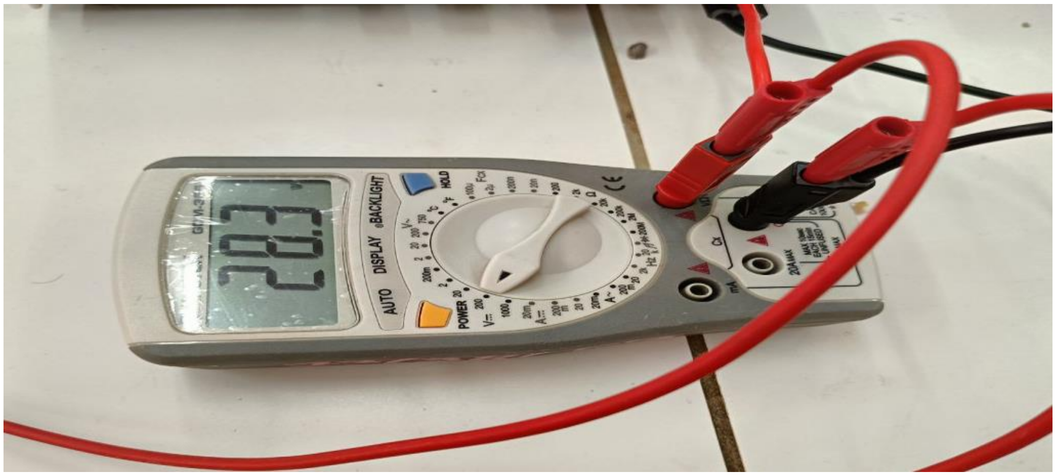

Figure II-3: Voltmeter.

b) Power Generator:

A power generator, also known as an electric generator or power source, is a device that converts one form of energy into electrical energy. The electrical energy is then supplied to electrical appliances or electronic circuits.

There are many different types of power generators, but they all work on the same basic principle: a magnetic field is created and moved through a conductor, which induces an electrical voltage. The voltage and current produced by the power generator depend on the type of generator, the strength of the magnetic field, and the speed at which the magnetic field is moved (17).

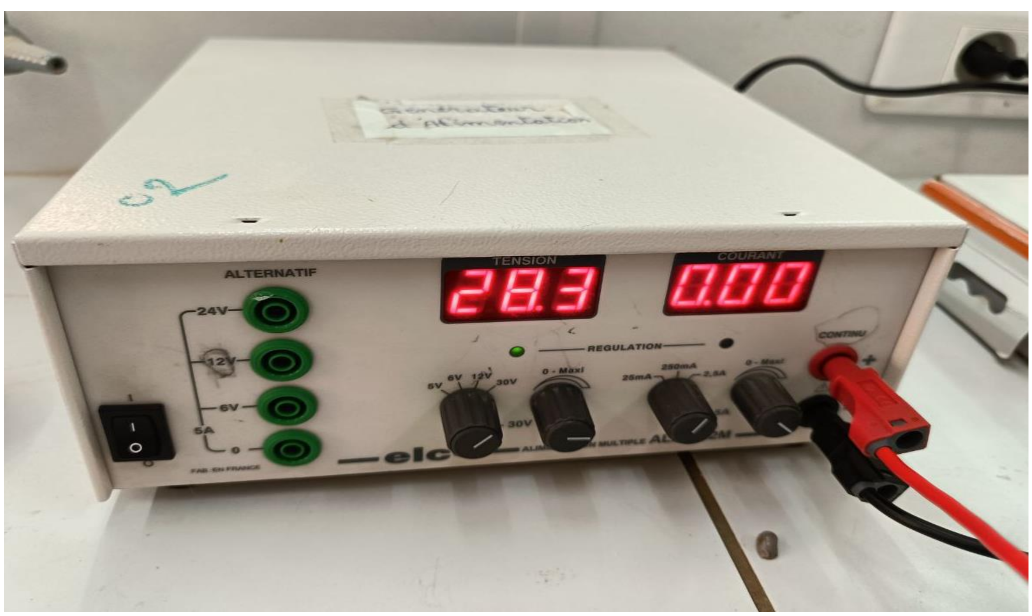

Figure II-4: Power generator.

c) Digital thermometer:

A digital thermometer is an electronic instrument used to measure temperature and display the reading on a digital screen.

Function:

- Measures temperature, a physical property indicating hotness or coldness.
- Uses a sensor to detect temperature changes and convert them into an electrical signal (18).

Figure II-5: Digital Thermometer.

d) Immersion heater:

An immersion heater, also known as an immersion element or thermo-plongeur (French), is an electric device used for heating liquids by directly submerging it in the liquid. It works by converting electrical energy into thermal energy through a heating element (19).

Figure II-6: Immersion heater (19).

e) Power cord:

Is an electrical cable that temporarily connects an appliance or electronic device to the mains electricity supply via a wall outlet or extension cord.

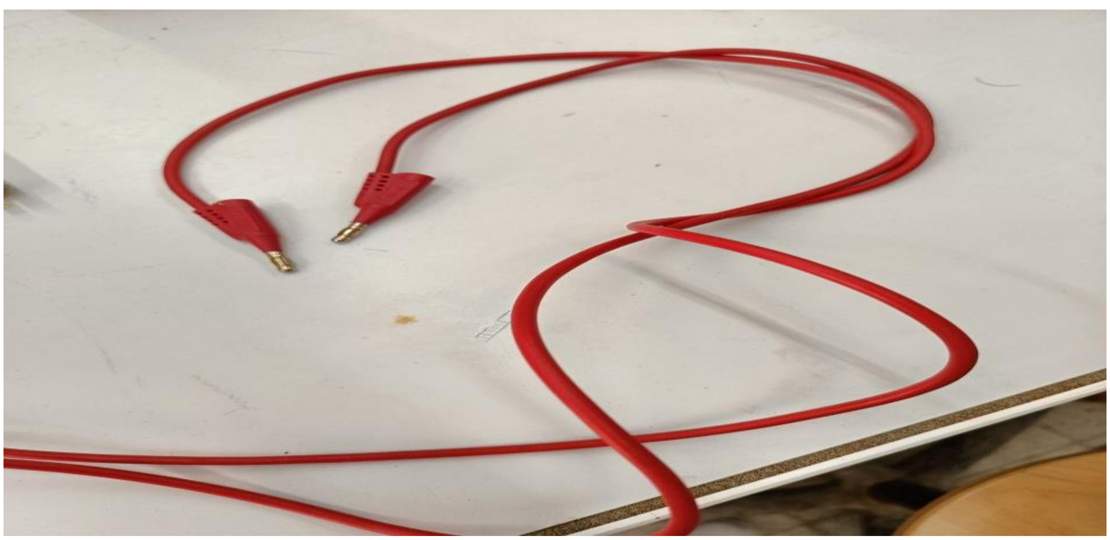

Figure II-7: Power cord.

f) Electrolyte:

An electrolyte is a device that uses electricity to split water molecules (H_2O) into its constituent elements, hydrogen (H_2) and oxygen (O_2), through a process called electrolysis. Electrolysis is a non-spontaneous chemical reaction that occurs when an electric current is passed through a substance

In the context of electrolyzers, electricity supplied by a power source drives the electrolysis process. The electrolyzer itself consists of two electrodes, an anode (positive electrode) and a cathode (negative electrode) submerged in a liquid electrolyte (a substance that conducts electricity). When the electric current flows through the electrolyte, it breaks down the water molecules at the electrodes. Hydrogen gas is produced at the cathode, and oxygen gas is produced at the anode (20).

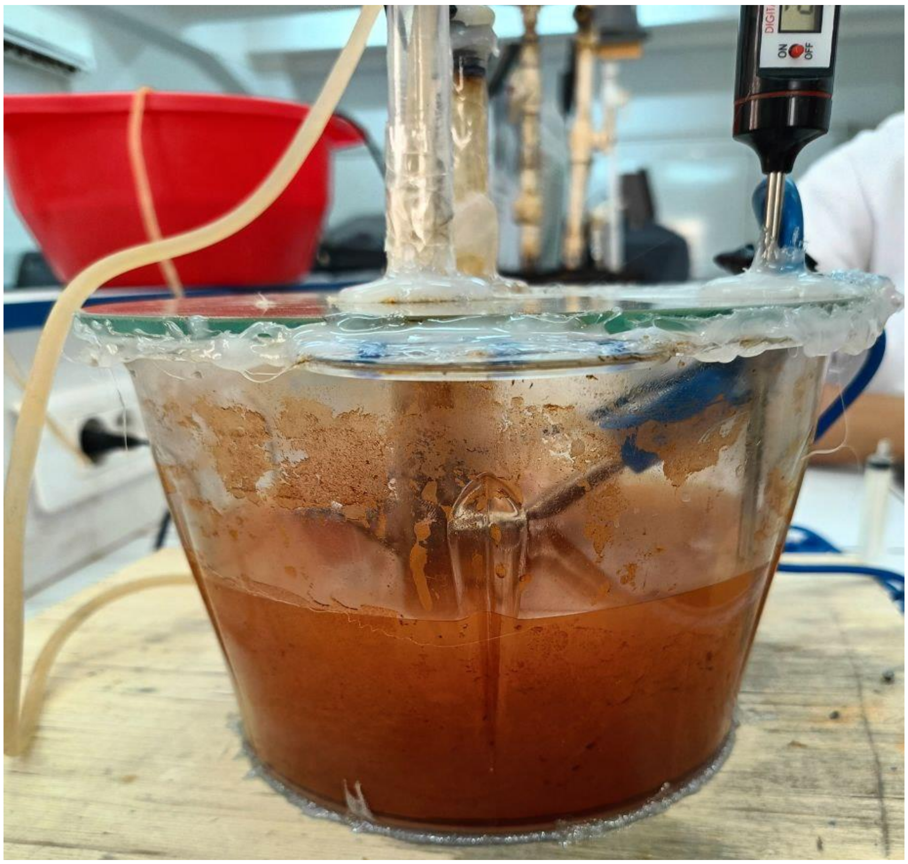

Figure II-8: Electrolyte.

II.6.2 General informations about HTF-14 well and ONM-23:

a) **Location and statue:**

Table II-1:Location and statue of HTF14.

Well	HTF-14
Zone	HZP
Date of Drilling	01/12/2012

Location	X : 819010.0907 Y : 85614.0441 Z_{SOL} : 157 (m) Z_{TABLE}: 165 (m)
Depth	3461 (m)
Statue	Artificial Lifting (Open)
Manifold/Sous-manifold	GOSP-HGA / HTFM2

b) Technical sheet of HTF-14 well and ONM-223:

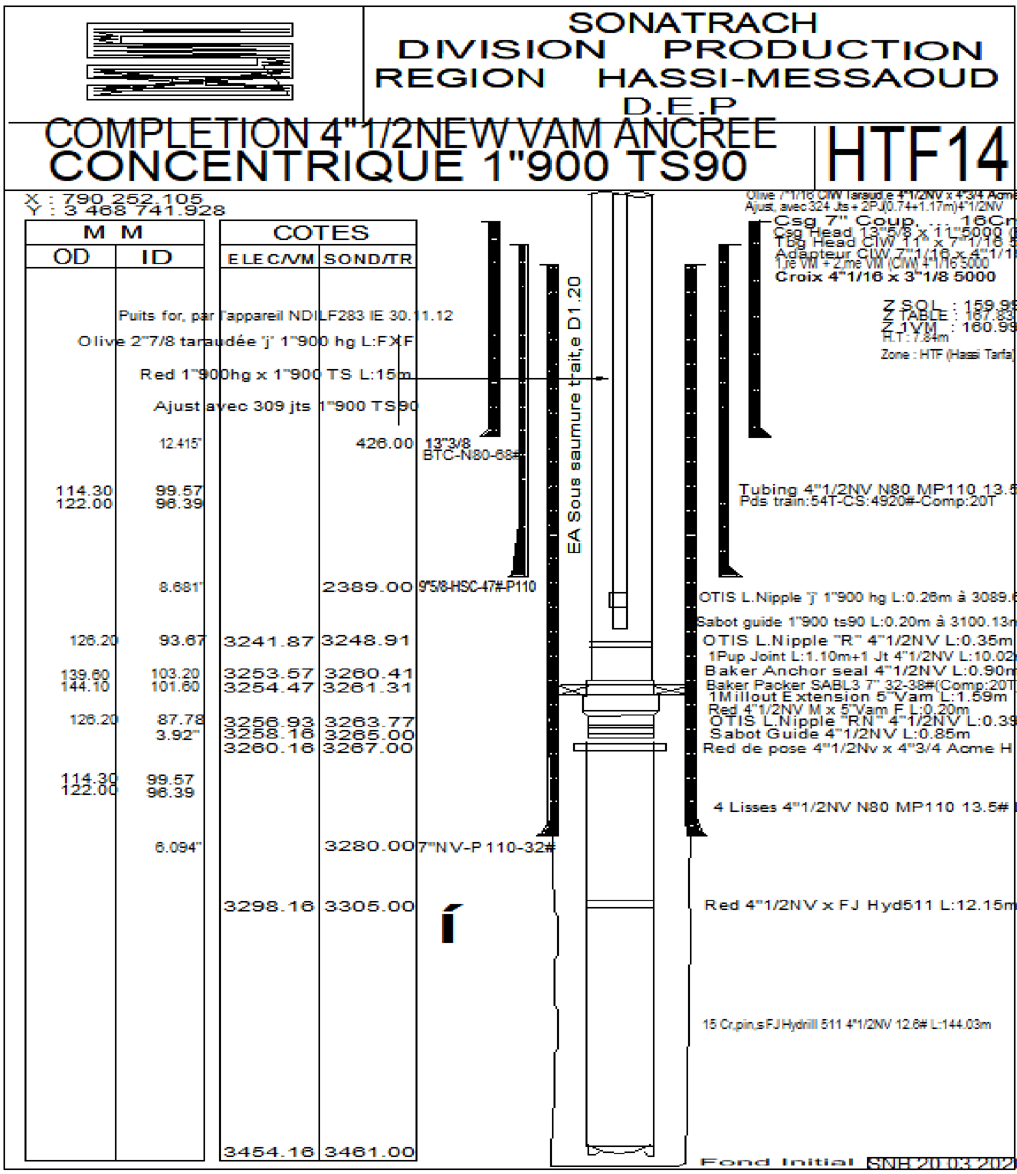

Figure II-9: Completion and technical sheet of HTF14.

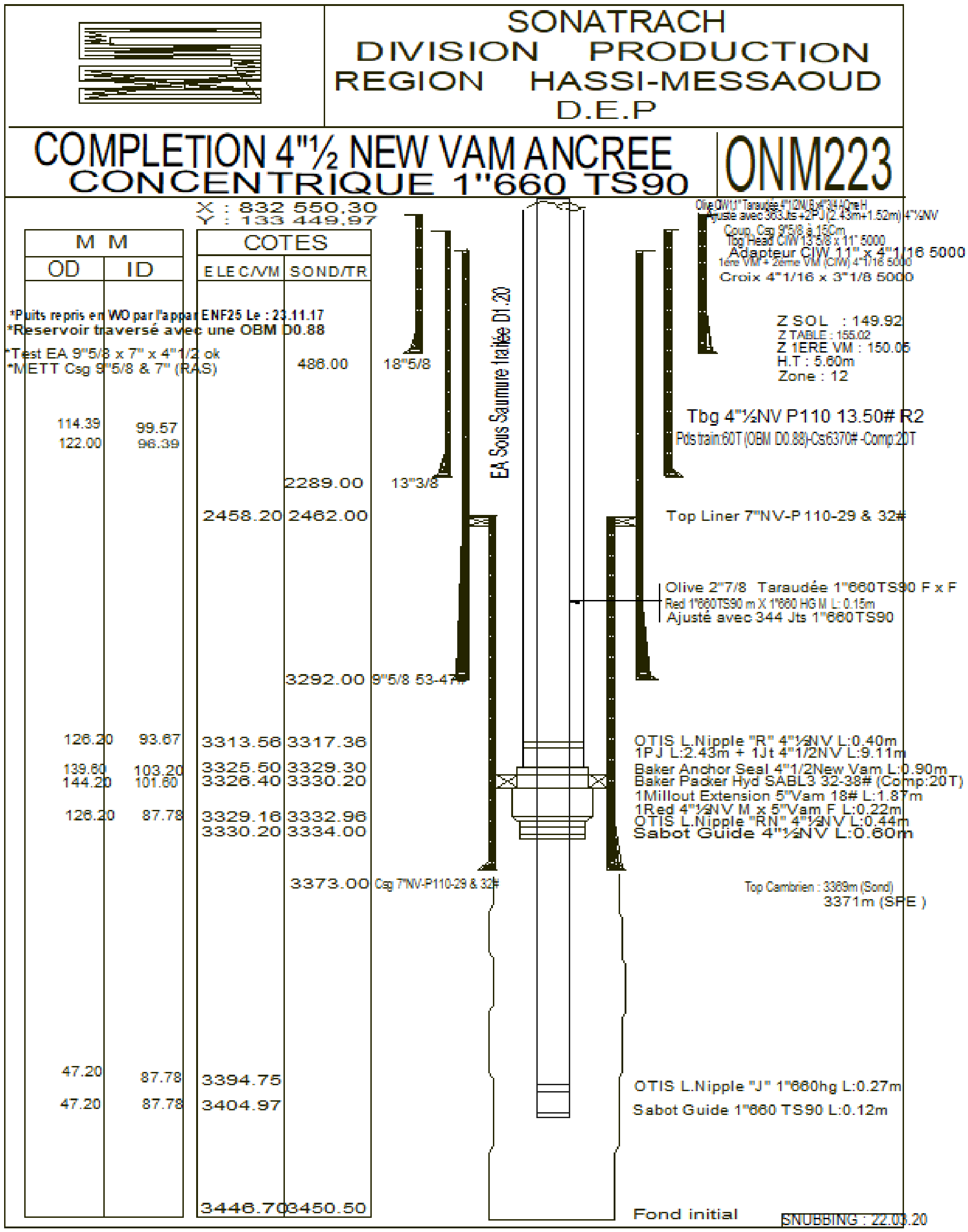

Figure II-10: Completion and technical sheet of ONM-223.

c) Water chemical compositions of water in ONM-223 and HTF-14:

The table presents the analysis of water before and after an experiment for two different samples, OMN-223 and HTF-14. The ion concentrations measured are N_2O, NH_4, Cl, F-O, and Zn.

Table II-2 Analyses of water before and after experiment.

WATER	**OMN-223**		**HTF-14**	
Ions	BEFOR	AFTER	BEFOR	AFTER
N_2O	3.4 mg/l	7.19mg/l	3.9 mg/l	7.77 mg/l
NH_4	1.44 mg/l	5.78 mg/l	3.1 mg/l	3.22 mg/l
Cl	0.09 mg/l	0.14 mg/l	0.12 mg/l	0.1 mg/l
F_2O	13.6 mg/l	13.6 mg/l	13.1 mg/l	13.5 mg/l
Zn	12 mg/l	26.1 mg/l	30.3 mg/l	12.8 mg/l

Interpretation of water analyses:

1. **N_2O (Nitrous Oxide) Levels**:
   - **OMN-223**: The concentration increased significantly from 3.4 mg/l to 7.19 mg/l after the experiment.
   - **HTF-14**: Similarly, there was an increase from 3.9 mg/l to 7.77 mg/l after the experiment.
   - **Interpretation**: Both samples show a considerable rise in N_2O levels, indicating that the experiment may have induced chemical reactions or processes that produce nitrous oxide.
2. **NH_4 (Ammonium) Levels**:
   - **OMN-223**: There was a substantial increase from 1.44 mg/l to 5.78 mg/l.
   - **HTF-14**: The increase was less pronounced, from 3.1 mg/l to 3.22 mg/l.
   - **Interpretation**: The ammonium concentration increased significantly in OMN-223, suggesting that the experimental conditions might have facilitated ammonium production or reduced its consumption.
3. **Cl (Chloride) Levels**:
   - **OMN-223**: Chloride levels slightly increased from 0.09 mg/l to 0.14 mg/l.
   - **HTF-14**: There was a slight decrease from 0.12 mg/l to 0.1 mg/l.

- **Interpretation**: Chloride levels remain relatively stable with minor fluctuations, implying that chloride ions were neither significantly produced nor consumed during the experiment.

4. **F-O (Fluoride Oxygen) Levels**:
   - **OMN-223**: The concentration remained unchanged at 13.6 mg/l.
   - **HTF-14**: There was a minor increase from 13.1 mg/l to 13.5 mg/l.
   - **Interpretation**: Fluoride levels are largely stable, suggesting minimal impact of the experimental conditions on fluoride ions.
5. **Zn (Zinc) Levels**:
   - **OMN-223**: Zinc levels more than doubled from 12 mg/l to 26.1 mg/l.
   - **HTF-14**: There was a significant decrease from 30.3 mg/l to 12.8 mg/l.
   - **Interpretation**: The divergent trends in zinc concentration imply different interactions or reactions in each sample. In OMN-223, zinc was either leached or produced in larger quantities, whereas in HTF-14, it was significantly reduced, possibly due to precipitation or adsorption processes.

The experimental conditions significantly affected the concentration of various ions in the water samples. Notably, there was a general increase in nitrous oxide and ammonium levels, while chloride and fluoride remained relatively stable. The changes in zinc levels were opposite for the two samples, indicating different chemical dynamics. This analysis provides insights into the chemical processes involved in the H_2 extraction experiment, suggesting potential areas for further investigation to optimize the process and control the ion concentrations.

II.6.3 Results:

we use in our installation those equipments, we variate in temperature and voltage in two different water OMN-223 and HTF-14, we use those conditions:
For temperature: 25, 42, 62.
For voltage: 5 V, 10 V, 12 V, 15 V, 17 V, 18 V, 20 V, 25 V, 29 V.
For pressure: with T=25 the pressure it's 1 atmosphere.
For the other temperature it's variable.

a) HTF-14 WATER:

Description of experiment:

We put our water (HTF-14) in electrolyzer we start to change in voltage with an ascending form in 1 min and we notice:

T=25C, P=1atm:

voltage	H2 volume (ml)
5	2.2
10	4.13
12	5.46
15	7.35
17	10.86
18	12.3
20	14.25
25	14.38
29	10.3

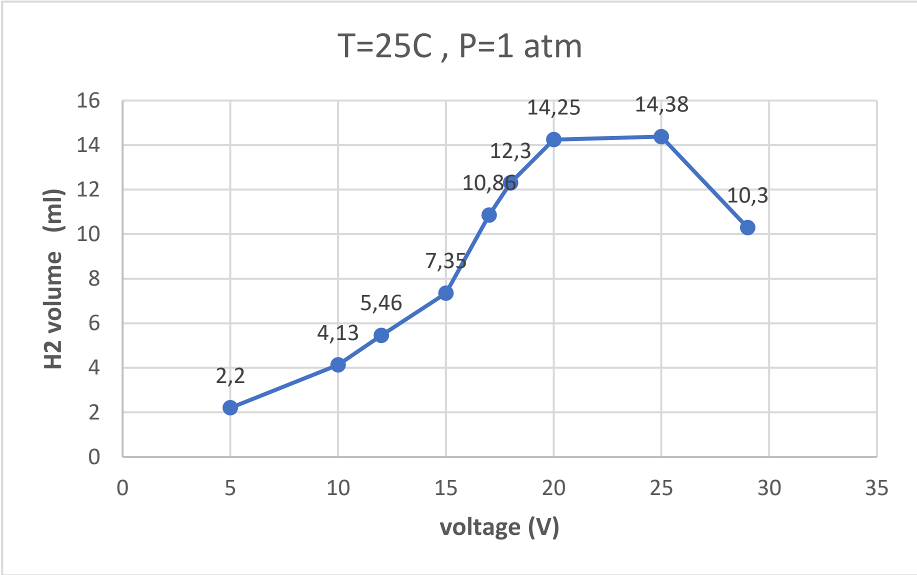

Table III-3 Electrolysis results of simple HTF-14 at different voltages and T 25C.

T=42C

voltage	H2 volume (ml)
5	2.3
10	3.74
12	6.37
15	8.25
17	10.1
18	10.83
20	10.55
25	10.54
29	11.1

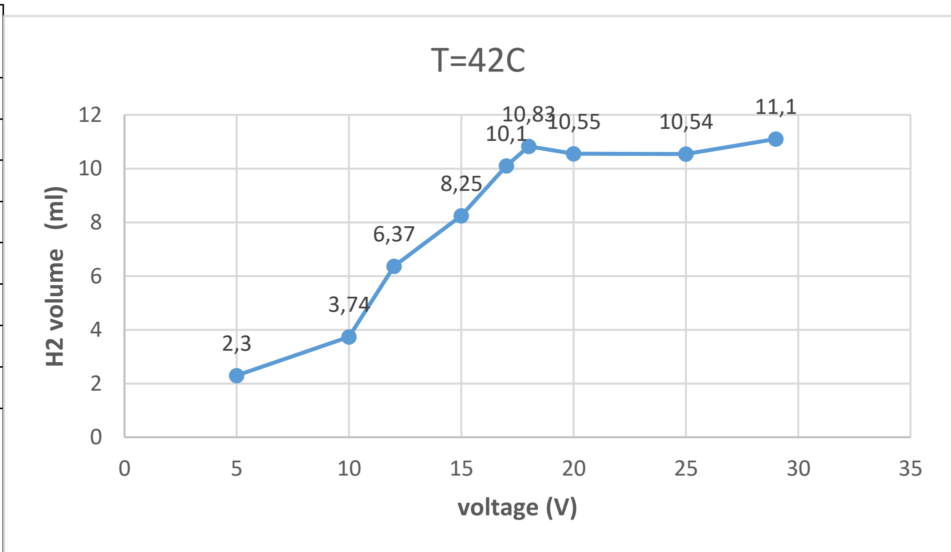

Table III-4: Electrolysis results of simple HTF-14 at different voltages and T 42C.

T=60 C:

voltage	H2 volume (ml)
5	3
10	8.82
12	13.99
15	17.41
17	19.5
18	17.29
20	23.54
25	14.28
29	

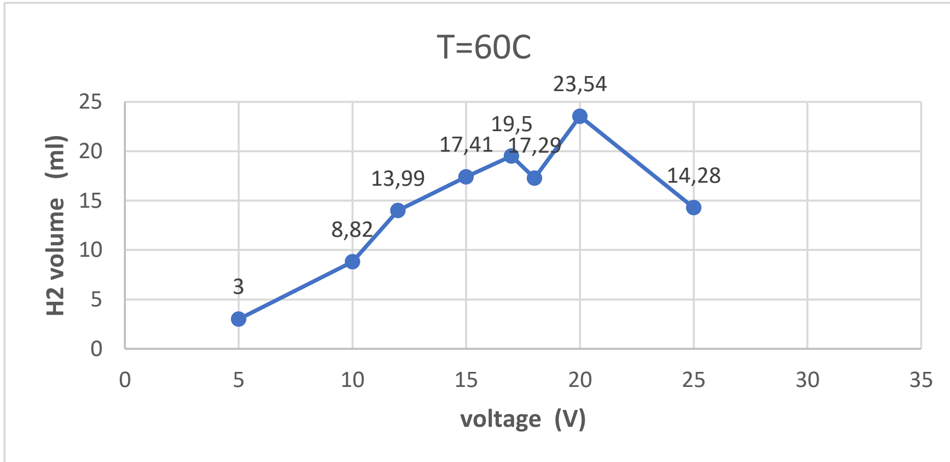

Table III-5: Electrolysis results of simple HTF-14 at different voltages and T 60C.

Curve of gain:

voltage	T=42/25	T=60/25
5	1.04545455	1.363636364
10	0.90556901	0.905569007
12	1.16666667	2.562271062
15	1.12244898	2.368707483
17	0.93001842	1.79558011
18	1.40569106	1.405691057
20	0.74035088	1.651929825
25	0.73296245	0.993045897
29	1.0776699	

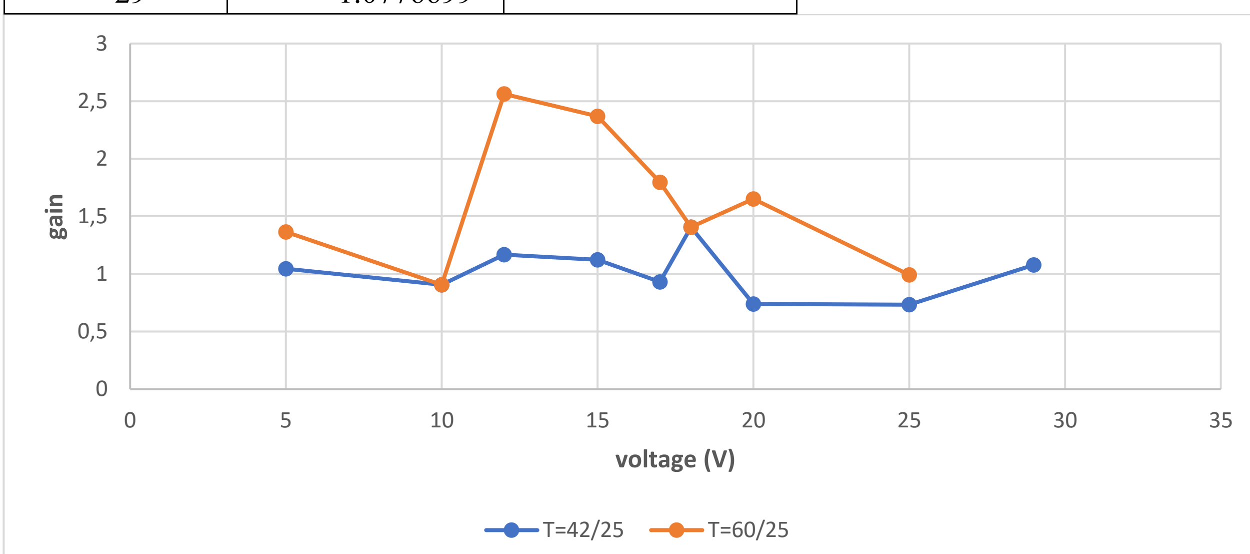

Table II-6:Curve of gain HTF-14.

b) ONM-223 WATER:

Description of experiment:

We put our water (ONM-223) in electrolyser we start to change in voltage with an ascending form in 1 min and we notice:

T=25C, P=1 atm:

voltage	H2 volume (ml)
5	2.2
10	4.13
12	5.46
15	7.35
17	10.86
18	12.3
20	14.25
25	14.38
29	10.3

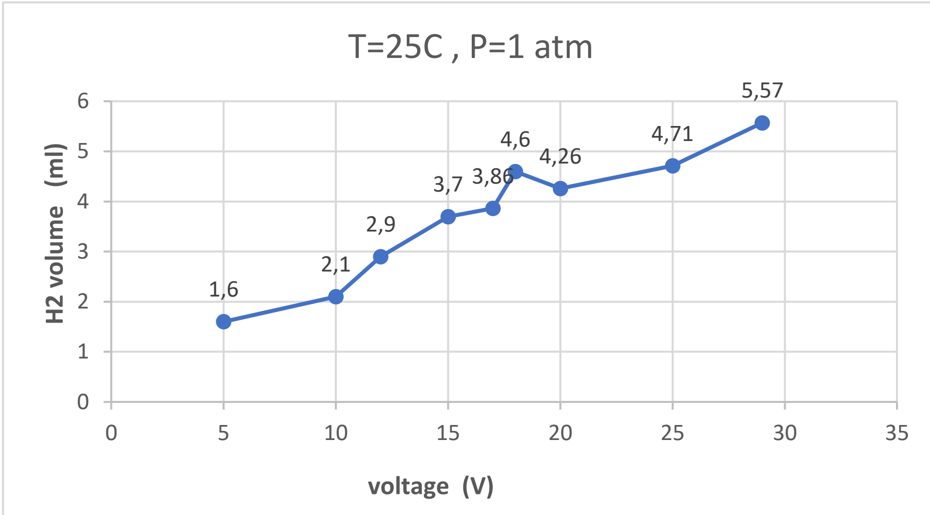

Table II-7: Electrolysis results of simple ONM-223 at different voltages and T 25C.

T=42C

voltage	H2 volume (ml)
5	2.3
10	3.74
12	6.37
15	8.25
17	10.1
18	10.83
20	10.55
25	10.54
29	11.1

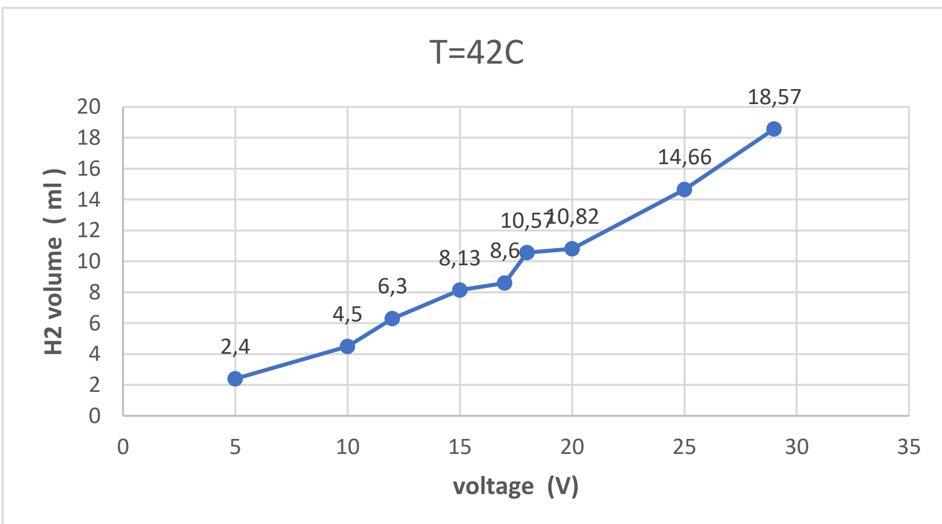

Table II-8 Electrolysis results of simple ONM-223 at different voltages and T 42C.

For T=60C**:**

voltage	H2 volume (ml)
5	3.2
10	6.08
12	8.42
15	10.53
17	12.92
18	14.28
20	16.72
25	22.54

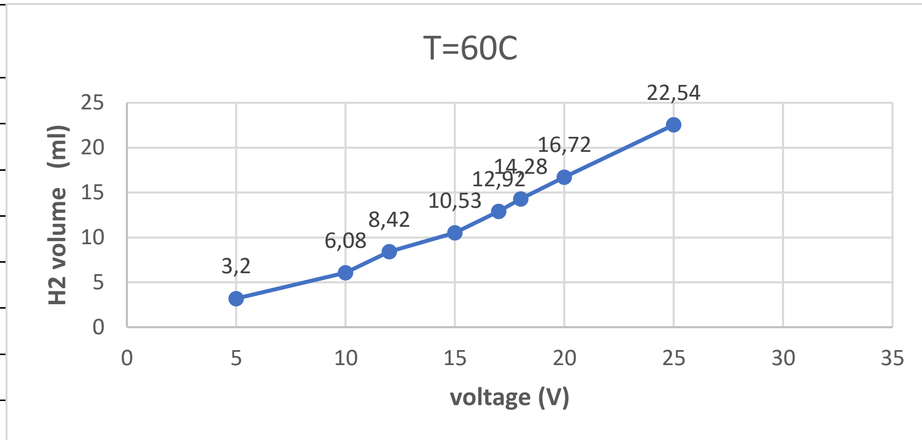

Table II-9: Electrolysis results of simple ONM-223 at different voltages and T 60C.

Curve of gain:

voltage	T=42/25	T=60/25
5	1.5	2
10	2.14285714	2.142857143
12	2.17241379	2.903448276
15	2.1972973	2.845945946
17	2.22797927	3.347150259
18	3.10434783	3.104347826
20	2.5399061	3.924882629
25	3.11252654	4.785562633
29	3.33393178	

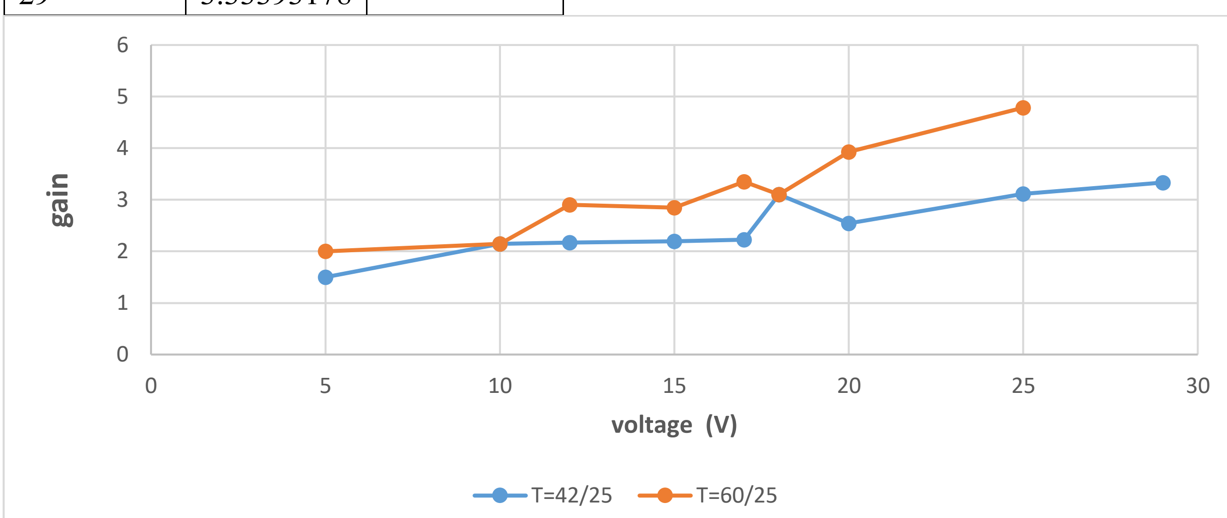

Table II-10: Curve of gain ONM-223.

II.6.3 Interpretation of results

Electrolysis stands as a pivotal technique in the realm of water analysis, offering insights into the intricate composition of aqueous solutions, particularly those found underground. In this investigation, nuanced variations in electrolysis gain within underground water samples are explored, with a specific focus on the influence of temperature fluctuations.

Experimental analysis revealed intriguing patterns in electrolysis gain across different temperatures. Notably, at 42°C, the distinct behavior of electrolysis gain at 42°C, characterized by an ascending form, contrasts with the peak-shaped curves observed at other temperatures. This divergence suggests temperature-dependent variations in ion activities and reaction kinetics.

Specifically, at 42°C, the heightened ion activities facilitate a continuous increase in gain, reflecting a favorable electrolysis environment. In contrast, deviations from this optimal temperature lead to the emergence of peaks in the gain curve, indicative of critical points where non-desirable reactions become prominent, thus limiting gain.

Interestingly, despite these temperature-induced fluctuations, the consistent presence of peak-shaped curves across different temperatures underscores the robustness of the electrolysis process. This uniformity implies a consistent pattern of ion interactions and electrochemical behaviors, irrespective of temperature variations. Such empirical evidence not only validates the reliability of the observed phenomena but also strengthens the predictive capabilities of the ML-01 model in forecasting electrolysis behavior across diverse environmental conditions.

In essence, the findings from this investigation offer valuable insights into the complex dynamics of electrolysis in underground water samples. By elucidating the temperature-dependent variability in electrolysis gain and identifying distinct patterns in gain curves, this study contributes to a deeper understanding of electrochemical processes in aqueous environments. Moving forward, leveraging these insights can inform the development of robust analytical techniques for water quality assessment and environmental monitoring, thus fostering more effective management strategies for underground water resources.

In conclusion, the investigation highlights the dynamic interplay between temperature, voltage, and electrolysis gain in underground water samples. The distinct patterns observed underscore the intricate nature of electrochemical processes in aqueous environments. Further exploration of these dynamics promises to enhance our understanding of water chemistry and refine analytical methodologies in environmental science.

In the quest for efficient and sustainable hydrogen production, the HSPEU unit stands at the forefront of innovation. A critical factor in the performance of the HSPEU is the quality of water used in the electrolysis process. The ML-01 model plays a pivotal role in optimizing this aspect by identifying and enhancing the mechanical and chemical properties of the water used.

1. Understanding the Role of Water in Electrolysis:

Electrolysis involves the decomposition of water (H_2O) into oxygen (O_2) and hydrogen (H_2) gas through the application of an electric current. The efficiency of this process is highly dependent on the properties of the water used. Impurities, ion concentration, pH levels, and the presence of specific electrolytes can significantly affect the electrolysis efficiency, energy consumption, and the longevity of the electrodes.

2. Mechanical Properties Optimization:

One of the mechanical aspects crucial for the water in electrolysis is its conductivity. High conductivity enhances the efficiency of the electrolysis process by reducing electrical resistance. The ML-01 model analyzes the relationship between water conductivity and factors such as temperature, pressure, and dissolved ion concentration.

By predicting the optimal range of these parameters, ML-01 helps in designing water treatment processes that ensure consistent and high conductivity, thus improving the overall efficiency of the HSPEU unit.

3. Chemical Properties Optimization

Chemical purity is another vital property. Impurities in water can lead to the formation of unwanted byproducts, electrode degradation, and reduced efficiency. The ML-01 model identifies the ideal chemical composition of water by considering the presence of beneficial electrolytes like potassium hydroxide (KOH) or sodium hydroxide (NaOH), which enhance the electrolysis process, while minimizing harmful contaminants.

Conclusion:

In conclusion, the experiments conducted on multiple underground water samples have yielded invaluable insights into the intricate phenomena of electrolysis, shedding light on the fundamental principles governing chemical transformations in aqueous environments. Through meticulous observation and analysis, we have elucidated the complex interplay of factors influencing the efficiency, selectivity, and kinetics of electrolytic reactions, paving the way for a deeper understanding of this essential process.

Crucially, these experiments have underscored the efficacy and reliability of the ML-01 model in capturing and predicting the behavior of electrolysis systems with remarkable accuracy. By comparing the experimental results with the simulations generated by the ML-01 model, we have demonstrated the model's ability to faithfully replicate observed phenomena and provide meaningful insights into the underlying mechanisms driving electrolytic processes.

Furthermore, the successful application of the ML-01 model in interpreting and rationalizing the experimental data highlights its utility as a powerful tool for enhancing our understanding of underground water electrolysis. Through its systematic approach and comprehensive mathematical framework, the ML-01 model offers a versatile platform for elucidating complex phenomena, guiding experimental design, and optimizing operational parameters to achieve desired outcomes.

Chapter III
Design of IHSPEU unit.

Introduction:

In this chapter, we delve into the realm of integrated power generation systems, exploring innovative approaches to enhance energy efficiency and sustainability. At the forefront of this endeavor lies the integration of two distinct yet synergistic facilities: methane cracking and electrolysis. Through the fusion of these technologies, we introduce a novel concept: the IHSPEU facility.

The IHSPEU facility represents a paradigm shift in energy production and utilization, leveraging the complementary strengths of methane cracking and electrolysis to maximize efficiency and minimize environmental impact. By integrating these processes into a unified system, we unlock unprecedented synergies, enabling the efficient conversion of methane and water into hydrogen, synthetic fuels, and other valuable products.

Moreover, the IHSPEU facility goes beyond conventional energy production paradigms by offering innovative solutions to mitigate CO2 emissions and reduce carbon footprint. Through the utilization of captured CO2 in Enhanced Oil Recovery (EOR) injection wells, we not only mitigate greenhouse gas emissions but also enhance oil recovery rates, thereby maximizing the economic and environmental benefits of the integrated system.

In this chapter, we explore the design, operation, and potential applications of the IHSPEU facility, highlighting its role as a transformative technology in the transition towards a more sustainable and resilient energy landscape.

By harnessing the power of integration and innovation, we pave the way for a brighter, cleaner, and more prosperous future for generations to come, and in first we are going to describe the simulation program aspen plus.

III.1 ASPEN PLUS:

Aspen Plus is a comprehensive process simulation software developed by Aspen Technology, Inc. It's widely used in industries such as chemical engineering, petroleum refining, pharmaceuticals, and other process-based sectors.

III.1.1 Modes of simulation in ASPEN PLUS:

Here's a detailed description of Aspen Plus along with its palette material and its uses:

- **Description**:

Aspen Plus is a process modeling tool used for simulating and optimizing chemical processes. It employs rigorous thermodynamic models to simulate various unit operations and chemical reactions within a process. It allows engineers to design, analyze, and optimize chemical processes, from conceptual design to detailed engineering.

Aspen Plus enables users to model steady-state and dynamic behavior of processes, facilitating the study of process dynamics and control strategies.

- **Key Features:**

Library of pre-defined unit operations such as reactors, distillation columns, heat exchangers, pumps, etc. Extensive thermodynamic databases for accurate modeling of phase equilibria and chemical reactions. Customizable process flowsheets for building complex process models.

Simulation capabilities for various industries including petrochemicals, chemicals, pharmaceuticals, and more.

Optimization tools for finding optimal operating conditions and process designs.

- **Applications:**

Aspen Plus is used in the design and optimization of chemical processes, including the production of fuels, polymers, pharmaceuticals, and specialty chemicals. It is utilized for process troubleshooting, debottlenecking, and revamping existing plants. Aspen Plus finds applications in environmental engineering for modeling and optimizing pollution control processes. It is used in research and development for process innovation and scale-up.

- **General simulations of ASPEN Plus:**

There are a lot of processes which can be modeled, See the model pallete here:

- Heat Exchanges.
- Reactors.
- Pressure Changers
- Absorption Columns.
- Separators & Mixers, etc.

More interestingly:

- Fluidized Catalytic Cracking.
- H2SO4 Alkylation.
- Catalytic Reformer.
- Hydrocracker.
- Sulfur Recovery Units.
- Alkaline electrolysis.

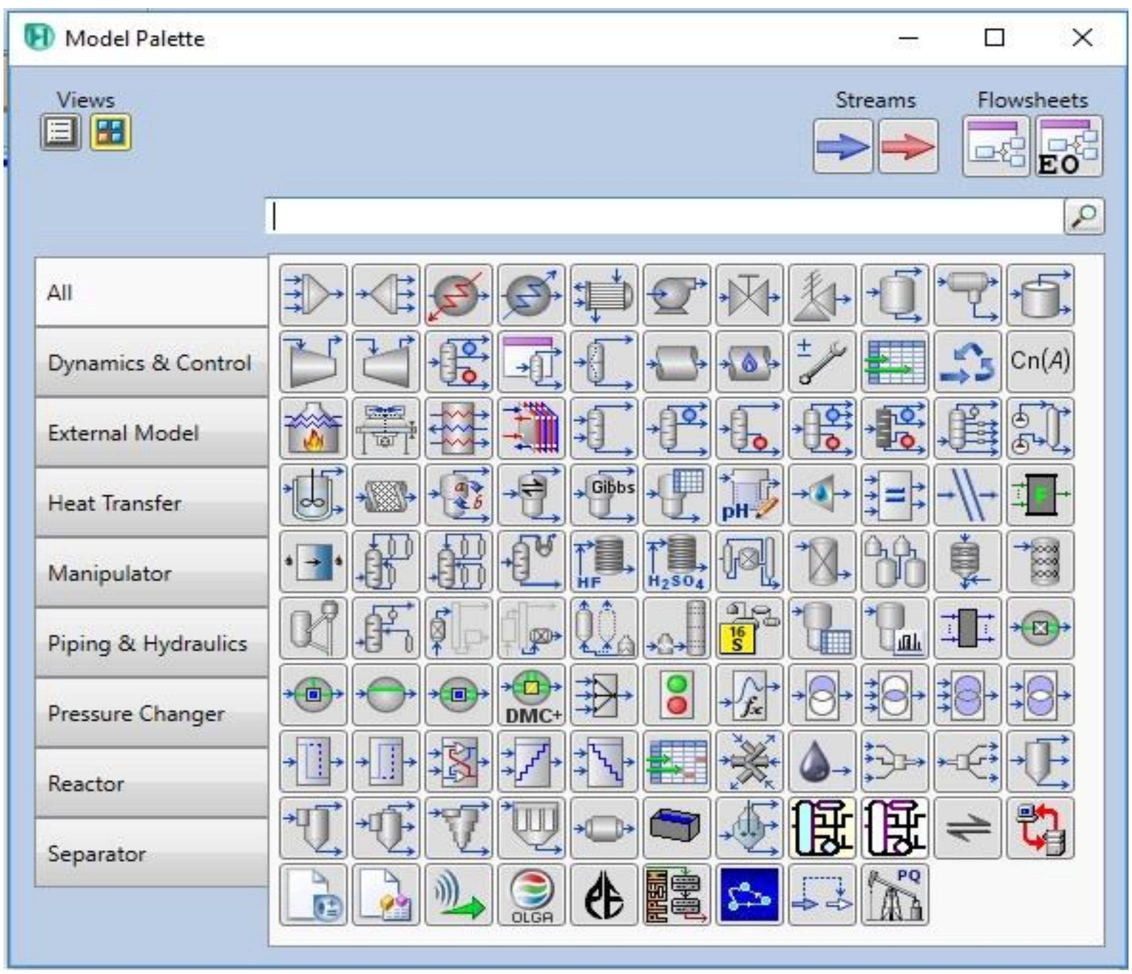

Figure III-1: Aspen plus Materials palette.

III.2 **Model cracking**

To create a model for methane combustion in Aspen Plus, you can follow these general steps:

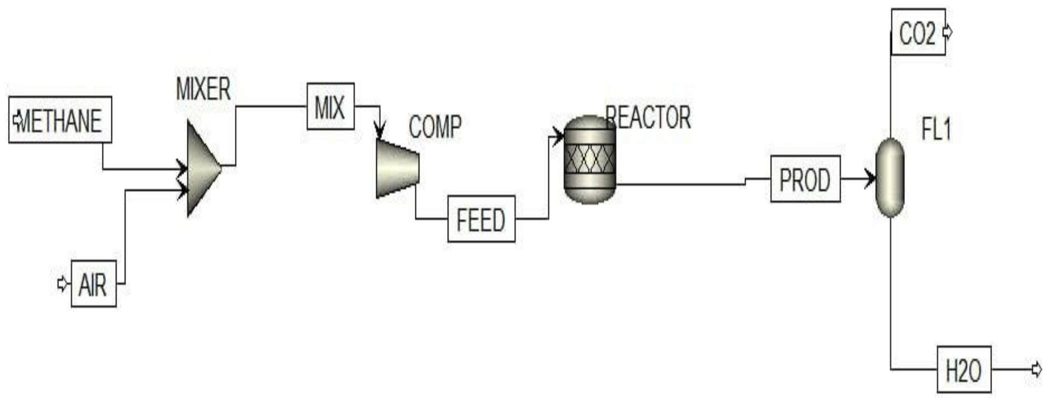

Figure III-2: Methane cracking model (Aspen Plus2024).

1. Start a new simulation in Aspen Plus and select the appropriate property method. For combustion reactions involving hydrocarbons and air.
2. Define the components involved in the process. For methane combustion, you will need to include methane (CH_4), oxygen (O_2), nitrogen (N_2), carbon dioxide (CO_2), and water (H_2O) as components.
3. Create a material stream for the feed, which will include methane and air (a mixture of oxygen and nitrogen). Specify the temperature, pressure, and composition of the feed stream:

Air 15 C ,1000Kpa (N_2 79%, O_2 21%) Flow rate 2000 kmol/h.

Methane 15 C, 1000Kpa 2000kg/h.

-Add a compressor (Isentropic): Feed compressed to 2900 Kpa

4. Create a reactor block for the combustion reaction type RStoic:

Adiabatic,2900Kpa, combustion conversion 100%.

5. In the reactor block, specify the reaction for methane combustion:

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

You can enter this reaction in the "Reactions" section of the reactor block.

6. Connect the feed stream to the inlet of the reactor block.

7. Create an outlet stream from the reactor block to represent the products of combustion.

8. Add a turbine type isentropic with: Discharge pressure=101Kpa, efficiencies=0,7.

9. Specify the desired output variables, such as temperature, pressure, flow rates, and compositions, for the streams of interest.

10. Run the simulation and analyze the results.

Table III-11 : Result of simulation methane cracking.

	A	B	C	D	E	F	G	H	I	J
1	Description									
2	From			FL1	COMP	FL1		MIXER	REACTOR	
3	To		MIXER		REACTOR		MIXER	COMP	FL1	
4	Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	
5	Maximum Relative Error									
6	Cost Flow	$/hr								
7	MIXED Substream									
8	Phase		Vapor Pha	Vapor Pha	Vapor Pha	Liquid Pha	Vapor Pha	Vapor Pha	Vapor Phase	
9	Temperat	C	15	-256,06	152,131	-256,06	15	14,9424	1976,42	
10	Pressure	bar	10	28	29	28	10	10	29	
11	Molar Vapor Fractio		1	1	1	0	1	1	1	
12	Molar Liquid Fractio		0	0	0	1	0	0	0	
13	Molar Solid Fraction		0	0	0	0	0	0	0	
14	Mass Vapor Fraction		1	1	1	0	1	1	1	
15	Mass Liquid Fractior		0	0	0	1	0	0	0	
16	Mass Solid Fraction		0	0	0	0	0	0	0	
17	Molar Ent	cal/mol	-85,846	-91489	-627,17	-32573	-17923	-1611	-627,17	
18	Mass Enth	cal/gm	-2,9756	-2117,3	-22,596	-1242	-1117,2	-58,043	-22,596	
19	Molar Ent	cal/mol-K	-3,8119	-15,486	-4,2966	-359,86	-24,186	-4,9747	10,1838	
20	Mass Entr	cal/gm-K	-0,1321	-0,3584	-0,1548	-13,721	-1,5076	-0,1792	0,36691	
21	Molar Der	mol/cc	0,00042	6,49E-05	0,00082	0,04126	0,00043	0,00042	0,00015	
22	Mass Den	gm/cc	0,01211	0,00281	0,02269	1,08222	0,00684	0,01166	0,00429	
23	Enthalpy F	cal/sec	-47692	-5E+06	-381006	-2E+07	-930997	-978689	-381006	
24	Average MW		28,8504	43,2109	27,7553	26,2267	16,0428	27,7553	27,7553	
25	Mole Flow	kmol/hr	2000	196,83	2187	1990,17	187	2187	2187	
26	Mole Fractions									
27	Mass Flow	kg/hr	57700,8	8505,21	60700,8	52195,6	3000	60700,8	60700,8	
28	Mass Fractions									
29	Volume Fl	l/min	79433	50535	44577,9	803,834	7314,19	86750,6	235900	
30	Vapor Phase									
31	Liquid Phase									

Sheet1

III.3 Model alkaline electrolysis system:

Creating an Aspen Plus model for an alkaline electrolysis system for hydrogen production involves several steps. Here's a step-by-step guide:

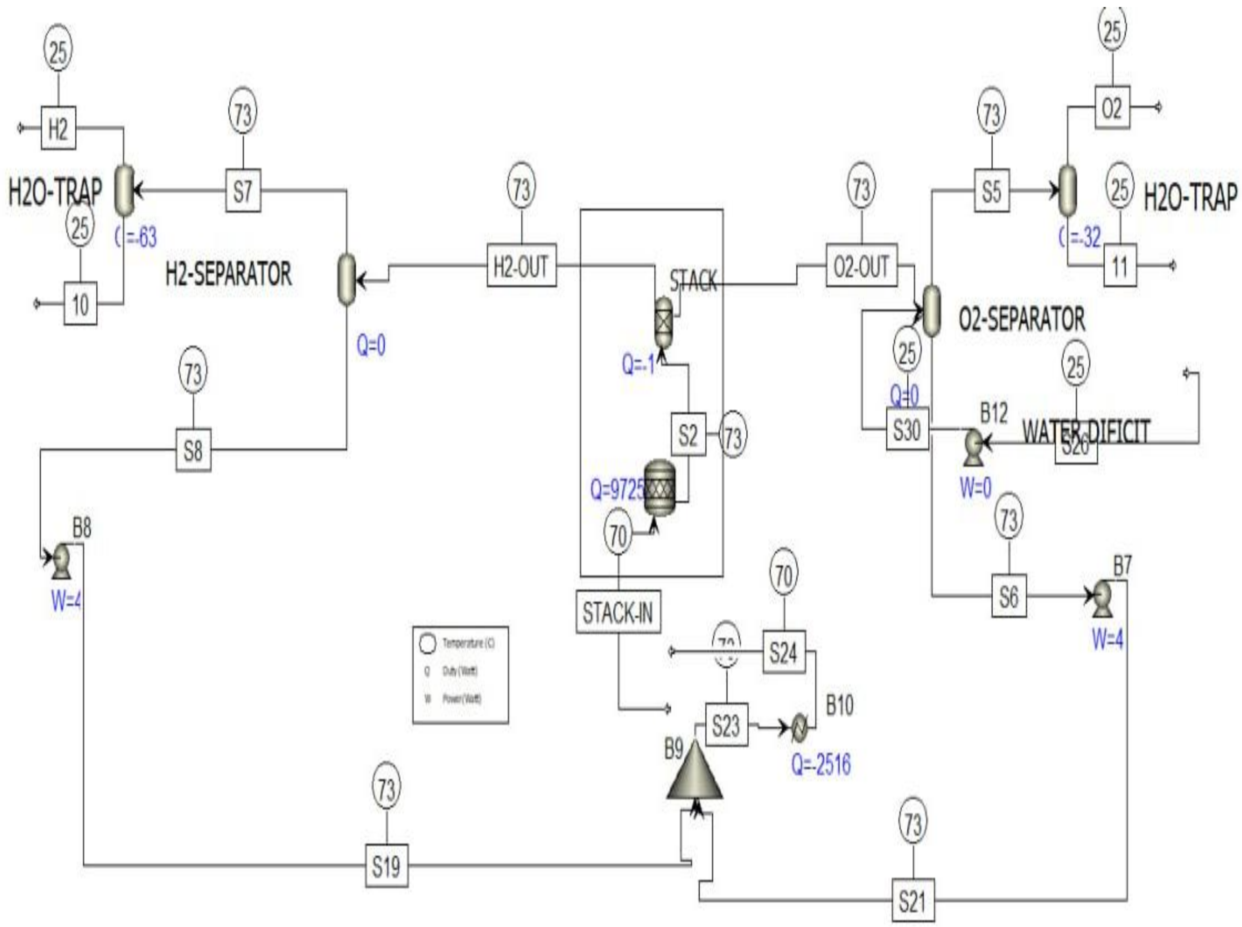

Figure III-3: Model alkaline electrolysis system (Aspen Plus2024).

1. Define Components:

- Launch Aspen Plus and start a new simulation.
- Define the components needed for the electrolysis process, including water (H2O), hydrogen (H2), oxygen (O2), H+, OH-, K+ and KOH.

- Set the appropriate property method for the components. For water, you can use the standard NRTL or RK model. Ensure the method is suitable for electrolyte solutions if ions are involved.

2. Define Electrolyte Solution:

- If your electrolysis system involves an electrolyte solution, set up the solution properties. Aspen Plus has options for modeling aqueous solutions with various electrolyte models.

- Define the concentrations of ions present in the solution, typically for an alkaline electrolysis system, you would have hydroxide ions (OH-) and perhaps other ions depending on the electrolyte used.

3. Specify Electrolysis Reactions:

- Define the electrochemical reactions occurring at the anode and cathode. For alkaline electrolysis, the overall reactions are typically:
  - Anode: $2H_2O(l) \rightarrow O_2(g) + 4e^- + 4OH^-$
  - Cathode: $4OH^- \rightarrow 2H_2O(l) + O_2(g) + 4e^-$
- You may need to specify kinetic data or use standard rate expressions for these reactions.

4. Set Up Mass and Energy Balances:

- Ensure that mass and energy balances are properly configured in your electrolysis unit operation block. This includes specifying feed streams, product streams, and any recycle streams if applicable.
- Specify any heat or energy inputs required for the electrolysis process.
- Specify the operating conditions such as temperature, pressure, and current density.

5. Create Electrolysis Unit:

- Add a reactor RSTOIC (T=70 C, P=7bar, Total Flow Rate =900 Kg/h) with mass fraction (H_2O = 0,65, KOH=0,35), this reactor product H_2 and O_2 from H_2O.
- Add separator 'sep1' to separate components based on specified flows or split fractions.
- Make connection between reactor RSTOIC and sep1 to create Cell Stack.
- Add 2 separators 'Flash2' (Two outlet flash, models flash drums, evaporators. Using rigorous VLL or VLL equil), one for H_2 and another one for O_2.
- Add 2 separators 'Flash2' (Two outlet flash, models flash drums, evaporators. Using rigorous VLL or VLL equil) for H_2O Traps.
- Connect first H_2O trap with H_2 separator.
- Connect second H_2O trap with O_2 separator.
- Add two pumps (Pressure changers) with (Efficiencies =0,7 and Discharge Pressure=7bar).
- Connect one pump with H_2 separator and second one with O_2 separator.
- Add mixer used to combine heat or work streams.
- Sub linking the mixer with last two pumps.
- Add heat exchanger (Heater) thermal and phase state changer.

-Connect the heater with mixer.

-Add new pump (Efficiencies =0,7, Discharge Pressure =7bar) for Water deficit (inlet T=25 C, inlet P=1bar).

7. Run the Simulation:

- Once your model is set up, run the simulation to obtain results.
- Check for convergence and troubleshoot any errors or warnings that may arise during the simulation.

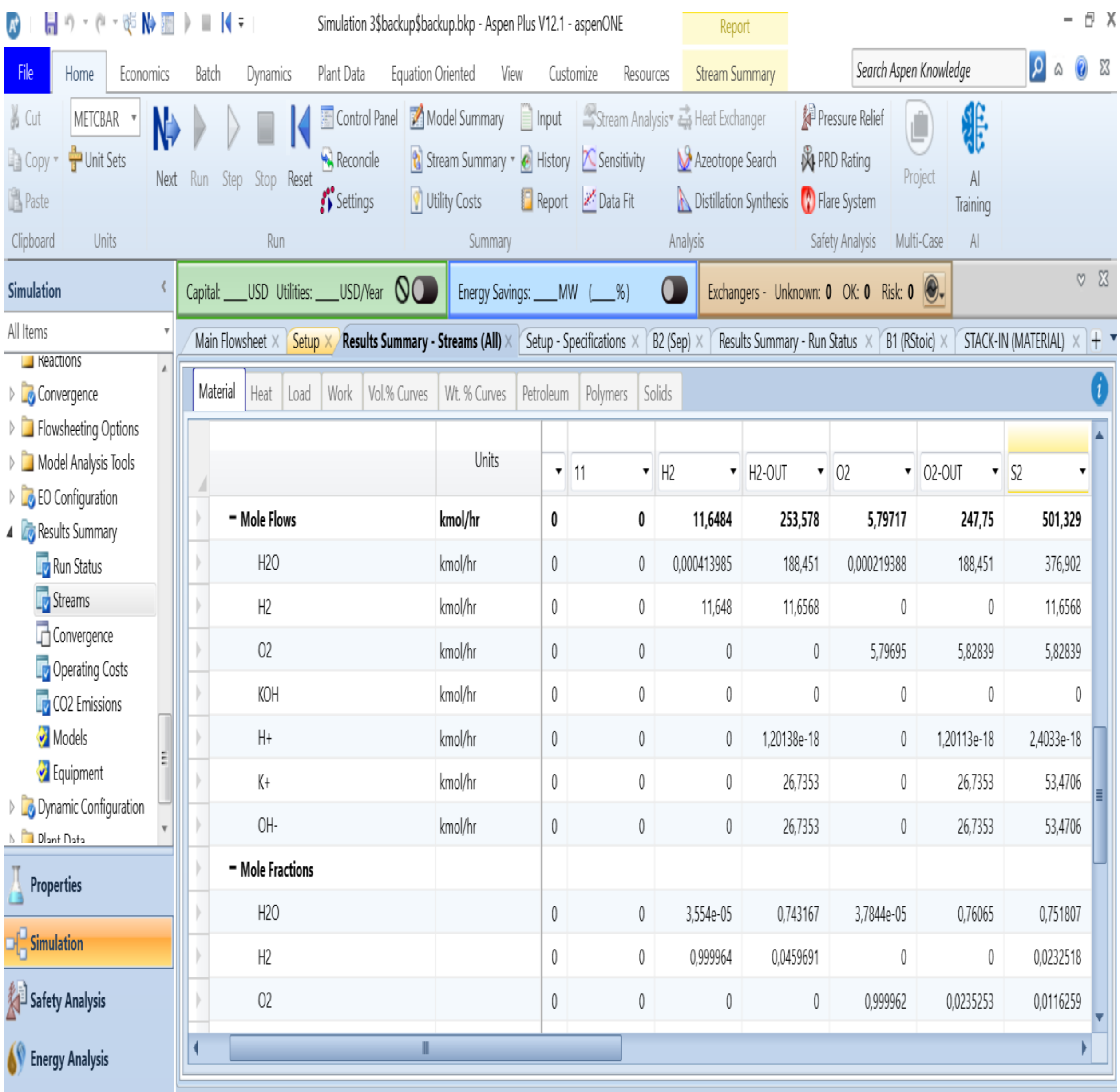

Figure III-4: Result of simulation electrolyser model in ASPEN PLUS.

8. Analyze Results:

- Review the simulation results to evaluate the performance of the electrolysis system.

- Look at hydrogen production rates, energy consumption, and other relevant parameters to assess the efficiency and feasibility of the process.

Table III-12: Stack in and H2 out with different % of H2O and KOH.

WATER PERCENTAGE		0,1		0,2		0,3		0,4		0,5		0,6		0,7		0,8		0,9		1	
Unit		H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN	H2-OUT	STACK-IN
H2O	Kmol/hr	26,921591	55,5084350	53,84318201	111,016	80,7647	166,52530	107,686364	222,033740	134,608	277,542175	9,99151	0	188,451	388,559045	215,372	444,067480	242,294	499,5759156	266,5237509	549,5335071
H2	Kmol/hr	1,66525305	0	3,3305061	0	4,99575	0	6,66101221	0	8,32626	0	0	0	11,6567	0	13,3220		14,9872	0	16,48600521	0
KOH	Kmol/hr	80,205840	160,411680	71,2940802	142,5881	62,3823	124,76464	53,4705602	106,941120	44,5588	89,1176003	35,6470	71,29408024	26,7352	53,4705601	17,8235	35,6470401	8,91176	17,82352006	0,891176003	1,782352006
V Flow	Cum/hr	2,5696148	5,19589280	2,6864757	5,493841	2,84066	5,8667205	3,0303836	6,30482212	3,25885	6,80227948			3,80577	7,96631511	4,12159	8,63619250	4,47059	9,376090007	4,82739181	10,13062166

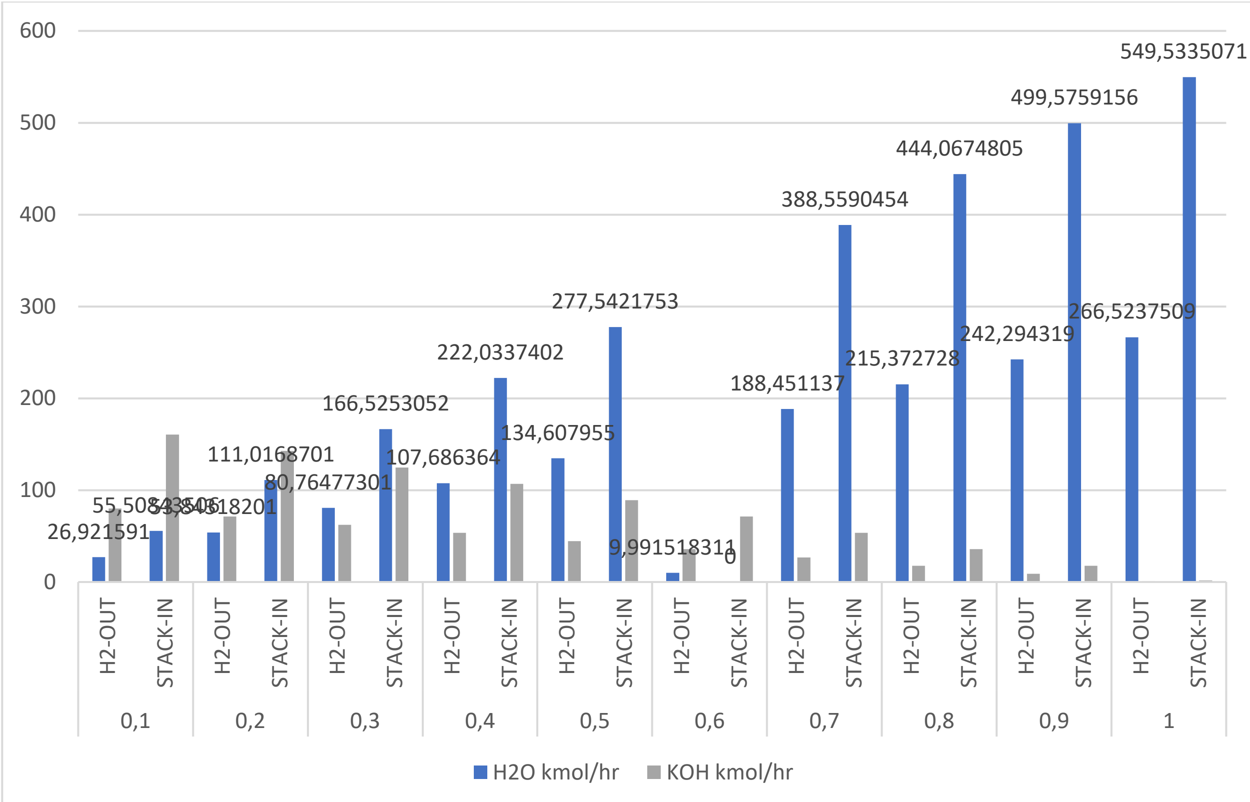

Figure 10: H2O stack in the unit.

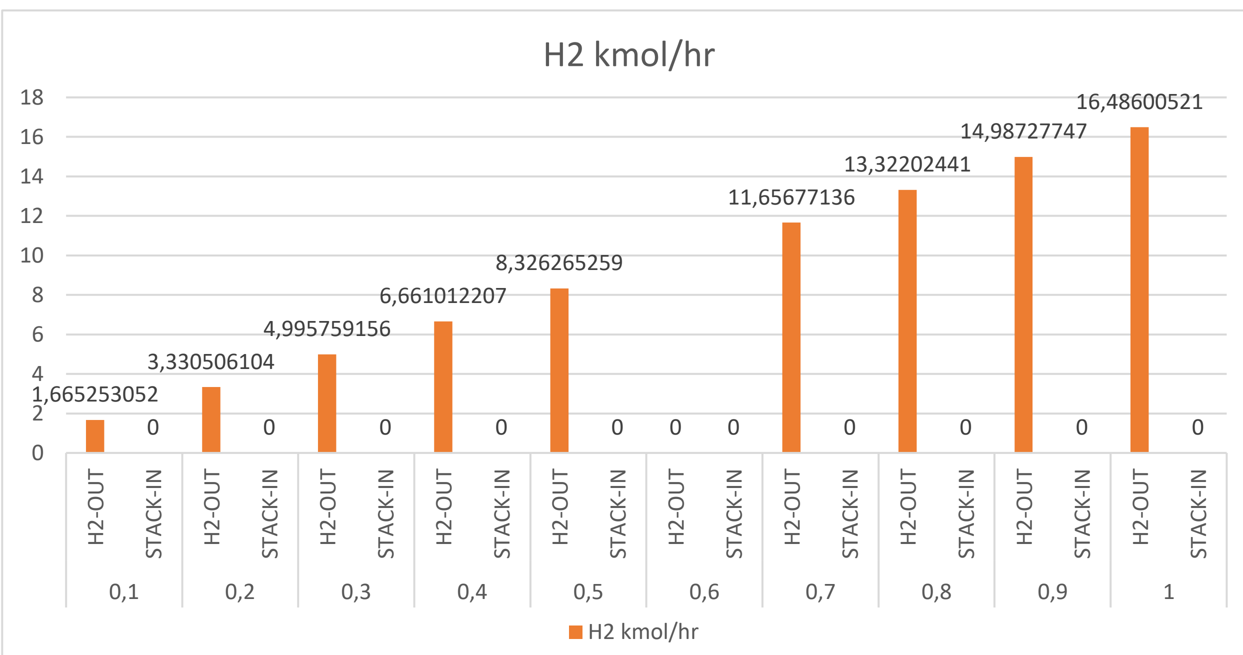

Figure III-6:H2 out from the unit.

9. Optimization (Optional):

- If desired, you can further optimize the electrolysis system by adjusting operating conditions or design parameters to improve performance.

10. Documentation:

- Document your model setup, assumptions, and results for future reference or sharing with others.

By following these steps, you can create an Aspen Plus model for an alkaline electrolysis system for hydrogen production. Adjustments may be needed based on the specific details and requirements of your system.

III.3.1 Analyses and interpretations:

- **Hydrogen Outlet (H2-OUT):**

  This represents the amount of hydrogen produced at the outlet of the electrolysis stack. The values are in kmol/hr (kilomoles per hour). Higher values indicate higher hydrogen production rates.

- **Stack Inlet (STACKIN):**

  This likely represents the amount of hydrogen entering the electrolysis stack. The values are also in kmol/hr. It is possible that some hydrogen is recirculated within the system, and this value reflects the total amount of hydrogen entering the stack, including both the fresh feed and the recirculated hydrogen.

Observations:

- **Impact of Water Percentage:**

  The data suggests a trend between water percentage and hydrogen production rate. In general, hydrogen production rates increase as the water percentage increases. This is likely because a higher concentration of water provides more reactant molecules for the electrolysis process to convert into hydrogen gas.

- **Data Fluctuations:**

  There are fluctuations in the hydrogen production rate (H2-OUT) for each water percentage. For example, at 0.1 water percentage, the H2-OUT values range from 1.66525 kmol/hr to 17.8235 kmol/hr. These fluctuations could indicate instabilities in the electrolysis process, such as variations in temperature, pressure, or current flow.

Overall, the data suggests that the electrolysis system is capable of producing hydrogen, and that the production rate increases with higher water percentages. However, the fluctuating production rates and lack of energy consumption data make it difficult to assess the overall performance and efficiency of the system.

Here are some additional points to consider:

- The type of electrolysis system: Different electrolysis systems have varying efficiencies and performance characteristics. Knowing the type of system would provide more context for interpreting the data.
- Operating conditions: Factors such as temperature, pressure, and current density can affect the efficiency of the electrolysis process. Information on these operating conditions would be helpful for a more comprehensive analysis.

By gathering additional data on energy consumption, operating conditions, and the specific type of electrolysis system, a more thorough evaluation of the system's performance could be conducted.

The graph shows the hydrogen production and influence of KOH in productivity and rate (H2O kmol/hr) on the y-axis and time on the x-axis. The stacked bar graph indicates that the electrolysis system produces hydrogen at a fluctuating rate. The hydrogen production rate starts at around 26.92 kmol/hr and increases to a peak of around 111 kmol/hr at around 30%. It then fluctuates around 100 kmol/hr before dropping to around 55.5 kmol/hr at the end of the simulation (around 90%).

KOH, or potassium hydroxide, plays a crucial role in electrolysis systems, but it's not directly involved in the core hydrogen production reaction.

Here's a breakdown of its influence:

Main Function: Increases Conductivity

- KOH is a strong electrolyte, meaning it readily dissolves in water to form ions (charged particles). These ions conduct electricity very well.
- In electrolysis, pure water is a poor conductor of electricity. KOH increases the conductivity of the solution, allowing the electrical current to flow more efficiently through the electrolyte. This translates to smoother operation and potentially less energy wasted on overcoming resistance within the system.

Secondary Effects:

- **Minimizes Side Reactions:**

  By improving conductivity and allowing the desired electrolysis reaction to proceed more efficiently, KOH can help minimize unwanted side reactions. These side reactions can consume energy and reduce hydrogen production.

- **Buffering Capacity:**

  In some electrolysis processes, KOH can act as a weak base, helping to maintain a slightly alkaline pH level in the electrolyte. This can be beneficial for certain types of electrodes by preventing them from degrading too quickly.

Important Note:

While KOH is commonly used, it's not the only option. Other electrolytes can be used, depending on the specific application and desired properties. For example, some systems might use acidic electrolytes for specific purposes.

Overall, KOH acts as a facilitator in the electrolysis process by:

- Enhancing conductivity for efficient current flow.
- Potentially reducing unwanted side reactions.
- Maintaining a suitable pH level for some electrode materials.

III.4 IHSPEU unit:

IHSPEU unit is an optimized solution where two energy production units (HSPEU for electrolysis + methane cracking unit) are combined together in a structural and organized matter.

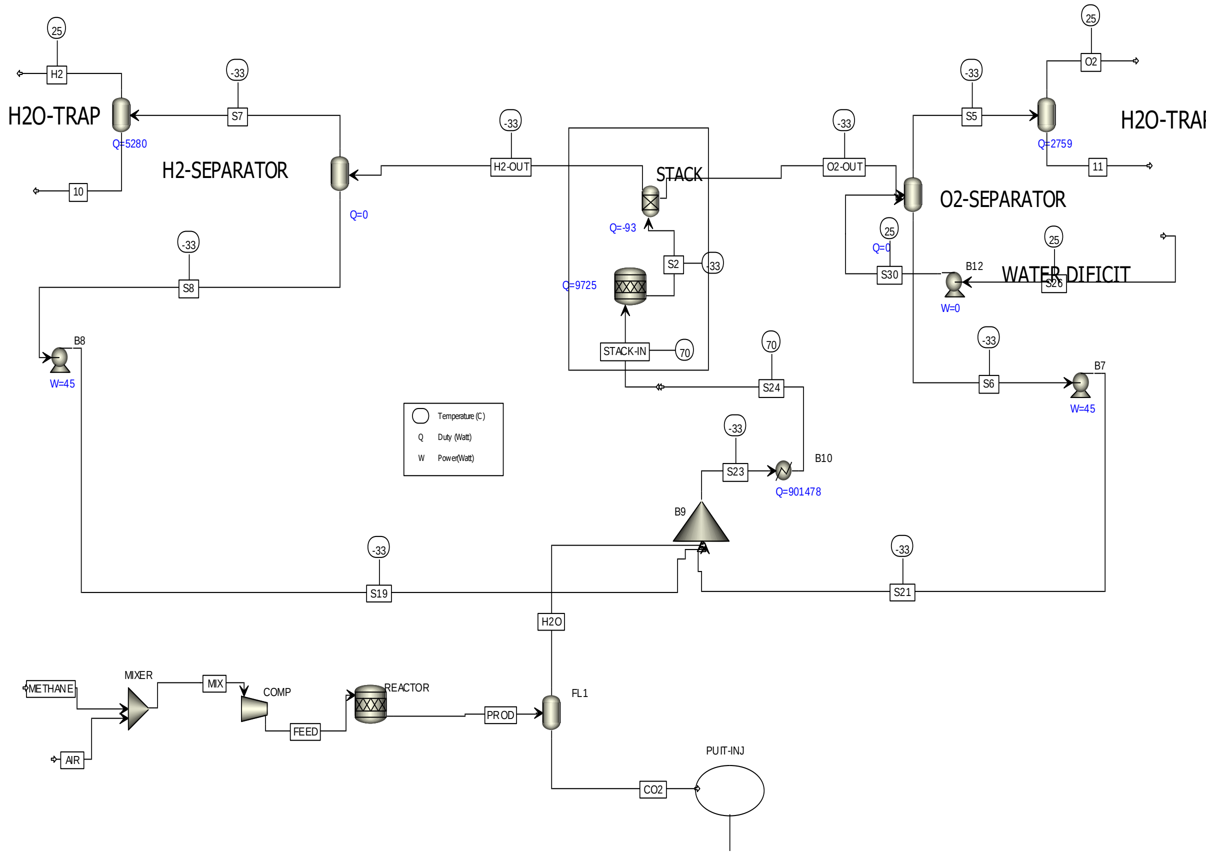

Figure III-7: Presentation of IHSPEU unit (ASPEN PLUS 2024)

III.4.1 Process of working in IHSPEU model:

Overall, this process model illustrates a system that converts methane into CO2 (which is captured), hydrogen, and oxygen through a combination of cracking/reforming and electrolysis steps. The hydrogen and oxygen produced could potentially be used as fuel gases or for other applications

This model appears to be a process flow for a system that takes methane as input, cracks it, separates the products (CO2 and H2O), and then further processes the H2O through an electrolyzer to produce hydrogen (H2) and oxygen (O2).

The main steps and components in the process are as follows:

1. Methane (CH_4) enters the system and goes through a compressor.
2. The compressed methane then undergoes cracking in the "STACK" unit operation, producing carbon dioxide (CO_2) and water (H_2O).
3. The CO_2 is sent to a "PUIT INJECTOR," which likely refers to a carbon capture and storage or utilization process.
4. The H_2O is fed into an electrolyzer, where it undergoes electrolysis to produce hydrogen (H_2) and oxygen (O_2).
5. The H_2 and O_2 streams leave the electrolyzer and pass through separate separators (H2-SEPARATOR and O2-SEPARATOR) for further processing or purification.
6. The system also includes water traps (H2O-TRAP) and a water reject stream to handle any excess water or condensation.

III.4.2 IHSPEU unit equipments:

The IHSPEU unit is composed of the main following equipments:

a) Electrolyser

Facilitate the electrolysis process by passing an electric current through an electrolyte solution. This causes chemical reactions, typically splitting water into hydrogen and oxygen gases. Electrolyzers consist of electrodes immersed in the electrolyte, where positive and negative ions migrate to the respective electrodes, generating the desired products. This technology is crucial for hydrogen production, energy storage, and various industrial processes aiming for sustainable fuel alternatives (21).

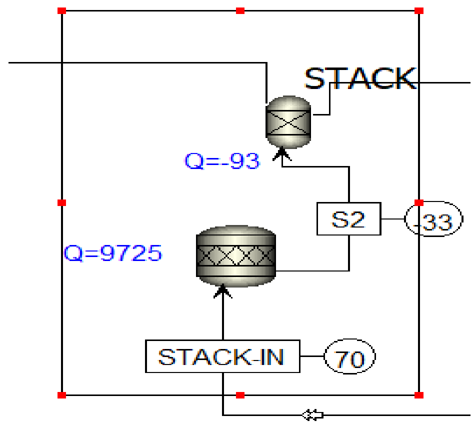

Figure III-8: Electrolyzer unit.

b) Cracking reactor:

Heats heavy hydrocarbon feedstock to high temperatures, inducing chemical reactions that break large molecules into smaller ones. These smaller molecules are then separated and refined to produce valuable products such as gasoline, diesel, and petrochemicals, playing a vital role in the petroleum industry's production process. The reactor's efficiency relies on precise control of temperature, pressure, catalysts, and reactor design (22).

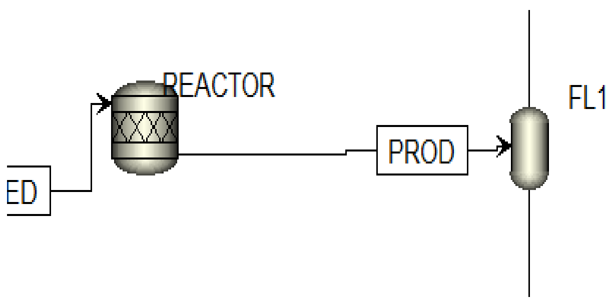

Figure III-9: Crackage Unit.

c) Auxiliary equipments:

•Pumps:

Pumps operate by converting mechanical energy into hydraulic energy, generating flow or pressure to move fluids from one location to another. They utilize rotating impellers or reciprocating pistons to increase fluid velocity or pressure, facilitating processes in various industries such as water supply, chemical processing, and oil refining. Pump performance depends on factors like speed, design, and fluid properties, ensuring efficient transport of liquids or gases (23).

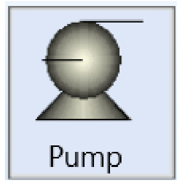

Figure III-10: Pump.

•Separator:

Divide mixed substances into distinct phases based on density or other properties. They typically employ gravity or centrifugal force to achieve separation. Separators operate by directing the phases into different outlets, ensuring efficient isolation of components such as oil, water, and gas in industries like petroleum refining, wastewater treatment, and food processing. (7)

Figure III-11: Separator flash2.

•Mixer:

Blend substances by agitating them together, promoting molecular intermingling for homogeneity. They typically employ rotating blades, paddles, or impellers to create fluid motion within a vessel. Mixing processes vary based on factors like speed, geometry, and rheological properties of the materials, ensuring thorough mixing for applications across industries like pharmaceuticals, food processing, and chemical manufacturing (9).

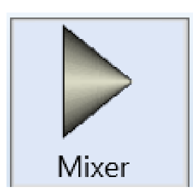

Figure III-12: Mixer.

•Heater:

Increase the temperature of a substance, typically by converting electrical or fuel energy into heat. They utilize heating elements or combustion chambers to transfer thermal energy to the substance being heated. Heater operation involves controlling temperature, ensuring safety, and optimizing energy efficiency for applications ranging from space heating and water heating to industrial processes like refining and manufacturing (24).

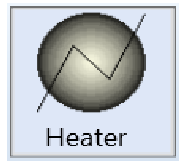

Figure III-13: Heater.

•Pipelines:

Transport liquids or gases over long distances through interconnected tubes or conduits. They rely on pumps or compressors to maintain flow and pressure, ensuring efficient transportation. Pipeline operations involve monitoring for leaks, controlling flow rates, and adhering to safety protocols to facilitate the movement of resources like oil, natural gas, water, and chemicals (25).

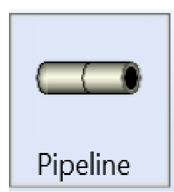

Figure III-14: Pipeline.

•Compressor:

Increase the pressure of gases by reducing their volume through mechanical means. They utilize rotating blades or pistons to compress gas, raising its pressure for transportation or processing. Compressor operation involves intake, compression, and discharge stages, ensuring efficient gas flow in applications such as refrigeration, air conditioning, and industrial processes (23).

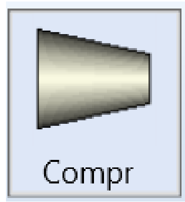

Figure III-15: Compressor.

III.5 CO2 injection:

III.5.1 Purposes of CO2 injection wells

CO2 injection wells have two main purposes:

a) **Enhanced Oil Recovery (EOR):**

This is the more established use. In EOR, CO2 is injected into depleted oil reservoirs. The CO2 mixes with the remaining oil, lowering its viscosity and making it easier to extract. This can significantly increase the amount of oil that can be recovered from a reservoir (26).

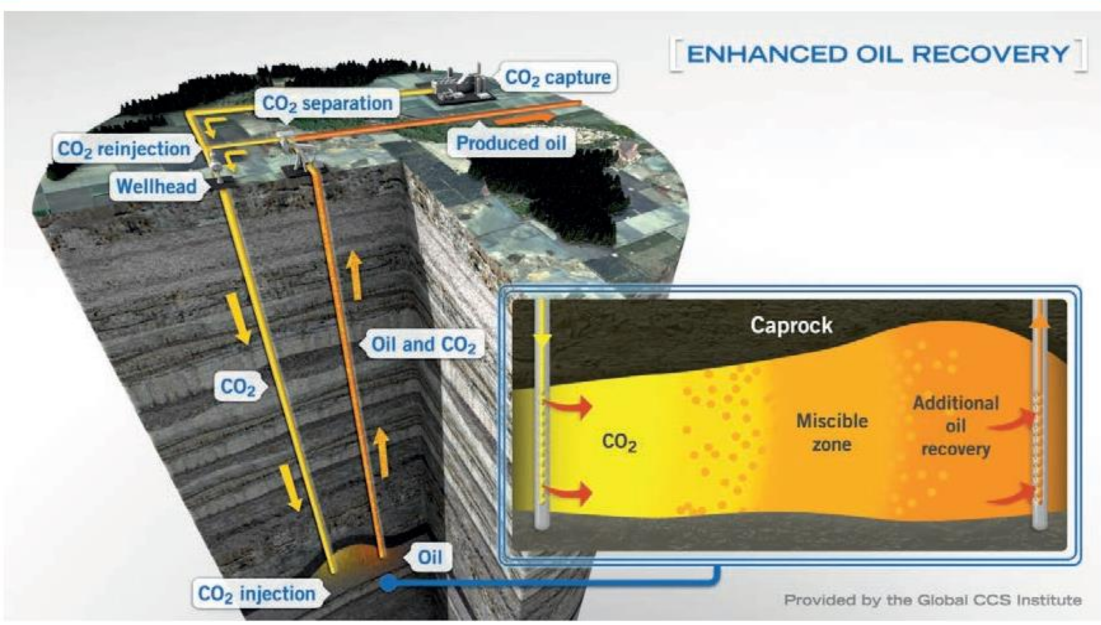

Figure III-16: CO2 enhanced oil recovery *(26)*.

b) **Carbon Capture and Storage (CCS):**

This is a technique for mitigating climate change. CO_2 is captured from industrial sources like power plants or factories. Then, the captured CO_2 is injected deep underground into suitable geological formations, where it is permanently stored. CO_2 injection wells are a key component of CCS projects.

Here's a breakdown of the key points:

- **EOR:** Increases oil production from depleted reservoirs.
- **CCS:** Stores captured CO_2 underground to prevent its release into the atmosphere.
- **CO_2:** injection wells are used for both EOR and CCS, but the purpose determines the specific design and operation of the well.

Here are some additional things to consider:

- **Safety and Regulation:**

  CO_2 injection wells need to be carefully designed and monitored to ensure they don't leak and contaminate groundwater or allow CO_2 to escape back into the atmosphere. Regulations are in place to govern the construction, operation, and closure of CO_2 injection wells.

- **Environmental Impact:**

  While CCS offers a potential solution for reducing greenhouse gas emissions, there are some environmental concerns associated with CO_2 injection wells, such as the possibility of induced seismic activity. Careful site selection and monitoring are crucial to mitigate these risks.

The effects of CO_2 injection in a gas well depend on the primary purpose of the injection. There are two main reasons for injecting CO_2 into a gas well:

a) **Enhanced Gas Recovery (EGR):**

This is similar to the Enhanced Methane Recovery (EMR) process mentioned previously. Here's how it works:

- **Increased Mobility:** CO_2 mixes with the remaining natural gas in the reservoir, causing it to swell and become less viscous. This makes the gas easier to flow towards the wellbore and ultimately be extracted.

- **Pressure Maintenance:** Injecting CO_2 helps maintain pressure within the reservoir, which can improve well productivity over time by preventing a decline in pressure as gas is extracted.

b) **Carbon Capture and Storage (CCS):**

In this scenario, the goal is to store captured CO_2 underground for climate change mitigation. Here's the impact on the gas well:

- **Storage Capacity:** Depleted gas wells can offer suitable geological formations for storing captured CO_2. The well itself acts as a conduit for injecting CO_2 deep underground.

Additional Considerations:

- **Technical Challenges:** Separating the CO_2 from the extracted gas stream and ensuring well integrity to prevent leaks require additional infrastructure and ongoing monitoring.
- **Economic Feasibility:** The cost-effectiveness of CO_2 injection for EGR depends on factors like the amount of recoverable gas, CO_2 availability, and processing costs.
- **Environmental Impact:** Similar to methane wells, there are risks of CO_2 leakage and potential for induced seismic activity. Careful planning and monitoring are crucial to minimize these risks (26).

III.5.2 CO2 Injection in Gas Wells: Modeling Considerations within PIPESIM

CO_2 injection into gas wells serves a dual purpose: Enhanced Gas Recovery (EGR) and Carbon Capture and Storage (CCS). PIPESIM, a commercial multiphase flow simulator, offers functionalities for modeling fluid flow in pipelines and wellbores. However, the specific approach to modeling CO_2 injection within PIPESIM requires examining the software version and available modules.

III.5.2.1 PIPESIM:

Developed by Schlumberger Limited, a leading global provider of technology for the energy industry, PIPESIM is a powerful computational fluid dynamics (CFD) software solution designed for modeling fluid flow in pipelines, networks, and production facilities.

PIPESIM is primarily targeted towards mid-sized to large enterprises operating in the oil and gas, petrochemical, and energy sectors. Its advanced capabilities and comprehensive features make it a valuable tool for engineers, researchers, and analysts involved in the design, analysis, and optimization of complex fluid systems. While the software is tailored for these specific industries, its robust modeling capabilities can also be applied to other sectors where fluid flow analysis is critical (27).

PIPESIM is a comprehensive solution that encompasses a wide range of features and modules tailored for fluid flow modeling and analysis. Here are some of the key components included in the software:

- **Multiphase Flow Modeling:** PIPESIM provides advanced multiphase flow modeling capabilities, allowing users to simulate and analyze the flow of multiple fluids (oil, gas, water) through pipelines, risers, and production facilities.
- **Thermal Hydraulic Analysis:** This module enables detailed heat transfer calculations and thermal hydraulic analysis, which is crucial for optimizing system performance and ensuring safe and efficient operations.
- **Pressure Drop Calculations:** PIPESIM offers accurate pressure drop calculations for various flow regimes.
- **Equipment Sizing and Selection:** The software includes tools for sizing and selecting appropriate equipment, such as pumps, compressors, and separators.
- **Network Modeling and Optimization:** PIPESIM allows users to model and analyze complex pipeline networks enabling optimization of flow rates, pressures, and system configurations.
- **Dynamic Simulation:** This feature enables users to simulate transient conditions, such as start-up, shutdown, and upset scenarios, providing valuable insights into system behavior and potential risks (27).

III.5.2.2 Modeling CO2 Injection in PIPESIM:

a) **Components and Properties:**

- PIPESIM likely allows you to define CO2 as a separate component within the wellbore and reservoir fluid mixture.
- You would need to specify the properties of CO2, such as its equation of state (EOS) parameters for accurate phase behavior calculations (28).

b) **Injection Well Definition:**

- PIPESIM might have functionalities to define an injection well where CO2 is introduced into the reservoir at a specific rate and pressure.

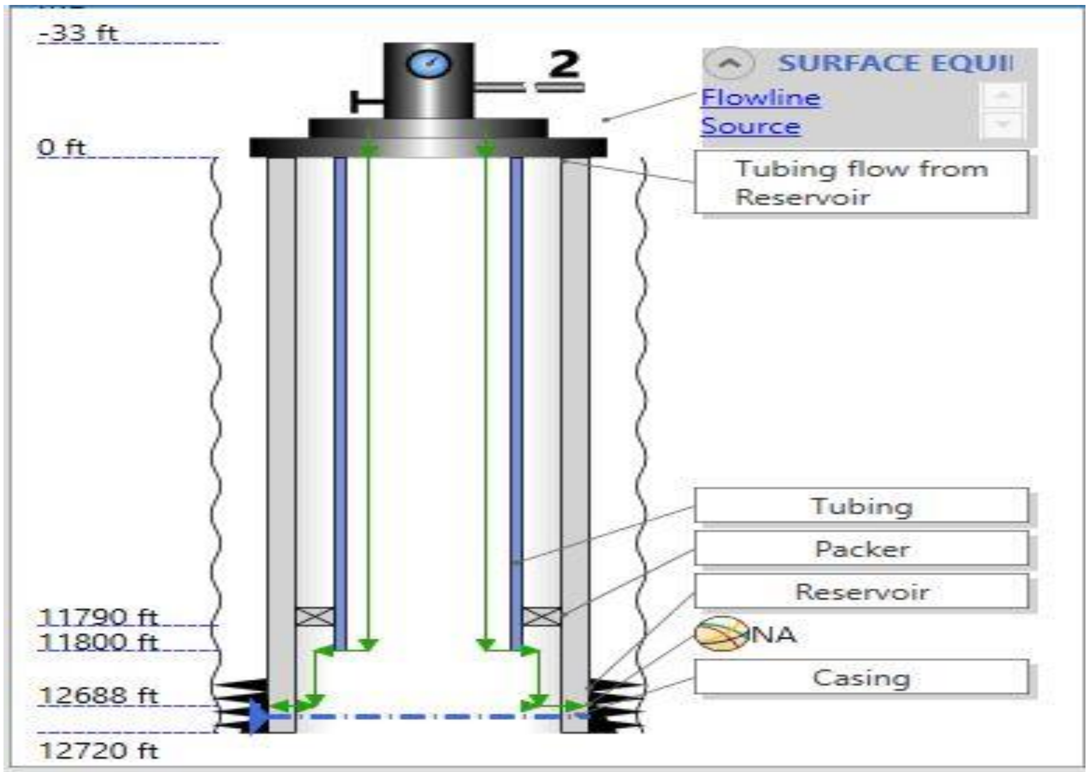

Figure III-17: CO2 Well injector model.

c) **Multiphase Flow Modeling:**

- PIPESIM is a multiphase flow simulator, meaning it can handle mixtures of gas, oil, water, and potentially other components like CO2.
- The program would likely simulate the interaction of CO2 with the existing reservoir fluids, including phenomena like:
  - **Mixing:** The CO2 would mix with the remaining natural gas, potentially affecting its viscosity and density.

- **Phase Behavior:** Depending on pressure and temperature conditions, CO_2 might partially dissolve in the oil phase or form a separate CO_2-rich phase (29).

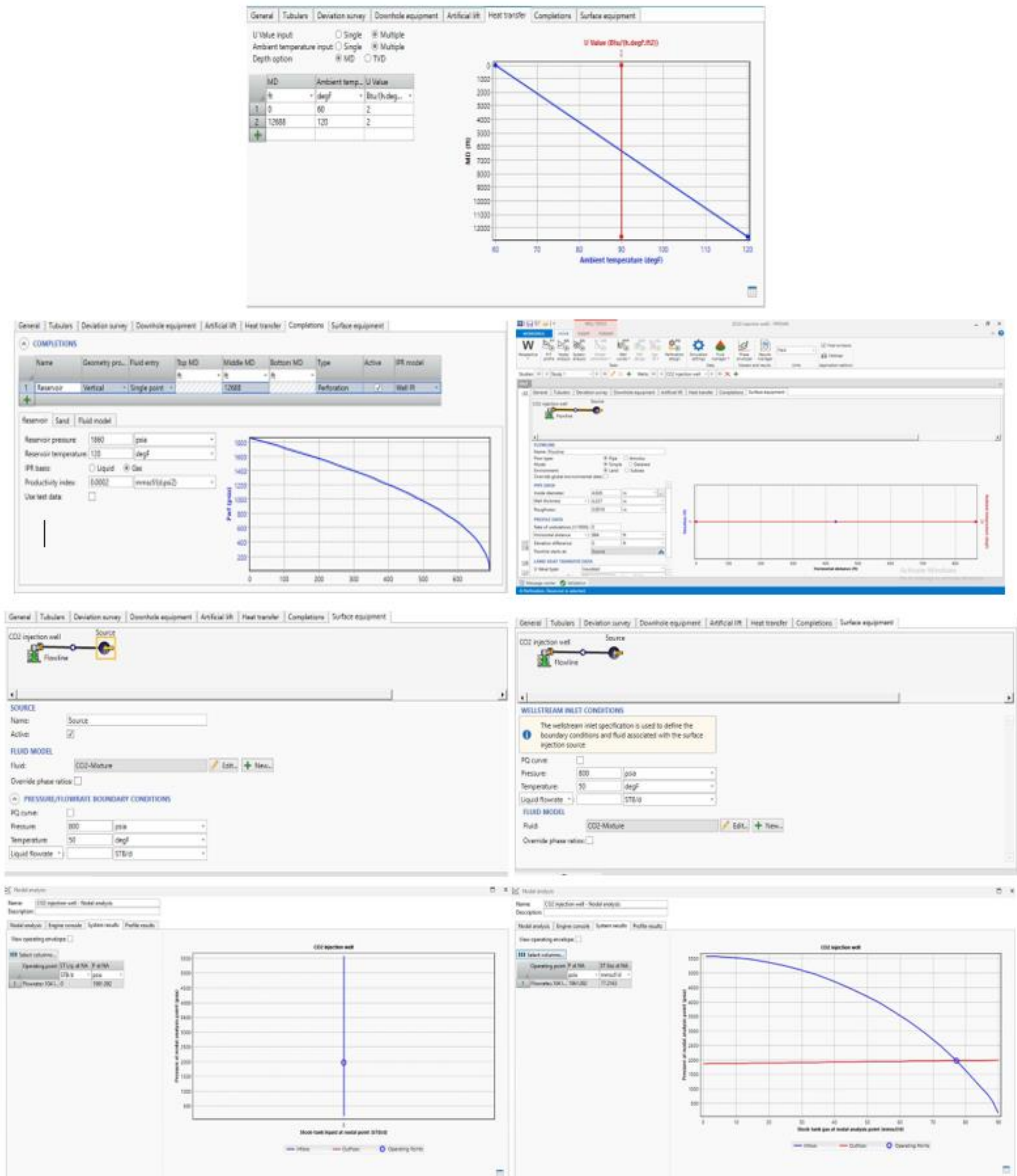

Figure III-18: steps to create CO2 Well injector.

d) **Enhanced Gas Recovery (EGR) Modeling:**

If PIPESIM has modules for reservoir simulation, it could potentially model the impact of CO_2 injection on gas recovery:

- **Relative Permeability:** The software might account for changes in relative permeability of the reservoir rock to gas and water due to the presence of CO_2. This would influence the flow of gas towards the wellbore.
- **Pressure Maintenance:** The injection of CO_2 could be modeled to help maintain reservoir pressure, leading to improved well productivity over time (29).

Injecting CO_2 into a methane well can have several effects, some positive and some negative. Here's a breakdown of the key impacts:

Positive Effects:

- **Enhanced Methane Recovery (EMR):** Similar to EOR with oil, CO_2 injection can enhance methane recovery from depleted methane wells. CO_2 mixes with the remaining methane, causing it to swell and become less viscous, making it easier to extract. This can lead to a significant increase in the amount of methane recovered from the well.
- **Improved Well Productivity:** CO_2 injection can improve the overall productivity of a methane well by maintaining reservoir pressure and displacing water that may be blocking methane flow paths (30).

Negative Effects:

- **Reduced Methane Quality:** The mixing of CO_2 with methane can dilute the methane content in the extracted gas stream. This reduces the quality of the methane product and requires additional processing to separate the CO_2 before it can be used as fuel.
- **Infrastructure Needs:** Processing the extracted gas stream to separate the CO_2 requires additional equipment and infrastructure, which can add to the cost and complexity of the operation.
- **Limited Application:** The effectiveness of CO_2 injection for EMR depends on various factors like the geologic formation and the properties of the remaining methane. It might not be suitable for all methane wells (31).

Environmental Considerations:

- **Leakage Risks:** There's a risk of CO2 leakage from the well, which could negate the climate change benefits of capturing CO2 from other sources. Careful well design, operation, and monitoring are crucial to minimize this risk.
- **Induced Seismic Activity:** In some cases, CO2 injection can trigger small-scale earthquakes. Careful site selection and monitoring of seismic activity are essential to mitigate this risk (32).

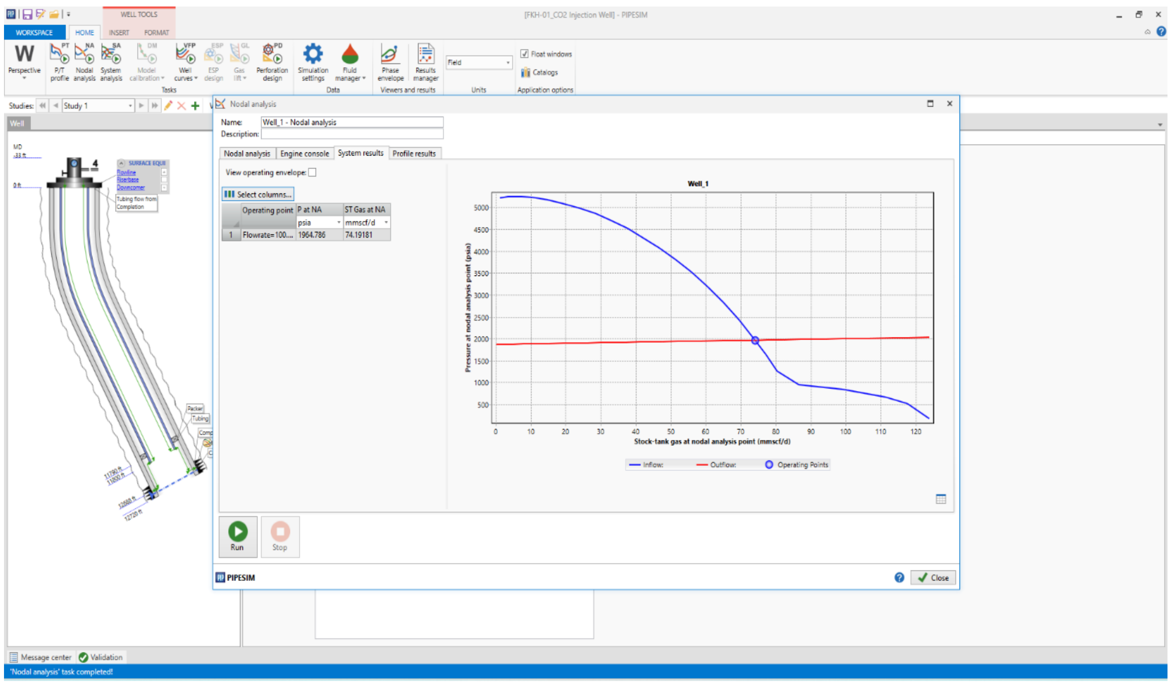

Figure *III-19:* CO2 Well injector model.

III.5.2.3 Description of the Graph:

The graph depicts the results of a nodal analysis performed using PIPESIM software. Nodal analysis is used to determine the optimal operating conditions for a well by analyzing the inflow and outflow performance (33).

Graph Components:

a) X-axis (Horizontal Axis):

Represents the stock-tank gas at the nodal analysis point in million standard cubic feet per day (mmscfd).

b) Y-axis (Vertical Axis):

Represents the pressure at the nodal analysis point in pounds per square inch absolute (psia).

c) Blue Line (Inflow Performance Relationship - IPR):

Shows the inflow performance of the well, indicating how much gas can flow into the wellbore from the reservoir at different pressures.

d) Red Line (Outflow Performance Relationship - OPR):

Represents the outflow performance of the well, showing the relationship between the pressure at the wellhead and the flow rate.

e) Operating Points:

The intersection of the inflow and outflow curves indicates the operating point of the well. In this case, the operating point is marked by a blue circle.

Key Values:

- **Operating Point:**

-Pressure at Nodal Analysis Point (P at NA): 1964.786 psia.

-Stock-Tank Gas at Nodal Analysis Point (ST Gas at NA): 74.19181 mmscfd.

III.5.2.4 Interpretation:

- **Operating Conditions**:

  -The well is currently operating at a pressure of approximately 1964.786 psia at the nodal analysis point, with a gas production rate of around 74.19181 mmscfd.

- **Flow Dynamics:**

  -The inflow curve indicates the reservoir's ability to deliver gas to the wellbore at various pressures. The steeper the curve, the more sensitive the inflow is to pressure changes.

-The outflow curve shows the ability of the well to transport gas to the surface. The intersection point signifies equilibrium between inflow and outflow, representing the well's current operating conditions.

- **Optimization:**

  -The nodal analysis helps identify if the well is operating efficiently or if there are opportunities to optimize production. Adjusting surface pressure, altering wellbore configurations, or enhancing reservoir performance can shift the operating point to improve production (32).

The well is producing gas at a flow rate of approximately 74.19181 mmscfd at a pressure of 1964.786 psia. The analysis suggests that current operations are balanced between reservoir inflow and wellbore outflow. Any changes in operating conditions, such as reducing wellhead pressure or improving reservoir stimulation, could potentially alter the production rate and efficiency (33).

Conclusion:

In conclusion, the Integrated Hydrogen Surface Production and Exportation Unit (IHSPEU) facility emerges as a beacon of hope and innovation in the quest for sustainable energy solutions. By seamlessly integrating fossil energy and renewable energy technologies into a unified system, the IHSPEU facility offers a transformative approach to energy production that transcends traditional boundaries and paradigms.

At its core, the IHSPEU facility embodies the principles of synergy and efficiency, harnessing the complementary strengths of methane cracking and electrolysis to maximize energy conversion efficiency and minimize environmental impact. Through the simultaneous generation of hydrogen, synthetic fuels, and CO2 capture for Enhanced Oil Recovery (EOR), the facility not only meets the growing demand for clean energy but also addresses the pressing need to mitigate greenhouse gas emissions and reduce reliance on fossil fuels.

Furthermore, the IHSPEU facility serves as a model for sustainable development, offering a blueprint for the integration of diverse energy sources and technologies into a coherent, resilient, and environmentally responsible framework. By leveraging the abundance of fossil energy resources alongside the inexhaustible potential of renewable energy, the facility embodies the transition towards a more balanced and sustainable energy mix that ensures energy security and mitigates climate change.

As we confront the challenges of a rapidly evolving energy landscape, the IHSPEU facility stands as a testament to human ingenuity and perseverance, offering a path forward towards a brighter, cleaner, and more prosperous future. Through continued innovation, collaboration, and commitment to sustainability, we can harness the full potential of integrated energy solutions like the IHSPEU facility to power the world towards a more sustainable and resilient tomorrow.

GENERAL CONCLUSION:

In conclusion, this dissertation underscores the pivotal role of models like ML-01 in enhancing water electrolysis efficiency. These models predict outcomes and address issues like energy consumption and electrode degradation, enabling more sustainable electrolysis systems and aiding the transition to a low-carbon economy.

Experiments on underground water samples have provided valuable insights into electrolysis, revealing the fundamental principles of chemical transformations in aqueous environments. The ML-01 model accurately replicated observed phenomena, providing insights into the underlying mechanisms driving electrolytic processes. This model's systematic approach and comprehensive mathematical framework make it a powerful tool for understanding underground water electrolysis, guiding experimental design, and optimizing operational parameters.

The ML-01 mathematical model is a key tool in advancing electrolysis technology, enabling precise control and optimization of electrolysis facilities. It provides a comprehensive understanding of electrolysis phenomena, enabling engineers to optimize processes, minimize energy consumption, and enhance product quality. This model will play a pivotal role in realizing electrolysis's full potential as a sustainable chemical synthesis and industrial production by performing electrolysis on two different water samples under various conditions. It also proposes a design for the HSPEU facility that combines electrolysis with methane cracking (probably to reduce dependence on fossil fuels) and suggests ways to make the process more environmentally friendly. The results obtained from this experiment show that the efficiency of the model reaches a temperature of 42°C and a voltage of 18V. finally these results are simulated by the ASPEN PLUS software.

Developing new models deepens our understanding of electrolysis and unlocks possibilities in clean energy production, guiding decision-making, optimizing resources, and reducing environmental impact. A multidisciplinary approach combining modeling techniques and empirical research can significantly improve electrolysis technology.

Moreover, integrating electrolysis with other energy sectors, such as methane cracking, offers solutions for sustainable energy challenges. The IHSPEU model uses surplus renewable electricity for electrolysis and hydrogen production, maximizing resource efficiency, stabilizing the grid, and facilitating cleaner energy transitions. This integration highlights the benefits of interdisciplinary collaboration in addressing complex energy issues.

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