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Mathematical modeling of mechanical properties in the permeation of green hydrogen through membrane separation materials

Hairch Y.[1,2], Medarhri I.[3], Jraifi A.[4], Elmlouky A.[1]

[1]*LPMC-Laboratory, University Chouaib Doukkali, El Jadida, Morocco*
[2]*ISTM-Laboratory, FS, Chouaib Doukkali University, El Jadida, Morocco*
[3]*MMCS Team, MAID-Laboratory, ENSMR-Rabat, Morocco*
[4]*MISCOM-Laboratory, ENSA-S, University Cadi Ayyad, Morocco*

The potential role of hydrogen in the future of energy has generated significant enthusiasm, despite the fact that it might not completely replace oil. Hydrogen, with its lengthy history and established place in long-term strategies and global perspectives, is seen as a pivotal player in the energy transition. Currently, hydrogen finds primary use in industrial applications like ammonia production, oil refining, and steel manufacturing, targeting energy-intensive sectors where ammonia and oil refinement are prioritized. However, the reliance on fossil fuels is contributing to economic vulnerability and a climate emergency within the ongoing energy crisis, spurring a global transition towards more sustainable and cleaner alternatives. Many countries are seeking to strengthen their energy security by pursuing renewable and clean energy sources, and classical polymer behavior is being utilized to drive this transition. In recent decades, membrane science has emerged as a powerful tool for developing new industrial processes that support sustainable industrial growth. In this study, we focus on the separation of hydrogen using membrane for hydrogen recovery. In particular, membrane technology has been widely accepted for gas separation to achieve high filtration. In this paper, we performed numerical calculations of the key physical parameters influencing hydrogen production: concentration, permeability and pressure. The verification of our study's credibility was using by comparing the experimental permeation flux and its responsiveness to alterations in hydrogen partial pressure.

Keywords: *modeling; green hydrogen; energy storage; separation membrane; permeability; MATLAB–simulation.*

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1. Introduction

In the current time, different energy storage systems are needed to secure the constant energy to reduce the release of greenhouse gas emissions that are warming our planet. To avoid the threat of climate change, fossil energy reserves are needed and today more capacity was added for renewable power [1–4]. Hydrogen is a versatile energy carrier that can be used for transportation and for short-term and long-term storage of renewable energy. With the advancements in technology, it is now possible to generate hydrogen using solar energy and wind power, making it a feasible option for energy storage. Hydrogen can be produced from any energy source [5–12], which further enhances its flexibility as an energy carrier. In 1671, Robert Boyle discovered what he called "flammable air," now known as green hydrogen, through the reaction between iron filings and dilute acids in cities in the UK [13–15]. Hydrogen is the most abundant chemical element in the universe, as discovered by Henry Cavendish between 1766 and 1781, and is a clean alternative to fossil fuels [16–19]. In June 1783, Lavoisier concluded that water is produced when hydrogen, which he referred to as the "water creator," is burned, and published a paper outlining the correct theory of this reaction involving hydrogen and oxygen [20].

For the first time (May 1898), James Dewar successfully liquefied Hydrogen using iterative cooling (dangerous process) to 252.87°C as the coldest substance produced at that time [21]. Finally, Harold Clayton Urey found heavy isotope of hydrogen in 1931 by measuring the small change in wavelength [22–24].

Emerging countries have committed to reducing carbon emissions and mitigating risks associated with methane emissions in order to limit the overall rise in temperature to 1.5°C by 2050. Deploying renewable energy sources and adopting clean hydrogen represent promising options for achieving the goal of a carbon-neutral 2050, as well as the European climate neutrality objective. These long-term solutions will ensure a secure energy future without adding more carbon dioxide to the environment [25–29]. Hydrogen is the most common chemical element in the universe, accounting for over 90% of all atoms. It is colorless, odorless, and has no neutrons. However, research indicates that hydrogen can be difficult to detect. The next generation of nuclear reactors will require immense energy to extract hydrogen from water. Despite this challenge, hydrogen production is seen as a promising pathway towards a clean, low-carbon energy system, due to its versatility as an energy carrier. Countries around the world are developing their own strategies for hydrogen exploitation, with a focus on international cooperation, bilateral coordination, and the establishment of agreements between governments. Multilateral initiatives and projects are also being developed to advance the use of hydrogen as a long-term solution for a secure energy future, as part of the neo-ecology movement [30–37]. The two most common methods for producing hydrogen are steam-methane reforming and electrolysis [38, 39]. Steam reforming, also known as steam methane reforming (SMR), is a process for producing syngas, which is a mixture of hydrogen and carbon monoxide. This is achieved through the reaction of hydrocarbons with water. Currently, steam reforming of natural gas is the predominant method for producing hydrogen worldwide, as it provides a zero-carbon energy source [40–45]. In the United States, steam-methane reforming is the most common method for producing hydrogen from hydrocarbons, which is carried out at high temperatures (850–950°C) and moderate pressures (20–30 bar) [46–50]. The presence of a catalyst, typically Nickel, facilitates an endothermic reaction, represented by the following equation:

$$C_nH_m + n\,H_2O \rightarrow n\,CO + \left(n + \frac{m}{2}\right)H_2. \tag{1}$$
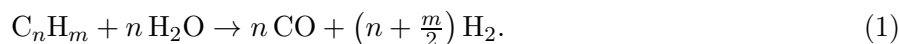
The steam reforming reaction is expensive and requires a large amount of energy for powering the grid. However, despite these challenges, hydrogen production has the potential to lead to a clean, low-carbon energy system as a versatile energy carrier.

Currently, there is an unprecedented level of interest and widespread popular support for using renewable energy sources, such as wind and solar energy, which are constantly improving and do not emit carbon dioxide. When fossil fuels, forests, and solid waste are burned, they release large amounts of greenhouse gases, such as nitrous oxide (N_2O) and carbon dioxide (CO_2), which make up the vast majority of greenhouse gas emissions. Green hydrogen is produced from renewable energy by water electrolysis fueled by renewable electricity. In an era of water insecurity, green hydrogen holds significant potential, as it can be produced using electricity through an association between wind turbines and electrolysis, which splits water molecules into hydrogen and oxygen. While hydrogen separation membranes are typically made from polymeric or metal materials and are used in a variety of applications, including the production of hydrogen fuel, purification of hydrogen streams, and hydrogen storage, the dehydrogenation of cyclic hydrocarbons in oil refineries is reversible.

One of the advantages of using a hydrogen separation membrane is its high selectivity for hydrogen. This allows for efficient separation of hydrogen from other gases, reducing the energy requirements and cost of the separation process. Additionally, many hydrogen separation membranes are lightweight and compact, making them well-suited for use in portable or on-demand hydrogen production and storage systems. However, a major challenge with the development of hydrogen separation membranes is the need for high permeability and selectivity simultaneously. Also, cost and durability are other factors that can be considered as a disadvantage. Overall, hydrogen separation membranes are a promising technology for the production, purification, and storage of hydrogen gas. Further research and development is needed to improve the performance and durability of these membranes, as well as to reduce their cost.

This paper presents technologies related to hydrogen production, including a numerical model for generating hydrogen via water electrolysis. The aim of the article is to introduce mathematical modeling approaches for membrane separation processes. Additionally, the paper presents a direct simulation study of a separation membrane for the hydrogen-membrane reaction under reasonable conditions. To achieve this, the mathematical model of the Arrhenius equation, the permeability, and the concentration of hydrogen into the separation membrane were developed from a theoretical study of the solution-diffusion model and implemented in MATLAB. The simulation results, under steady-state conditions, show that membranes are permeable to gases such as hydrogen through a single-layer separation membrane.

2. Hydrogen production and background

This part reviews the hydrogen production technologies through a diverse, domestic resources including thermal, electrolytic and photonic ones. At present, the majority of hydrogen produced via steam methane reforming and obtained from natural gas. The principle is to heating a methane from natural gas, with steam, to produce a mixture of carbon monoxide and hydrogen at high-temperature steam (700–1000°C). In this process, methane reacts with steam under 3–25 bar pressure in the presence of a catalyst to produce hydrogen, carbon monoxide, and a relatively small amount of carbon dioxide in what is called the "water-gas shift reaction" [51–56]. In a second process, impurities and carbon dioxide are removed from the gas (pressure–swing adsorption), leaving pure hydrogen. Methane steam reforming (MSR) contributes about 50% of the world's hydrogen production. Nevertheless, (MSR) is expensive and suffers from issues such as deposition during the reaction, mass, heat transfer and coke. Industrially, several steps are necessary in this process: purification devices, the reduction of carbon monoxide content and pressure swing adsorption. In summary, detailed steps for the SMR process can be broken down into five distinct steps: Furnace – Steam Production, Reforming Reaction, Water Gas Shift Reactor (WGS Reactor), Gas Purification – Pressure Swing Absorption (PSA) and Recycling and Output. Now, a different means of producing hydrogen is needed such as photobiological water splitting and fermentation.

Today and by using biological systems such as sunlight energy, several approaches are possible could be used for hydrogen production from algae cultures or either isolated cellular components and wastes. Bio-photolysis process proceeds in two different ways: direct bio-photolysis in the microalgae and indirectly by stored the electrons from water. The easiest approach to produced hydrogen are through photovoltaic (PV) electricity by converting solar energy to hydrogen chemical energy. At high-temperature heat (500–2000°C), series of chemical reactions use to produce hydrogen and oxygen within each cycle (Thermolysis process) an indirect method. Solar thermochemical water-splitting cycles use high-temperature heat for hydrogen production [57]. Consequently, the S–I cycle consisting of three steps (Figure 1).

This separation process involves steam and SO_2, hydriodic acid and sulfuric acid, and iodine and hydrogen. This cycle is technically feasible for hydrogen production. Additionally, hydrogen can be effectively produced using high-temperature steam from intermediate liquid biofuels through renewable liquid reforming, allowing for distributed hydrogen production at fueling stations. However, the cost of biomass-derived liquids and the operation and maintenance costs need to be reduced to make this method more economically feasible. An-

Fig. 1. Block diagram of the sulfur-iodine cycle.

other potential method for hydrogen production is photo-catalytic hydrogen production using photonic energy. On a large scale, semiconductor materials such as new gold/titanium dioxide are promising
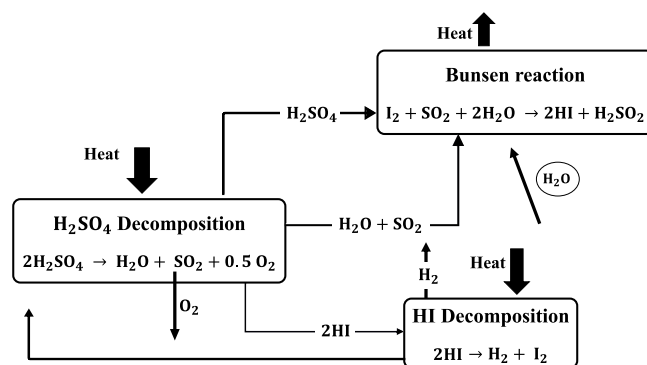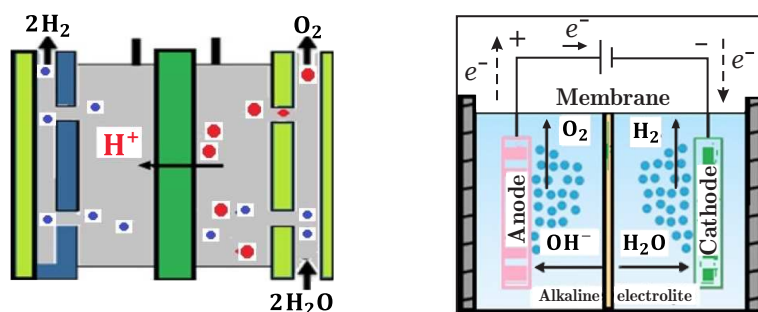
photocatalysts for hydrogen production, as they require the interaction between photons (sunlight) and semiconducting materials.

*a* Polymer electrolyte membrane (PEM)　*b* Alkaline electrolysis schematic

Fig. 2. Green hydrogen production via water decomposition.

The electrolysis of water has attracted great attention as an important part of industrial electrochemical processes and as sustainable and renewable chemical technology. Indeed, water is an ideal source for producing hydrogen and as one of the environmentally friendly alternatives to produce hydrogen is to use water electrolysis as feedstock, in which water is broken down into oxygen and hydrogen. During processing, water reacts at the anode to form oxygen and the hydrogen ions move to the cathode. The hydrogen produced through the decomposition of water by a renewable energy source is called green hydrogen (Figure 2).

In an alkaline electrolysis, the half-cell reaction at the anode is shown in following equation:

$$2OH^- \to H_2O + \tfrac{1}{2}O_2 + 2e^-. \tag{2}$$

As for the cathode:

$$2H_2O + 2e^- \to H_2O + 2OH^-. \tag{3}$$
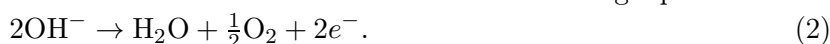
The overall reaction is represented by equation:

$$H_2O \to H_2 + \tfrac{1}{2}O_2. \tag{4}$$

Alkaline water electrolysis is a key technology and the most efficient methods for the hydrogen production, although it is relatively expensive technology when compared to thermo-chemical and photo-catalytic methods using only renewable. Structurally, the permeable membrane is a critical component for the performance of alkaline water electrolysis (such as asbestos). Hence, prevents the product gases from mixing and it ensures the ionic contact between the electrodes. To maintain a high ionic conductivity, the membrane require a highly concentrated electrolyte solution. On the other hand, the asbestos is toxic and causes mesothelioma and cancer. Consequently, there has been a global drive seeking renewable and clean alternatives to separation membrane as perfluorosulfonic acid polymer membranes (such as Nafion).

3. Materials and methods

Numerical simulations for transport in membranes involve using mathematical models and computational methods to study the movement of molecules across a membrane. This can include simulating the diffusion of small molecules, the transport of ions, and the movement of macromolecules such as proteins. These simulations can be used to understand the underlying mechanisms of transport, to predict the behavior of transport systems, and to design new transport systems. They can also be used to study the effects of different variables such as membrane composition and temperature on transport. Accordingly, numerical modeling of transport in membranes involves using mathematical equations and computational methods to simulate the movement of molecules across a membrane. The mathematical equations used in these models can include partial differential equations (PDEs) or ordinary differential equations (ODEs) that describe the transport of molecules based on factors such as concentration gradients, electric potentials, and protein-mediated transport. These models can be solved using various numerical methods such as finite element method (FEM), finite difference method (FDM), finite volume method and boundary element method (BEM).

There are several different models that can be used to simulate transport in membranes, including: continuum models, which treat the membrane as a continuous entity and use macroscopic transport

equations to describe the movement of molecules across the membrane. Furthermore, lattice models, which treat the membrane as a discrete entity and use molecular dynamics or explicit method simulations to describe the movement of molecules across the membrane. Finally, hybrid models, which combine elements of both continuum and lattice models to provide a more realistic description of transport in membranes.

4. Results and discussion

It is important to note that while palladium-based membranes have shown great potential for hydrogen separation, they are still relatively expensive and require careful handling to prevent degradation. In addition, the presence of impurities such as sulfur and chlorine can also significantly reduce the performance of these membranes. As a result, there is ongoing research to develop alternative materials and improve the performance and durability of these membranes. High-performance electrolyte membranes based on organic polymers, such as Nafion, have been widely studied and have shown good selectivity for hydrogen. However, they also have limitations in terms of mechanical and thermal stability, which can affect their long-term performance. Overall, the development of advanced separation membranes for hydrogen production and purification is an active area of research, and there is still much to be learned and improved in this field [58–60].

The proton conductivity or proton permeability is a measure of the ability of a material to conduct protons through it. This parameter is influenced by various factors, including the membrane material, the presence of water, temperature, humidity, and other environmental factors. It is an important parameter for the performance of membranes in various applications, including fuel cells, electrolysis cells, and other electrochemical processes. In general, higher proton conductivity or permeability leads to better membrane performance in these applications. In the case of a proton exchange membrane (PEM) electrolyte, the proton conductivity is typically in the range of (10^{-4}) to $(10^{-2})\,\text{S/m}$. The conductivity of the PEM is influenced by the concentration of protons at the electrolyte/membrane interface and the activation energy for proton transport. The permeability coefficient is a measure of how easily hydrogen ions can pass through the membrane and is a function of factors such as the membrane material, temperature, and the applied pressure. Therefore, the hydrogen permeability of dense membranes is strictly related to their flux Φ of the gas through the membrane:

$$\Phi = P\frac{(P_{SH} - P_{SL})}{L}. \tag{5}$$

In this expression, P is the permeability, P_{SH} and P_{SL} are the partial pressures of hydrogen on the high-pressure (feed) side, the low pressure (permeate) side and L the thickness, respectively. Where the mass flux describes the relationship between the flux through the membrane and the difference in partial pressure. The flux is independent from the total pressure and is inversely proportional to the membrane thickness. Different types of mathematical models can be used to predict hydrogen permeation, including kinetic models, which describe the transport of hydrogen through the membrane based on the movement of individual molecules, and continuum models, which treat the membrane as a porous medium and describe the transport of hydrogen in terms of macroscopic fluxes. Additionally, the properties of the membrane, such as its thickness and porosity, can also have an impact on hydrogen permeation and must be considered in the modeling. Because of the sensitivity of polymeric materials to high temperatures, many modeling attempts, Arrhenius models were developed have been done to take into account the effects of temperature and pressure on the properties of membranes. In addition, the permeability in polymeric membrane is temperature $(T[K])$ dependent and this dependence is described by an exponential equation of Arrhenius relationship:

$$P_{SH} = P_{SL} \exp\left\{\frac{E_p}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right\}, \tag{6}$$

E_p is the activation energy for the permeability and $R\,[\text{J mol}^{-1}\,\text{K}^{-1}]$ is the gas constant. The separation membrane of polymers with a low permeability and low barrier has a high permeability to gases.

While the principle for this equation is to measure the pressure difference on each side of a separation membrane. On the other hand, hydrogen partial pressure is assumed affecting fermentative hydrogen pathways. This model (Eq. (6)) shows the consumption of hydrogen inside a membrane. Therefore, the hydrogen permeability measured as a function of pressure as well as temperature for the membrane (Figure 3).
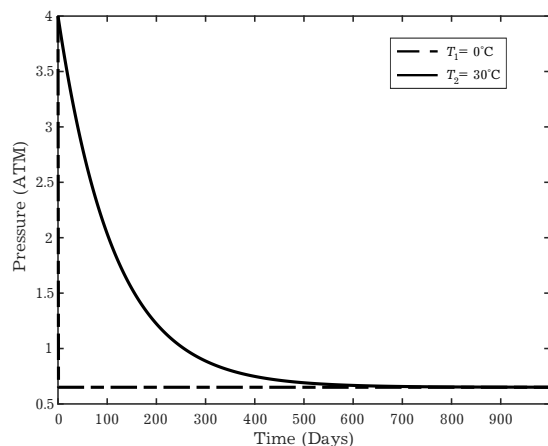

Fig. 3. The time estimated for the consumption of Hydrogen through electrolyte membrane.
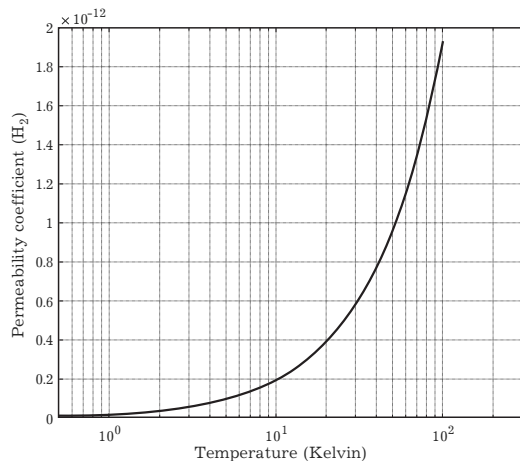

Fig. 4. The permeability coefficients of Hydrogen in separation membrane from $0 - 30°C$.

The hydrogen permeability of membrane is decreases with decreasing temperature and is strictly related to their lattice structure, while the input hydrogen flow rate constant after 1000 days. Physically, the permeability of permeate hydrogen in membrane is really affected by a variation of pressure. Nevertheless, the temperature have a large effect on the transport of small penetrants in the polymeric membrane. Because of the concentration gradient, the transport of hydrogen occurs at the upstream side of the separation membrane. In physical chemistry, the Arrhenius equation is a simple formula but remarkably accurate, for the temperature dependence of reaction rates.

The hydrogen permeation coefficient is estimated to be approximately $(9.65 \cdot 10^{-9}$ mol $H_2 \cdot$ m$^{-1} \cdot$s^{-1}Pa$^{-0.5})$ and the molar volume of hydrogen gas is 22.4 (L/mol). As expected, the permeability coefficient of Hydrogen increased with increasing temperature in a range of $0 - 30°C$ for separation membrane (Figure 4).

Due to plasticization effects, the increase of gas temperature can have a positive impact on membrane performance. The Hydrogen permeability dependant on pressure and temperature and not affected by the presence of nitrogen and carbon monoxide. At higher pressure and real process conditions, in the membrane a fixed amount of sorption sites are present, which are saturated at a certain pressure, thereby leading to a decrease in solubility. This may be explained by the model of dual-mode sorption in polymeric membranes was used to describe Hydrogen permeation behavior for binary gas mixtures. As expected, with the pressure's increase, the Hydrogen permeability slightly decreases and can induce a swelling process of natural polymer matrix,

$$P = P_0 \exp\left(-\frac{E_p}{RT}\right), \tag{7}$$

where P_0 is the pre-exponential factor. For the activation energy:

$$E_P = E_S + E_D, \tag{8}$$

where E_S is the activation energy for solubility and E_D is the activation energy for diffusion.

In general, the proton conductivity increases with increasing temperature and decreasing pH. Additionally, the application of an electric potential across the membrane can also increase the proton conductivity by promoting the transfer of protons from one side of the membrane to the other. It is important to note that, the proton conductivity assumed in the example provided above is a constant, in reality, it is a function of many factors and it is not always constant. In real systems, it is often difficult to obtain a precise measurement of the proton conductivity due to the complexities of the system, so it is often estimated using mathematical models or empirical relationships.

In one dimension, the concentration of hydrogen can be described by a partial differential equation that accounts for diffusion and any other relevant chemical or physical processes. Hence, the concentration can be roughly predicted by the rearranged equation in Eq. (9):

$$\frac{\partial C}{\partial x} = D_0 \left(\frac{\partial^2 C}{\partial x^2} \right) e^{\alpha t} - \Phi, \tag{9}$$

where Φ is the flux of hydrogen ions through the membrane and at $30°$C, the diffusion coefficient of hydrogen is $D_0 = 4.9 \cdot 10^{-5}\, \text{m}^2/\text{s}$ and $\alpha = \frac{-E_D}{RT}$.

Under reasonable conditions, the concentration of hydrogen distributed uniformly prior in the separation membrane. Initially, we use the following initial condition:

$$C(x,0) = C_0. \tag{10}$$

The boundary conditions are constraints necessary for the solution of a boundary value problem:

$$C(0,t) = C(L,t) = 0. \tag{11}$$

We suppose that the diffusion rate increases exponentially over the time and only occurs in one dimension. In order to solve this partial differential equation (Eq. (9)), we use the Fourier method with linear homogeneous boundary conditions, in which allows to rewrite the final analytical solution;

$$\sum_{n=1}^{\infty} A_n \sin \frac{n\pi}{L} \big(1 - \cos(n\pi)\big), \tag{12}$$

where

$$A_n = \frac{2C_0 \exp\left(D_0 \beta^2\right)}{n\pi} \exp\left\{ \frac{-\beta D_0}{\alpha} e^{\alpha t} \right\} \quad \text{and} \quad \beta = \frac{n\pi}{L} \quad (n = 1, 2, 3, \ldots).$$

The concentration of hydrogen into the separation membrane could be seen as a side reaction of the overall reaction, which is a product of a cathodic polarization. The concentration profile of hydrogen in separation membrane is shown in (Figure 5). Accordingly, the diffusion of hydrogen in a membrane can be described with transport law, which the flux of a molecule is directly proportional to its thermodynamic activity. Therefore, there are an equilibrium between both diffusible and trapped hydrogen due to stress-induced defects due to an effective diffusion coefficient.
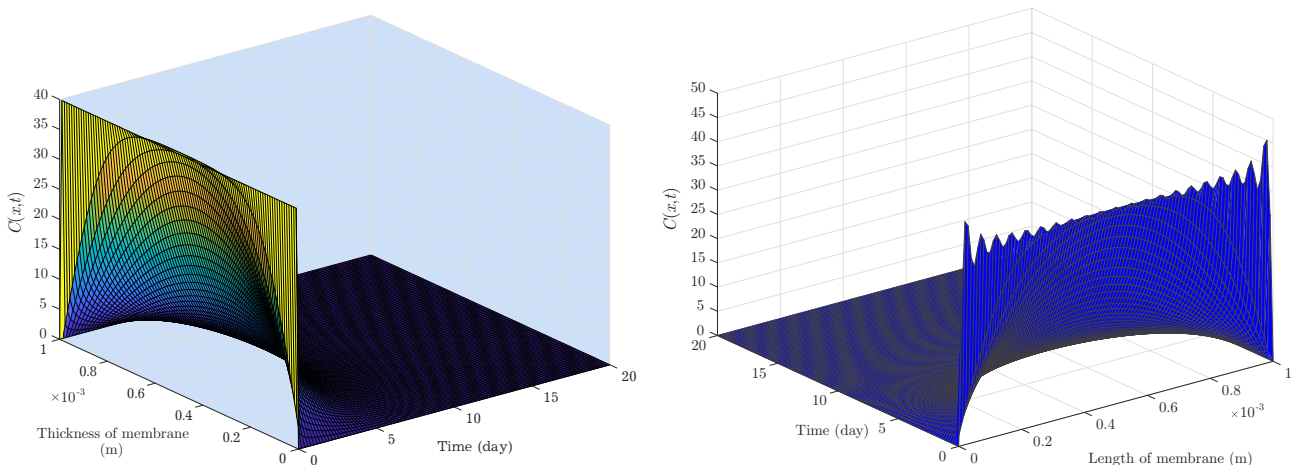

Fig. 5. The concentration of hydrogen in separation membrane.

Furthermore, the concentration of hydrogen because of the film chemical composition and the selective hydrogen removal along the separation membrane length was found to become significant with increasing membrane permeability. Typically, transportation of Hydrogen through separation membranes is governed by the higher solubility in the polymer matrix, the size and the shape of the molecules as well as their interaction with the membrane. In one dimensional, we can also examine the concentration of Hydrogen in the separation membrane for the one-dimensional using finite-difference numerical method. We used a forward difference approximation for the time derivative (Figure 6).
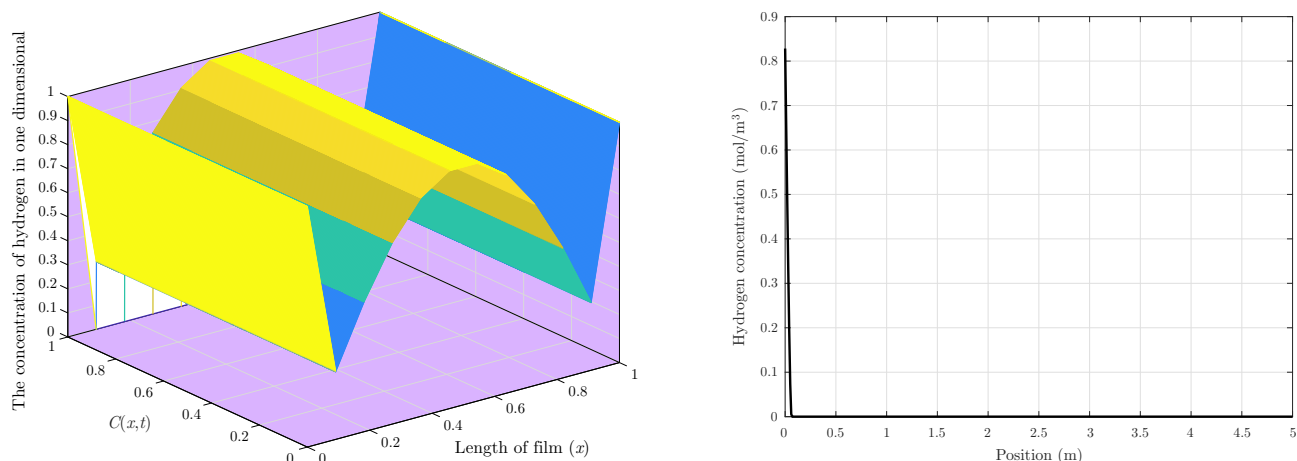
Fig. 6. The concentration of Hydrogen in one dimensional.

In one dimension, we can also consider the concentration of hydrogen changes only in one direction x and it is constant in other directions. If we assume a steady state and perfect membrane with a high separation factor, the concentration of hydrogen on the permeate side will be much lower than the feed side. The concentration of hydrogen on the feed side will be close to the inlet concentration and the concentration on the permeate side will be close to zero. It is important to note that in reality, membrane separation processes are more complex, and many factors such as temperature, pressure, and the presence of other gases will affect the concentration of hydrogen on both sides of the membrane. Additionally, membranes are not perfect, and have a certain degree of permeation, which means that some hydrogen will pass through the membrane regardless of the concentration difference between the feed and permeate sides. The above one dimensional model serves as a simplified representation of the process, and the performance of the process will depend on the specific design and operating conditions of the system.

The concentration of hydrogen in a palladium membrane can be determined by measuring the amount of hydrogen that has been absorbed by the palladium. This can be done through a variety of methods, including gravimetric analysis, which involves measuring the weight of the palladium membrane before and after hydrogen absorption, or through spectroscopic methods such as infrared spectroscopy or nuclear magnetic resonance spectroscopy. In addition, the concentration of hydrogen in a palladium membrane (Figure 7) can also be calculated by using mathematical models that describe the kinetics of hydrogen absorption and desorption. These models can take into account factors such as temperature, pressure, and surface area of the palladium membrane.
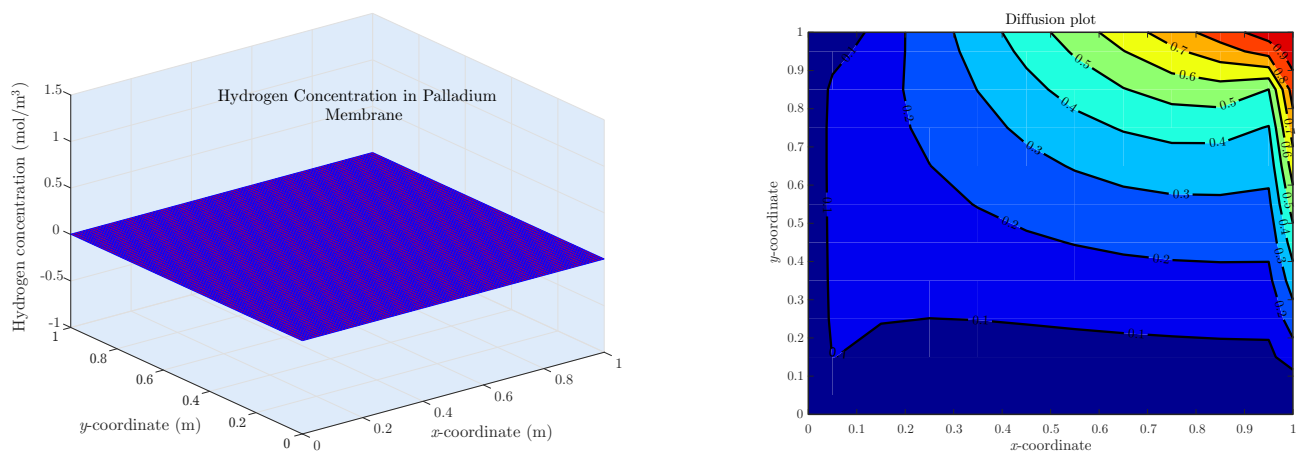

Fig. 7. Concentration of hydrogen in a palladium membrane.

The hydrogen concentration within a palladium membrane is influenced by various factors (see Figure 8). Now, let us delve further into the explanation of a few of these factors:

— Pressure and temperature: the concentration of hydrogen in a palladium membrane increases with increasing pressure and decreasing temperature.
— Surface area: a larger surface area of the palladium membrane can increase the concentration of hydrogen that can be absorbed.
— Impurities: the presence of impurities, such as oxygen or carbon monoxide, in the palladium can decrease the concentration of hydrogen that can be absorbed.
— Kinetics of absorption and desorption: the rate at which hydrogen is absorbed and desorbed by the palladium membrane can affect the concentration of hydrogen that can be absorbed.
— Saturation: palladium can become saturated with hydrogen, meaning it can no longer absorb any more hydrogen. This process is known as poisoning and can decrease the concentration of hydrogen that can be absorbed.
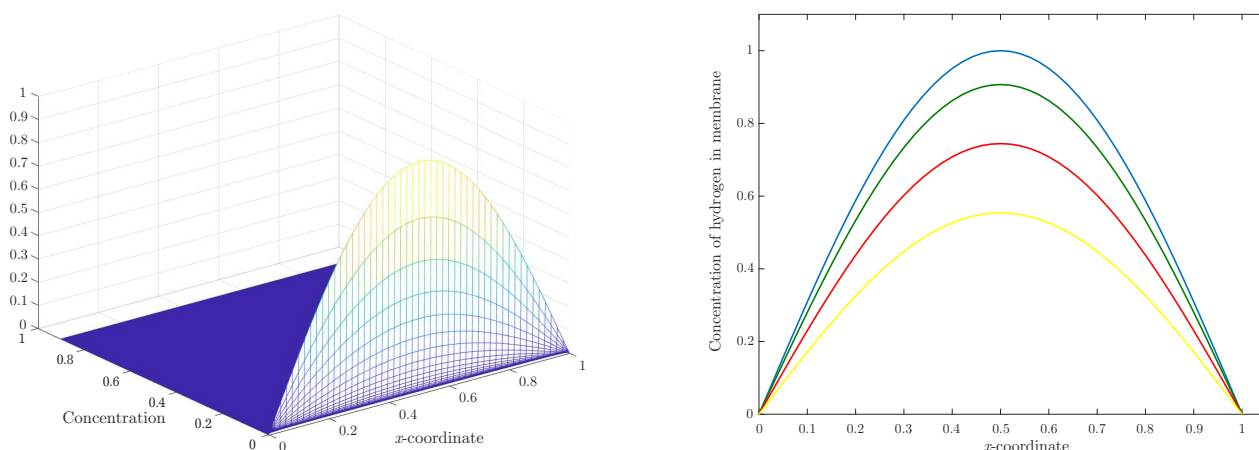

Fig. 8. The concentration of hydrogen in a palladium membrane (one dimensional).

On the other hand, hydrogen permeation through palladium membranes is a process in which hydrogen gas molecules pass through a palladium membrane due to a pressure difference on both sides of the membrane, and are usually operated at normal pressure on the permeate side with a single outlet. Palladium is a preferred membrane material because of its high selectivity and permeability for hydrogen, and its ability to maintain its structural integrity at high temperatures. The process is used in various industrial applications, such as hydrogen purification, hydrogen recovery, and hydrogen separation. In a membrane separation process of hydrogen, the pressure applied on one side of the membrane affects the hydrogen flow density through the membrane. As the pressure increases, the hydrogen flow density through the membrane also increases. This relationship is known as the ideal gas law, which states that the product of pressure, volume, and temperature is constant for a given mass of gas.

The membrane material also plays an important role in determining the hydrogen flow density. The permeance of the membrane, which is a measure of

Fig. 9. Dependence between hydrogen flow density and pressure on the surface of membrane.

the membrane's ability to allow hydrogen gas to pass through it, affects the hydrogen flow density. Membranes with higher permeance will allow for a higher hydrogen flow density at a given pressure. It is important to note that the relationship between hydrogen flow density and pressure in a membrane separation process is not linear and may be affected by other factors such as temperature, pressure, and concentration of hydrogen on the feed side and the permeate side (Figure 9).
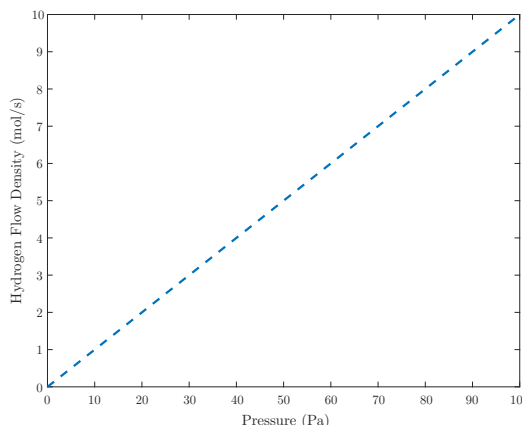
In addition, the membrane separation process of hydrogen can be affected by other factors such as the pressure drop across the membrane, the membrane's selectivity, and the effects of impurities or contaminants.

With rising concerns related to climate change issues and peak oil scenarios. Presently, a global drive seeking renewable and clean alternatives to fossil fuels. In this context, Hydrogen is being used as feedstock in different industrial applications, such as refineries to ammonia and methanol production mainly by catalytic steam. Hydrogen production will lead to a clean, low-carbon energy system as a versatile energy carrier. Hence, the steam reforming reaction is too expensive and requires a large amount of energy for powering the grid, although hydrogen is the available abundant in its pure form on Earth's surface. A widespread development of green hydrogen requires an amount of water electrolysis fuelled by renewable electricity.

Presently, there is unprecedented interest and widespread popular support for using renewable energy, as sources of sustainable energy, particularly wind energy and solar which is constantly improving and without giving rise to any carbon dioxide emissions. Furthermore, when fossil fuels, forests and solid waste are burned, they release large amounts of greenhouse gases trap heat in our atmosphere as nitrous oxide (N_2O), carbon dioxide (CO_2) which makes up the vast majority of greenhouse gas emissions. Green Hydrogen is produced from renewable energy by water electrolysis fuelled by renewable electricity. In an era of water insecurity, green hydrogen holds significant, produced by using electricity by achieving an association between wind turbines and electrolysis, which splits water molecules into hydrogen and oxygen. In oil refineries, dehydrogenation of cyclic hydrocarbons are reversible.

5. Experimental validation

In this section, we compare our numerical results with those already existing in the literature. The previous study involved the use of a tested membrane that was compressed between two alumina collectors. Additionally, a vermiculite gasket commonly available in the market was employed on either of the collectors [61]. The membrane's active region being tested is defined as the space enclosed by the seal, measuring $1.38\,\text{cm}^2$. Gases are introduced to both sides of the membrane through tiny quartz inlet tubes (not depicted) located wi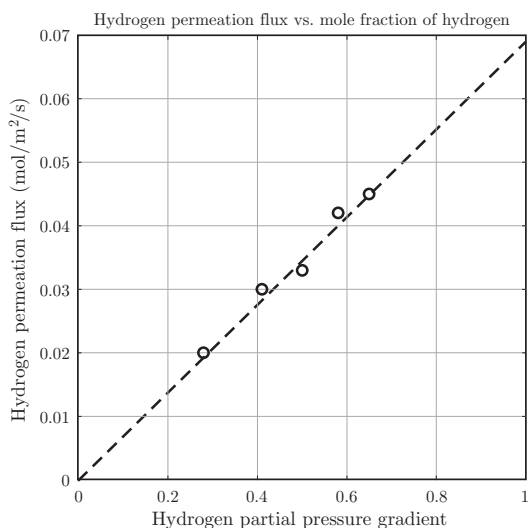thin the alumina support tubes. The input (permeant) and output (permeate) flows are directed through the gap between the support tube and the quartz inlet tube. Gas flow rates are regulated using Alicat mass flow controllers that receive high-purity gases. The assembly of the manifold and membrane is introduced into a clam-shell furnace under PID control, and it is compressed using a spring at the top and a hydraulic jack at the bottom. The feed side of the membrane receives gas mixtures containing H_2, He, and Ar, either humidified or dry. Helium is employed as the tracer gas for identifying membrane leaks, with the partial pressures of H_2 and He in the feed gas maintained at equality throughout the experiments. On the sweep side of the membrane, pure Ar is supplied, either humidified or dry, and the resulting exhaust passes through a desiccant (calcium sulfate) before entering an Agilent 3000 micro gas chromatograph (GC). The rate of permeation demonstrates a

Fig. 10. Plots of H_2 permeation fluxes through ($BaCe_{0.8}Y_{0.2}O_{3-d} - Ce_{0.8}Y_{0.2}O_{2-d}$) membrane as a partial pressure gradient at 900°C.

linear increase concerning the hydrogen partial pressure. This characteristic of a half-order relationship is in accordance with Norby and Larring's hydrogen-permeation model for single-phase materials, assuming the negligible occurrence of oxygen-ion conduction. In the simulation section, the flow density of hydrogen within the membrane signifies the quantity of hydrogen gas traversing the membrane per

unit area and time. This measurement gauges the pace at which hydrogen molecules permeate the membrane material. Our calculation employs the subsequent formula:

$$\text{Flow density} = \frac{\text{Permeance} \cdot \text{Pressure}}{\text{Membrane area}}. \tag{13}$$

Where the permeance is $(0.1 \, \text{mol/m}^2 \cdot \text{Pa} \cdot \text{s})$, the membrane area is $(1 \, \text{m}^2)$ and the pressure is the rate of change of permeation with respect to the gradient in hydrogen's partial pressure. Similar to the findings in the experimental results, the permeation rate demonstrates a linear increase corresponding to changes in the hydrogen partial pressure (Figure 10).

The observed half-order relationship aligns with Norby and Larring's model for hydrogen permeation through a material with a single phase. This model assumes that the influence of oxygen-ion conduction is negligible.

6. Conclusion

Indeed, the development of a sustainable hydrogen economy requires not only scientific and technological advancements but also an understanding of the social, economic, and political contexts in which it will operate. This includes the development of appropriate regulations, policies, and standards for the safe production, storage, transportation, and use of hydrogen. Additionally, the public acceptance and awareness of the benefits and potential risks of hydrogen as an energy carrier are also crucial for the success of a hydrogen economy. Furthermore, the integration of renewable energy sources such as solar and wind energy for hydrogen production can enhance the sustainability of the overall process, as it reduces the carbon footprint and reliance on fossil fuels. However, the intermittent nature of renewable energy sources can pose a challenge to the stable and continuous production of hydrogen, and thus, the development of efficient and cost-effective energy storage technologies will be critical. In summary, the development of a sustainable hydrogen economy requires a multi-disciplinary approach that includes scientific and technological advancements, policy and regulation development, public awareness and acceptance, and the integration of renewable energy sources and energy storage technologies. The permeability coefficients of hydrogen in a separation membrane refers to the quantitative measures that represent the ease with which hydrogen gas can pass through the membrane material. These coefficients indicate the efficiency of the membrane in allowing hydrogen molecules to permeate from one side to the other, usually in response to differences in pressure or concentration. A higher permeability coefficient indicates a more permeable membrane for hydrogen gas. The numerical fluctuations in hydrogen concentration within the separation membrane pertain to the computed adjustments in the density of hydrogen gas within a membrane employed for separation procedures. These alterations are ascertained through mathematical calculations and symbolize the deviations in the dispersion of hydrogen molecules throughout the membrane's framework. The changes in hydrogen flow density and pressure across the membrane's surface refers to the fluctuations or alterations in both the density of hydrogen gas flowing through the membrane and the pressure of that hydrogen across the external face of the membrane. In the final section, a strong concurrence was observed between the numerical and experimental findings.

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Математичне моделювання механічних властивостей під час проникнення зеленого водню через мембранні роздільні матеріали

Хаірч Ю.[1,2], Медархрі І.[3], Джрайфі А.[4], Ельмлуки А.[1]

[1]*Лабораторія LPMC, Університет Шуайб Дуккалі, Ель-Джадіда, Марокко*
[2]*Лабораторія ISTM, FS, Університет Шуайб Дуккалі, Ель-Джадіда, Марокко*
[3]*Команда MMCS, Лабораторія MAID, ENSMR-Рабат, Марокко*
[4]*Лабораторія MISCOM, ENSA-S, Університет Каді Айяд, Марокко*

Потенційна роль водню в майбутньому енергетики викликає значний ентузіазм, незважаючи на те, що він не може повністю замінити нафту. Водень, який має тривалу історію та місце в довгострокових стратегіях і глобальних перспективах, вважається ключовим гравцем в енергетичному переході. На даний час водень знаходить головне застосування в промислових цілях, таких як виробництво аміаку, нафтопереробка та виробництво сталі, орієнтуючись на енергоємні сектори, де пріоритетними є аміак і переробка нафти. Однак залежність від викопного палива сприяє економічній вразливості та надзвичайному клімату в умовах триваючої енергетичної кризи, що стимулює глобальний перехід до більш стійких і чистіших альтернатив. Багато країн прагнуть зміцнити свою енергетичну безпеку шляхом використання відновлюваних і чистих джерел енергії, і для стимулювання цього переходу використовується класична поведінка полімерів. В останні десятиліття дослідження мембран стало потужним інструментом для розробки нових промислових процесів, які підтримують стале промислове зростання. Це дослідження зфокусоване на відділенні водню за допомогою мембрани для відновлення водню. Зокрема, мембранна технологія широко поширена для розділення газів з метою досягнення високої фільтрації. У цій статті чисельно розраховано основні фізичні параметри, що впливають на виробництво водню: концентрації, проникності та тиску. Перевірка достовірності виконаного дослідження здійснена шляхом порівняння експериментального потоку проникнення та його реакції на зміни парціального тиску водню.

Ключові слова: *моделювання; зелений водень; накопичення енергії; роздільна мембрана; проникність; MATLAB–моделювання.*