Modeling of Water Generation from Air Using Anhydrous Salts

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Abstract: The atmosphere contains 3400 trillion gallons of water vapor, which would be enough to cover the entire Earth with a one-inch layer of water. As air humidity is available everywhere, it acts as an abundant renewable water reservoir, known as atmospheric water. The efficiency of an atmospheric water harvesting system depends on the sorption capacities of water-based absorption materials. Using anhydrous salts is an efficient process in capturing and delivering water from ambient air, especially under a condition of low relative humidity, as low as 15%. Many water-scarce countries, like Saudi Arabia, receive high annual solar radiation and have relatively high humidity levels. This study is focused on the simulation and modeling of the water absorption capacities of three anhydrous salts under different relative humidity environments: copper chloride (CuCl$_2$), copper sulfate (CuSO$_4$), and magnesium sulfate (MgSO$_4$), to produce atmospheric drinking water in water-scarce regions. By using a mathematical model to simulate water absorption, this study attempts to compare and model the results of the current computed model with the laboratory experimental results under static and dynamic relative humidities. This paper also proposes a prototype of a system to produce atmospheric water using these anhydrous salts. A sensitivity analysis was also undertaken on these three selected salts to determine how the uniformity of their stratified structures, thicknesses, and porosities as applied in the mathematical model influence the results.

Keywords: atmospheric water; anhydrous salts; solar cells; water vapor; solar energy

1. Introduction

1.1. Overview

About 4 billion people, or two-thirds of the world’s population, suffer from water scarcity [1]. About 13 sextillion (10$^{21}$) liters of water exist in the atmosphere at any given time [2]. Unfortunately, this atmospheric water, which is considered a substantial renewable source or reservoir of water, enough to satisfy everyone’s needs in the world, has been overlooked [3]. Atmospheric water usually exists in three basic types [4]: clouds floating in the sky, fogs that are close to the land, and water vapor in the air. Clouds and fogs are all made up of tiny drops of water, typically with a diameters of 1 to 40 mm, compared with the sizes of rain droplets, which vary from 0.5 to 5 mm. Nonetheless, the concentrations of water droplets in fogs are usually larger.

Water vapor is a renewable natural resource that has the ability to provide water to arid areas around the world [5]. Real challenges are being faced by Saudi Arabia due to the depletion of the rapidly used renewable groundwater. In Saudi Arabia, water is extremely scarce due to arid climatic conditions. The high water demand in the agricultural sector is exacerbating the water scarcity situation in the Kingdom. Urban water and sanitation services incur high costs to the government [6]. Moreover, there is always plenty of water available in the atmosphere, even in the very dry desert regions [7]. Methods to harvest water from humid air are known [3–11], and currently, 25 countries worldwide
are capturing atmospheric water droplets from fogs in remote villages [9–13]. However, fog harvesting techniques require the frequent presence of high relative humidity (RH), typically 100%, in the air, making it only viable in limited locations. This restrains this technology to be applied in any other site, unless the site has a very high RH [14,15].

There have been efforts with limited success to harvest water vapor from low RH air to produce water with a self-sustained energy source [3,16]. Water harvesting by vapor absorption was demonstrated in 2017 by Yaghi et al. [17], using a porous metal-organic structure that operates in a low RH of 20% and delivers water using low-grade heat natural sunlight, aided by a photothermal content. More recently, Li et al. [18] fabricated an all-in-one bi-layered composite disk device to integrate water vapor collection and photothermal-assisted water release, using anhydrous salts: copper chloride (CuCl₂), copper sulfate (CuSO₄), and magnesium sulfate (MgSO₄), with low relative humidity, as low as 15%.

This paper reports on a project that simulated and modeled an atmospheric water-generation unit using anhydrous salts: copper chloride, copper sulfate, and magnesium sulfate, to produce atmospheric water from thin air. In a sensitivity analysis test, the effects of the main parameters of the mathematical model under various RH modes and their effects on the water absorption mechanism were investigated. Due to the lack of published data about the hygroscopicity of anhydrous salts to generate water from thin air, as most data from vapor adsorption focus only on other porous material and none was found on the anhydrous salts nor was there modeling on it, we modeled and simulated the adsorption of water vapor, and the computed model was compared with the actual data of the laboratory results [18] to verify our calculations.

Statement of the Problem

In its Vision 2030, Saudi Arabia targets a national transformation program towards renewable energies and redirects oil and gas exploration to other higher-value uses. Saudi Arabia has significantly increased its renewable energy targets and its long-term visibility. The goal could be achieved by setting an energy roadmap to supply 10% of its energy demands from renewable sources, with an initial target of generating 9.5 GWs of renewable energy by 2023 and 3.45 GW by 2020 [19]. In 2019, the Saline Water Conversion Corporation consumed 40 million megawatt-hours of electricity to produce freshwater: 14.7% in desalination plants, located in the west coast, and 85.3% in the east coast. 32 From a total production of 1883.6 million m³ of freshwater, 44.8% was used in the west coast and 55.2% in the east coast [20].

Saudi Arabia has an excellent source of renewable energy because it lies within the world’s solar belt and enjoys clear skies, with 3000 h of sunshine yearly and high solar radiation [21,22] and with an average rate of 8.9 h of sunshine a day across most of the provinces [23]. However, due to environmental issues and rising costs, the production of water is declining. However, the expansion of water resources is an inevitable necessity in economic development [24]. Although desalination is a known solution to this problem, it has the highest energy consumption in the water use cycle [25], thereby delimiting its application.

Water resources exist regionally, but the only source of water accessible all around the Earth is the moisture in the air [24]. The amount of atmospheric water is estimated to be 12,900 cubic kilometers, while the amount of water in all lakes is 91,000 cubic kilometers [26]. Depending on relative humidity, various methods have been proposed for the harvesting of atmospheric water (AWH), including fog collecting [27], direct cooling [28], dew collecting [29], membrane separation [30], and the use of anhydrous salts to produce atmospheric water. Each of these technologies, their feasibilities, and functionalities depend on the region’s climate. Methods, like dewing and fog collecting, are only applicable in high relative humidity areas, as they are not feasible in arid areas, like in most areas of Saudi Arabia. Membrane separation and direct cooling are capable of generating water
in dry lands. Still, it is not rational to use them, since energy consumption is significantly high in low dew point temperatures [31].

The potential of using anhydrous salts to produce atmospheric water is immense, as it works with low relative humidity, as low as 10%. It was identified as an asset that still needs to be utilized for sustainable atmospheric water generation. Due to low relative humidity, the salts can absorb humid air, serving as cost-effective water absorbents in the production of drinking water in water-scarce regions. No modeling and simulation has been conducted in Saudi Arabia to investigate the potential to produce atmospheric water using anhydrous salts. Therefore, no current programs consider this as a viable choice, as Saudi Arabia did not plan to use this alternative to produce atmospheric water.

1.2. Outline of the Paper

This paper is divided into six sections. In Section 2, the state of water scarcity in the world, the alternative sources of water, and an extensive literature review on the production of water from the atmosphere, its development, investigation, and assessment are presented. Section 3 evaluates the characteristics of the anhydrous salts, and it presents the atmospheric water-generation prototype from this study. Section 4 describes the methodology that was adapted in this study. Results and discussion are presented in Section 5, which include the sensitivity analysis of the computed model and the validation of the model using static and dynamic relative humidities. Finally, Section 6 draws the main conclusions of this paper and the suggested future works.

2. Study Background and Literature Review

2.1. Overview of Water Scarcity and Alternative Sources of Water

Water scarcity is one of the most severe issues in the world. Approximately around 97.5% of the Earth’s water content is seawater, which means that only 2.5% of the existing water is freshwater. Almost 70% of this amount is frozen water in the form of polar ice caps, and around 30% exists as moisture in the air or in underground aquifers. Therefore, only less than 1% of the Earth’s freshwater is accessible for direct human use [32]. The annual global average relative humidity indicates that the Middle East suffers from water scarcity and has a low relative humidity of less than 25%. The Global Horizontal Irradiance (GHI) in Saudi Arabia, where most solar irradiance falls, consequently results to water scarcity [33]. Two technologies that overcome the obstacle posed by limited water capacity and the relatively continuous expensive water delivery are: the desalination of saline water (groundwater) and the extraction of water from the air [34]. The source of the water is usually chosen based on its availability and costs. The current water desalination methods include dew evaporation, reverse osmosis, electro-dialysis, and electrosorption [25,35]. Hence, these technologies on small-scale applications require an accessible brackish water source and expert labor for their operations and maintenance, which narrow down the application conditions of these technologies [35–37]. In contrast, harvesting water from the atmosphere is accessible everywhere, and the water harvester can be easily operated with a local renewable energy source, especially in arid regions, like Saudi Arabia [38].

Water vapor and liquid water cannot coexist at the same ambient pressure, so the vapor’s partial pressure must exceed the pressure of the liquid molecules on the water’s surface [39]. If the liquid water pressure is higher than the partial pressure of the water vapor, then liquid water evaporates until the pressures are in equilibrium. When the vapor’s partial pressures are higher than the pressure of the liquid water, the vapor will start to condense into liquid water, until the pressures are in equilibrium with one another. The equilibrium point changes in different locations due to changes in temperature, specific volume, and pressure. These dynamic factors directly affect the humidity of the air in any region. For example, the atmosphere holds more moisture at a higher temperature, which affects the humidity level in that area [40].
2.2. Previous Studies

Many different methods are utilized to extract water vapor from the atmosphere, which is done by altering pressure, volume, or temperature to force condensation within the system [39]. All devices for atmospheric water generation rely on the same thermodynamic fundamentals, i.e., capturing moisture from the air, then condensing the captured moisture into liquid water. Renewable energy contributes to the separation process and the condensation process that requires energy consumption.

There are many advanced technologies that are applied to harvest atmospheric water nowadays, like refrigeration-based atmospheric water generators (AWGs). In these a refrigerant passes through a condenser and an evaporator coil that cools the air that surrounds it. This causes the water to condense. The fans blow purified air over the coil, which then passes through the tank for purification, before being filtered to remove viruses and bacteria that were obtained from the environment [41]. The water production of the AWG depends on the relative humidity, the size of the compressors, and the ambient air temperature. They are not efficient at relative humidities, i.e., between 30% and 40% or at temperatures below 18.3 °C (65 °F), making this refrigeration-based AWGs impossible to harvest atmospheric water in dry regions with very low relative humidities, as the dew point temperatures in these regions may reach sub-zero temperatures.

Fog water collectors work effectively under high relative humidities, typically in arid coastal areas. Fog water collectors are made by placing a rectangular mesh that is perpendicular to the wind. The mesh collects the fog droplets, while the wind blows the high humid air to it, and as the water droplets become larger, they sink into the tank due to gravity [34,42]. This works in areas with very high relative humidity, as high as 100% for fog to form [43], which limits their application to areas with high relative humidities only.

The need to reduce dependency on fossil fuels drove researchers to use solar energy-driven AWG. Various investigations have reported two methods: a dew water harvesting using solar-powered sorption chiller [44] and the sorption generation condensation method [45]. The sorption generation condensation method uses desiccants to capture water vapor from the air in the shade and under the sun. It desorbs the water out. Like in the metal-organic frameworks (MOFs), they are porous materials with sorbents made of metal groups that are linked together with organic molecules. They absorb water from dry air, condense it, and collect it for drinking. The solar-assisted water collection and the absorption processes take place in a MOF sheet and a condenser. The desorbed vapor is concentrated at ambient temperature and delivered through a passive heat sink during water harvesting (left), requiring no additional energy input. The vapor is adsorbed on the MOF layer during the water capture, rejecting the heat to the ambient (right) [17]. Yaghi and Wang [17] reported that the MOF-based device could capture water vapor from the ambient air, with a relative humidity of as low as 20%, as the water is delivered using heat from natural sunlight. This paper simulated their efforts to find other cost-effective materials, with water absorbent capacities under lower relative humidities.

2.3. Significance of the Study

The Renewable Energy Project Development Office (REPDO) of Saudi Arabia’s Ministry of Energy, Industry, and Mineral Resources (MEIM) announced a plan to increase the share of renewable energies to generate 40 GW of solar energy over the next decade [32]. Solar energy can be utilized to operate the water-harvesting device in arid areas or to reduce its grid’s dependency. Furthermore, harvesting water from the air shows a great promise in supplying water for the communities in dry areas, where the sea, rainfall, lakes, springs, rivers, and groundwater are not viable water sources. Hence, a sustainable onsite water supply technology for these communities is more promising and practical.

The water vapor in the atmosphere provides a sustainable and innovative solution to produce water using anhydrous salts. Atmospheric water is available everywhere, and there are no restrictions in using anhydrous salts. Devices to harvest atmospheric water can be easily operated with a renewable energy source, like solar energy. During the last
few decades, there has been significant development in water production from the air as a new and sustainable water source, driven by the requirement of finding alternative sources of water in arid areas or by the need to decrease the emissions of greenhouse gases. Using anhydrous salts to produce atmospheric water is expected to play a role in supplying arid areas in Saudi Arabia, instead of depending on the scarce groundwater or on water from the desalination plants.

3. Anhydrous Salts and System Prototype

3.1. Anhydrous Salts

These are also a well-known group of hydrated salts, especially their dry and anhydrous counterparts. The anhydrous salts can absorb water vapor from the air to become hydrated, and they have been well utilized in trace water removals from organic solvents [18]. Proposed materials, such as zeolites, silica gels, and MOFs, can harvest water from the air by absorption over a wide range of humidity values [46–48]. These materials suffer from the low uptake of water, which is unlike the uptake of water vapor by anhydrous salts, which is a chemical process known as a hydration reaction with absorption heat that is desirably higher than 60 kJ/mol [17,46].

In 2018, Li et al., screened 14 common anhydrous and hydrated salt using a fabricated all-in-one bi-layered composite disk device, for integrated water vapor collection photothermal-assisted water release. Among the salt couples they investigated, copper chloride, copper sulfate, and magnesium sulfate stood out due to their water absorption/release capabilities and their chemical and physical stabilities. The results showed that the three salts have a high (>20%) available water capacity, and this water capacity after 10 cycles does not change [49]. The thermal gravimetric analysis (TGA) results, with 80 °C dehydration, proved that they could release a significant amount of their hydration water at temperatures between 70 °C and 85 °C, implying that they are good candidates for the application. The results of their work indicate that copper chloride works better in regions with very low ambient RH, as low as 15% but with abundant sunlight irradiation, such as in deserts. In comparison, copper sulfate and magnesium sulfate are more suitable in areas with high humidity, like 35% but low sunlight irradiation, such as in island or mountainous areas. Their work proved that anhydrous salts are cost-effective water absorbents that can be used in producing drinking water in water-scarce regions.

When using anhydrous salts to capture water from the air, a hydration reaction occurs between the salt and the water molecules. Copper chloride becomes hydrated, as it binds to a limit of two moles of water molecules. In their hydrous states, copper sulfate and magnesium sulfate bind to more than three moles of water molecules (five and four molecules, respectively) [50]. Mossab mentioned that such hydration reactions have an enthalpy of reaction that thermodynamically describes the extent to which a particular reaction direction is favored. The higher the absolute value of the enthalpy of reaction is, the easier this reaction is achieved.

These enthalpy values help in choosing the appropriate type of salt for a specific application, when evaluated based on the Clausius–Clapeyron Equation (1) [18,50].

\[
\Delta H_m = \frac{RT_1 T_2}{T_2 - T_1} \ln \frac{P_2}{P_1}
\]

where \(\Delta H_m\) is the enthalpy of reaction (absorption heat), \(R\) is the gas constant, and \(P_1\) and \(P_2\) are the partial pressures at temperatures \(T_1\) and \(T_2\), respectively. In the water capture and release scenario, \(T_1\) is the temperature at night time during summer, and \(T_2\) is the temperature at which the photothermal desorption process happens, i.e., 290–298 K and 343–358 K, respectively, with RH values between 1% and 25%. As indicated in literature [18], the minimum absorption heat in those temperature ranges was calculated to be in the range of 60 to 130 kJ/mol. The chosen salt should have an enthalpy of reaction not lower than 60 kJ/mol. In Table 1, it can be inferred that some salts do not fall within these ranges, making them unsuitable for the application [50].
Table 1. The initial data on the static relative humidity (RH) that were used for the current model.

| Parameter | Copper Chloride (CuCl$_2$) | Copper Sulfate (CuSO$_4$) | Magnesium Sulfate (MgSO$_4$) | Unit |
|-----------|-----------------------------|---------------------------|-------------------------------|------|
| $Y_e$     | 0.9                         | 0.099                     | 0.009                         | (kg L/kg S) |
| $t$       | 1                           | 1                         | 1                             | (day) |
| $d$       | 3.4                         | 4                         | 3.2                           | (dimensionless) |
| $\varnothing$ | 15                         | 35                        | 35                            | Relative Humidity in % |
| $x_{ra}$  | 0.0015                      | 0.0015                    | 0.0015                        | (m)  |
| $D_{ps}$  | 0.002720402                 | 0.068666526               | 0.098730463                   | m$^2$ kg S/kg L day$^d$ |

3.2. Atmospheric Water Generation System Prototype

A suggested, absorption-based atmospheric water harvesting system that utilizes the absorption property from the hydrated slats. The working concept starts during the night, when the humidity becomes high, sorption occurs as the anhydrous salts capture the water within the salt’s porous material. During the daytime, the sun rays heat the salts using the solar thermal layer, where the salts release the adsorbed water. A simple device is warranted to integrate these features in one device, as shown in Figure 1. Water vapor is absorbed at an ambient temperature. The water release happens with the help of externally heated and cooled appliances within the module to increase the process of generating the atmospheric water from the air. The water vapor is then passed through a condenser to a filter to make sure the water is fit for human consumption, and minerals are added to enhance its taste as it is collected in a tank.

![Figure 1](A)
From Figure 1A, following the system concept, the water vapor diffuses into the anhydrous salt layer (the adsorbent layer), filling the pores of the adsorbent, when the fan is on, allowing the air to flow through the adsorbent layer. During the day, the fan is switched off to stop the air flow, as the system is closed and heated from the top by the sunlight that is received from the solar absorber. Desorption happens as the temperature and the concentration difference occur between the adsorbent layer and the condenser. As the heat conducted through the device from the latent heat of the condenser, desorption happens (Figure 1B) in one layer of anhydrous salt (the adsorbent layer). The adsorbent layer is in contact with a solar absorber that is insulated by a transparent convection cover. The bottom of the adsorbent layer is in contact with the condensation surface that consists of an array of fins, cooled by small fans. The AWH using anhydrous salts can operate in arid climates at 10–35% RH, as desorption can occur under natural sunlight at low temperatures, at around 65 °C [17,50]. This system can operate using one single layer of anhydrous salt, using a single condenser for heat rejection and a single solar absorber for the system heat input.

4. Mathematical Modelling

In this section, the mathematical model is developed to simulate water vapor absorption by the anhydrous salts, namely, copper chloride, copper sulfate, and magnesium sulfate. The following comparisons were conducted to establish a cost-effective water absorbents analysis:

- Model comparison of the salts;
- Model validation under different relative humidity modes;
- Sensitivity analysis on the computed model.

A range of vapor diffusion in porous materials represents the vapor’s absorption and release from the absorbent materials. Based on a kinetic process that is controlled by the vapor diffusion through the porous material, depending on the relative humidity, we can analyze and estimate the absorption rates and the rates of release of water vapor from the anhydrous salts. In this paper work, the model developed by Cesek et al. [51] was considered, which originally was used to describe vapor absorption in porous cellulosic
fiber web. The one-dimensional diffusion of molecules in the perpendicular direction of the porous material into thin layer (Figure 2) is described by Fick’s first law as:

\[-i_d = -D \times \text{grad} \, c = c \times v\]  \hspace{1cm} (2)

where \(i_d\) is the one-dimensional diffusion flow of the component molecules and \(\text{grad} \, c\) is equal to \(\frac{dc}{dx}\); \(v\) is equal to \(\frac{dx}{dt}\); \(x\) is the distance achieved by the molecules penetrating the salt molecules at time, \(t\); and \(c\) is the concentration of the component in the measured solution (mol/L). By simple arrangement of Fick’s law, a basic differential equation can be obtained [51]:

\[D \frac{dC}{dt} = C_0 \left(\frac{dx}{dt}\right)^2\]  \hspace{1cm} (3)

where \(C\) is the actual vapor concentration, and \(C_0\) is the saturated vapor concentration. \(D\) is the diffusion coefficient, \(\varphi\) is the relative humidity, and \(x\) is thickness of the absorbent material.

![Figure 2. Schematic diagram of the system under consideration.](image)

The variation of diffusion and absorption in the porous material is proportional to the relative concentration variation of the condensed water inside the absorbent, which can be described as:

\[D \frac{dY}{dt} = \frac{C_0 \varphi M \varepsilon}{\rho_p} \left(\frac{dx}{dt}\right)^2\]  \hspace{1cm} (4)

where \(M\) is the molecular weight of the water, \(\rho_p\) is the apparent density, and \(\varepsilon\) is porosity of the salt. Assuming that the concentration gradient at the boundary of the porous material is constant, the velocity of penetration at the boundary becomes:

\[\frac{dx}{dt} = k^{0.5} \left(\frac{x}{t + \varepsilon}\right)\]  \hspace{1cm} (5)

where \(k\) is the proportionality coefficient, which was taken as \(k = 1\) in our calculations. The parameter, \(\varepsilon\), characterizes the uniformity of the stratified structure of the porous material. Moreover, \(k\) is a dimensional parameter can be used to balance the dimension of Equation (5) based on the value of the parameter \(\varepsilon\). When \(\varepsilon = 1\), the porous material is
uniformly stratified. However, if $d > 1$ or $d < 1$, the porous material is non-uniformly stratified [51]. From the above equations, a simplified differential equation can be obtained as:

$$D \frac{dY}{dt} = \frac{kC_0\varphi M \varepsilon}{\rho_p} \left( \frac{x_{ra}}{Y_e} \right)^2 \frac{1}{t^{d+1}}$$

which is a separable equation that can be solved easily to give [51]. Here, $Y_e$ is the moisture content of the condensed component at a time, $t \to \infty$, while $Y$ is the moisture content of the condensed component at any time, $t$, and $x_{ra}$ is half of the thickness.

$$Y = Y_e t^d + t^d$$

such that $D_{ps} = D\rho_p / kC_0 M\varepsilon$.

5. Results and Discussion

The hydration processes in the anhydrous salts until they are fully saturated with water vapor, depending on their absorption rates. Each type of salt has a different RH, e.g., copper chloride (CuCl$_2$) has a low relative humidity of 10% and copper sulfate (CuSO$_4$) and magnesium sulfate (MgSO$_4$), 35%. Static and dynamic relative humidity modes were applied on each salt to generate accurate results. Furthermore, the sensitivity analysis was applied on the computed model to observe its effects on the water contents of the salts.

A preliminary kinetic study was necessary to compare the computed model with the laboratory data [18]. A detailed analysis of the model validation using static and dynamic relative humidities was performed, along with the sensitivity analysis of the parameters that were used. The results of the model absorption validation was calculated using the data on the water contents in percentages that were measured in hourly intervals per day. The static and dynamic RH modes were conducted to thoroughly investigate the water absorption properties of the three salts with different absolute errors due to the physics of each salt. Comparing the results on the dynamic and static RH hydration processes showed a good agreement with the with experiment results. That the three salts are capable of capturing a good amount of water vapor from the air under the different RHs.

5.1. Model Validation Statistics for Relative Humidity

In order to validate our computed model using the model developed by Cesek et al. [51] Equation (7), a comparison between the computed water contents against the experimental data that were obtained from literature, using a static and dynamic RHs for each of the three salts [18] was undertaken. From the literature in the laboratory settings using the water vapor generator with a programmed output of nitrogen flow with static RH [18], the RH rises from 87% to a predetermined number, i.e., there is no RH ramp, and it stays there for 17 h to allow for hydration [18]. A constant temperature of 24 °C was set for the hydration processes for both modes, based on the fact that water vapor absorption in arid areas happens at night.

It can be noted in Figure 3A that the computed model represents the moisture content of the copper chloride under around RH of 3.4%. It reached the maximum saturation rate of 95.748 kg L/kg S after 17.4 h of hydration, compared with the experimental results [18], with an 6% maximum absolute error. In Figure 3B, copper sulfate showed no absorption at 21% RH, and its onset of absorption is at 35% RH. In our model, absorption reached a maximum saturation rate of 81.797 kg L/kg S after 17.4 h of hydration, with a maximum absolute error of 2.8902%. For the anhydrous MgSO$_4$ (Figure 3C), the onset of water absorption was at 35% RH, under which the weight of the salt increased to 76.825 kg L/kg S, with a maximum absolute error of 10.196%. Table 1 presents the parameters that were used in the model simulation for the three salts.
5.2. Model Validation for Dynamic Relative Humidity

From the literature, the laboratory settings for the dynamic mode the water vapor generator was programmed with output of the nitrogen flow with different RH, that is gradually increased from 1.5% to 9%, with a 1.5% step interval and a 60-min equilibration period between each step. The step interval was 3% and the equilibration time was 30 min.
for the RH range of 9% to 21%, while the step interval was 6% and the equilibration time was 30 min for the RH range of 21% to 80% [18]. Figure 4 shows the dynamic relative humidities, compared with the laboratory results, using the same mathematical model to ensure the accurate results for the three salts. The corresponding values are listed in Table 2.

![Figure 4](image-url)
Table 2. The initial data on the dynamic RH for the current model.

| Parameter | Value of the Parameters |
|-----------|-------------------------|
|           | Copper Chloride (CuCl₂) | Copper Sulfate (CuSO₄) | Magnesium Sulfate (MgSO₄) |
| Yₑ       | 1                       | 1                       | 1                         |
| t        | 1                       | 1                       | 1                         |
| d        | 12                      | 12.85                   | 12                        |
| φ        | 15                      | 35                      | 35                        |
| xₑ       | 0.0015                  | 0.0015                  | 0.0015                    |
| Dₛ       | 0.002329022             | 0.002329022             | 0.002329022               |

For the dynamic RH mode, Figure 4A presents the computed model for the moisture content of the copper chloride whereby the absorption happens around 10% RH. It reaches a maximum saturation rate of 98.6115 kg L/kg S, compared with the experimental results [18], with a 2.7935% maximum absolute error. In Figure 4B, with copper sulfate as the anhydrous salt under a dynamic RH, the absorption of water happens around 35% RH, and in our model it reached a maximum saturation rate of 75.3989 kg L/kg S, with maximum absolute error of 2.3508%. In Figure 4 for the anhydrous magnesium sulfate, the onset of the water absorption under the dynamic RH mode happens around 35% RH, in our model, and the weight of the salt has increased to 78.6886 kg L/kg S, with a maximum absolute error of 1.9616%. Table 2 presents the parameters that were used for the current model simulation for the three salts.

5.3. Sensitivity Analysis

5.3.1. Sensitivity of the Porosity (ε)

The ε resembles the total porosity of the pore sample, because it can be calculated by knowing the apparent density of the porous material, ρₚ [51].

\[ ε = 1 - \frac{ρ_p}{ρ_s} \]  

where ρₛ is the density of the solid part of the porous material. The density of the three salts are listed in Table 3.

Table 3. Densities of the three salts.

| Salt Type               | Density (ρₛ) | Unit     |
|-------------------------|--------------|----------|
| Copper chloride (CuCl₂) | 3386         | kg/m³    |
| Copper sulfate (CuSO₄)  | 3600         | kg/m³    |
| Magnesium sulfate (MgSO₄)| 2660        | kg/m³    |

All parameters of the current model were fixed as constants (Table 2), except for ε, which was tested with different values as shown in Figure 5. As shown, the more uniform the salt, the more water content it held. The smaller the pore volume (smaller porosity), the faster the salt diffusion rate due to the decrease in the diffusion path, which increased the water contents of the salts.
Figure 5. Water content curves of the three salts: (A) copper chloride, (B) copper sulfate, and (C) magnesium sulfate under different porosities, \( \varepsilon \).

5.3.2. Sensitivity of Thickness (\( x_{ra} \))

The \( x_{ra} \) resembles the half-thickness of the sample, as this parameter has an essential effect on the absorption rates of the three salts. The initial value used was 1.5 mm. Other values were also used, as shown in Figure 6, to observe the behavior of the water content on the salts.
Figure 6. Water vapor absorption curves of the three salts: (A) copper chloride, (B) copper sulfate, and (C) magnesium sulfate under different thicknesses.

The thicknesses of the salt layers played an important role in the absorption time and the water contents of the salts. As the thickness decreased, the salt absorbed the water vapor faster and, thus, its water content was increased.
5.3.3. Sensitivity of the Uniformity of the Stratified Structure (d)

The d resembles the uniformity of the stratified structure of porous web materials. The results in Figure 7 showed that more water were gained by the salt in lesser time, when the salt was more uniform. The salt took more time and gained less water content, when it was less uniform. The uniformity of the stratified structures of the three salts: copper chloride, copper sulfate, and magnesium sulfate, played a role in the kinetics of the absorption process.

![Graph A](image1)

![Graph B](image2)

**Figure 7. Cont.**
5.4. Discussion

When the salt becomes dehydrated again [50]. Solution becomes higher than the vapor pressure in the air, leading to desorption. That is, in the vapor reached equilibrium. By inputting energy, the water’s partial pressure in the absorb is reached. For deliquescent salts, water hydrates the crystals and forms a solution, when the weight of the salt increased to 78.6886 kg L/kg S, with a maximum absolute error of 1.9616%.

For non-deliquescent salts, such as copper chloride, water hydrates the crystals until the maximum number of water molecules that the crystals can absorb is reached. For deliquescent salts, water hydrates the crystals and forms a solution, until the partial pressure of the water in the solution and the vapor pressure of the water in the vapor reached equilibrium. By inputting energy, the water’s partial pressure in the solution becomes higher than the vapor pressure in the air, leading to desorption. That is, when the salt becomes dehydrated again [50].

This observation confirms that the diffusion of the vapor into the porous material is the dominant process that controls the absorption kinetics, that is, the condensation of the vapor in the porous material, but it is dependent on its uniformity and structural homogeneity [51]. The water vapor diffuses until it reaches the surface of the material. When it comes to chemical absorption, the water molecules fill the salt crystals, once they contact the pores. The limit to this is that the water hydrates the crystals, depending on the type of the salt that is involved. For non-deliquescent salts, such as copper chloride, water hydrates the crystals until the maximum number of water molecules that the crystals can absorb is reached. For deliquescent salts, water hydrates the crystals and forms a solution, until the partial pressure of the water in the solution and the vapor pressure of the water in the vapor reached equilibrium. By inputting energy, the water’s partial pressure in the solution becomes higher than the vapor pressure in the air, leading to desorption. That is, when the salt becomes dehydrated again [50].

5.4. Discussion

The main outcomes of this paper are: (a) the model and the simulation of the absorption process of water vapor from thin air using anhydrous salts; (b) the results of the comparison of the computed model with the data from experimented laboratory results; and finally, (c) the results of the sensitivity analysis on each of the selected salt to obtain more accurate results for evaluation, the variables of which have greater impact in the computed model. Generally, it was shown in the static RH model validation mode that the moisture contents of the copper chloride under an RH of 15% reached a maximum saturation rate of 88.748 kg L/kg S after 17.4 h of hydration, with a maximum absolute error of 8.3%. The copper sulfate under a 35% RH reached a maximum saturation rate of 81.797 kg L/kg S after 17.4 h of hydration, with maximum absolute error of 2.8902%. The third salt, magnesium sulfate, under a 35% RH had increased its saturation rate to 76.825 kg L/kg S, with a maximum absolute error 10.196%. In the dynamic RH model validation mode, copper chloride reached a maximum saturation rate of 98.6115 kg L/kg S, with a 2.7935% maximum absolute error. The anhydrous copper sulfate reached a maximum saturation rate of 75.3989 kg L/kg S, with a maximum absolute error of 2.3508%. The anhydrous magnesium sulfate had an onset water absorption under a dynamic RH mode, when the weight of the salt increased to 78.6886 kg L/kg S, with a maximum absolute error of 1.9616%.

Figure 7. Water vapor absorption curves of the three (A) copper chloride, (B) copper sulfate, and (C) magnesium sulfate under different uniformities of their stratified structures (d).

Water vapor absorption curves of the three (A) copper chloride, (B) copper sulfate, and (C) magnesium sulfate under different uniformities of their stratified structures (d).
Sensitivity analysis was conducted on each of the main parameters that affected the water contents of the salt in our computed model, like porosity ($\varepsilon$), thickness ($x_{ra}$), and the uniformity of the stratified structure ($d$). It was observed from the computed model that the salt held more water, if it was more uniform. The porosities also differed, based on the type of salt that was involved. Copper chloride reached its maximum absorption at $\varepsilon = 0.35$, for copper sulfate and salt magnesium sulfate, $\varepsilon = 0.1$, indicating that faster diffusion rate of the salt was due to the reduction in the diffusion direction, which increased the water content of the salts. This mechanism became more monodisperse as the porosities were increased, and vice versa. Also, the thickness ($x_{ra}$) had a critical impact on the three salts’ absorption rate activities. The more water the salt contained, the thinner the salt layer, with $x_{ra} = 1.5$ mm, based on the computed model. Furthermore, the uniformity of the stratified structure ($d$) vapor absorption was influenced not only by the porous structure of the salt, but also by its uniformity across the salt layer width. Values of the uniformity parameter, $d \rightarrow 1$, describes a salt with a high uniformity of stratified structure, but this parameter is highly affected by the amount of condensed water in the porous structure of salt.

6. Conclusions and Recommendations

6.1. Conclusions

In this study, the modeling and simulation of water absorption using anhydrous salts were conducted using a comprehensive mathematical model to represent the absorption process. The computed model was compared with real data from experimented laboratory results. Different relative humidity modes were presented and a sensitivity analysis was undertaken on the computed model using the three salts to observe the effect of the main parameters on the computed model and the results on the simulated model. The goal was to validate our mathematical model through modeling and simulating the absorption process. The computed model was validated through the data from the real laboratory experiment. Different sensitivity analyses were obtained, including different porosities, thicknesses of the samples, and uniformities of the stratified structures. These key parameters were selected to examine the effects of the efficiency of the absorbent materials. Based on the results, under an RH of 15%, the moisture content in the copper chloride registered the highest saturation rate of 88.748 kg L/kg S) after 17.4 h of hydration, with a maximum absolute error of 8.3% in the static RH model validation mode. After 17.4 h of hydration, copper sulfate achieved a maximum saturation rate of 81.797 kg L/kg S under a 35% RH, with a maximum absolute error of 2.8902%. Under a 35% RH, the weight of the third salt, magnesium sulfate rose to 76.825 kg L/kg S, with a gross absolute error of 10.196%.

In the dynamic relative humidity mode, copper chloride achieved a maximal saturation rate of 98.6115 kg L/kg S, with a 2.7935% maximum absolute error. The overall saturation limit of the anhydrous copper sulfate was 75.3989 kg L/kg S), with a maximum absolute error of 2.3508%. For the anhydrous magnesium, the onset of water absorption caused the weight of the salt to increase to 78.6886 kg L/kg S, with a maximum absolute error of 1.9616%. Through the sensitivity analysis, the computed model revealed that the salts held more water when they were more uniform, and their porosities varied, depending on the type of salt, with copper chloride reaching its maximum absorption at 0.35, copper sulfate at 0.1, and magnesium sulfate at 0.1. The higher salt diffusion rate was due to a decrease in the diffusion path, which increased the water content in the salts. As porosities were increased, the process became more monodisperse, and vice versa. Also, thickness had a significant effect on the absorption rates of the three salts. More water was absorbed by the salt when the salt sheet was thinner. The stratified structure’s uniformity ($d$) vapor absorption was affected not just by the salt’s porous structure, but also by its uniformity throughout its sheet length.
6.2. Recommendations

Anhydrous salts, which are inexpensive and readily available, can capture atmospheric water vapor and become hydrated. They have been successfully used to remove trace water from organic solvents. Producing atmospheric water from anhydrous salts can solve the water problems of areas where relative humidity is as low as 10%. The production of atmospheric water in Saudi Arabia is a new concept. It needs only a thermal source to produce water. This solution requires research on conducting a sensitivity analysis on the different RHs to determine the viability of installing and implementing water harvesting devices in different sites in Saudi Arabia. A mathematical model is needed to simulate the dehydration mechanism and the subsequent release of water vapor from the anhydrous salts. It is also recommended here to add another source of heat and a condensing device to simulate the process of the model, and to compare the results with the photothermal material laboratory experimental results. Finally, to determine the performance of the proposed method in this study, an actual prototype of the anhydrous salt production of atmospheric water from thin air must be built and tested.

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Abbreviations

- AWG: Atmospheric Water Generators
- AWH: Atmospheric Water Harvesting
- CNT: Carbon Nanotubes
- GHI: Global Horizontal Irradiance
- GW: Giga Watt
- KJ: Kilo Joule
- MEIM: Ministry of Energy Industry and Mineral Resources
- MOF: Metal-Organic Frameworks
- REPDO: Renewable Energy Project Development Office
- RH: Relative Humidity
- TGA: Thermal Gravimetric Analysis

List of Symbols

- $\Delta Y_e$: Steady-state increment of moisture: equilibrium value (kg L/kg S)
- $D_{ps}$: Pseudo diffusion coefficient of the vapor of diffusing component through the porous web material (m$^2$ kg S/(kg L day$^d$))
- $Y_e$: Steady-state moisture content, equilibrium value (kg L/kg S)
- $c_0$: complete concentration of the separated component (mg/L or mmol/L)
- $c_{at}, n_{at}$: concentrations of adsorbed components retained by oxycellulose, pulp, and so forth at times, $t \rightarrow \infty$ and $t$, respectively (mg/L or mmol/L)
- $c_r$: equilibrium solution phase concentration (mg/L or mmol/L)
- $i_d$: one-dimensional diffusion flow of component molecules (mmol m/L s or mg m/L s)
- $x_{rd}$: Half of sample thickness (m)
- $\rho_p$: Apparent density of paper mass, that is, grammage of the paper sample divided by the thickness of the sample (kg/m$^2$)
ΔY Increment of the moisture content (kg L/kg S)
A Outer surface of the pore sample given by its geometry (m²)
a Parameter in (1) (kg L/kg S)
b \((=x_{2}\varphi)/(dD_{p}a_{c})\) parameter in (1) (day⁻¹)
v Condensation or moistening rate at the beginning of vapor condensation or moistening of web pore sample (kg L/(kg S day))
Yi Initial moisture content (kg L/kg S)
Δr Interval of pores \((r \min \leq r \leq r(\varphi))\) filled in steady state by condensed water at a given \(\varphi(\psi/\upsilon)\)
ζr Interval of pores \((0 \leq r \leq r(\varphi))\) filled in steady state by condensed water at a given \(\varphi(\upsilon/\psi)\)
D Density of condensed liquid (kg/m³)
Dp Density of solid part of porous web material (kg/m³)
C, C₀ Vapor and saturated vapor concentration (kmol/ m³)
D Diffusion coefficient of the vapor of diffusing component through the porous web material (m²/day)
M Molar mass (kg/kmol)
Y Current moisture content (kg L/kg S)
c \((=\Delta \gamma_{c})\) parameter in (1) (kg L/kg S)
d Parameter characterizing a uniformity of stratified structure of porous web material (dimensionless)
k Proportionality coefficient (day⁻¹)
t Time of sample storage at given relative humidity (day)
ψ Relative humidity of air

References
1. Mekonnen, M.; Hoekstra, A. Four billion people facing severe water scarcity. Sci. Adv. 2016, 2, e1500323. [CrossRef]
2. Gleick, PH. Water and Conflict: Fresh Water Resources and International Security. Int. Secur. 1993, 18, 79–112. [CrossRef]
3. Wahlgren, R.V. Atmospheric water vapour processor designs for potable water production: A review. Water Res. 2001, 35, 1–22. [CrossRef]
4. Beysens, D.; Milimouk, I.; Schweitzer, A. The Case for Alternative Fresh Water Sources. Pour Resour. Altern. Secher. 2000, 11, 1–16.
5. Fathbieh, F.; Kalmuztki, M.J.; Kapustin, E.A.; Waller, P.J.; Yang, J. Practical water production from desert air. Sci. Adv. 2018, 4, eaat3198. [CrossRef]
6. National Water Strategy Homepage. In Ministry of Environment Water and Agriculture. Available online: https://www.mewa.gov.sa/en/Ministry/Agencies/TheWaterAgency/Topics/Pages/Strategy.aspx (accessed on 5 January 2021).
7. Schneider, S. Encyclopedia of Climate and Weather; Oxford University Press: New York, NY, USA, 2012.
8. Park, K.C.; Chhatre, S.S.; Srinivasan, S.; Cohen, R.E.; McKinley, G.H. Optimal Design of Permeable Fiber Network Structures for Fog Harvesting. Langmuir 2013, 29, 13269–13277. [CrossRef] [PubMed]
9. Zhang, L.; Wu, J.; Hedhili, M.; Yang, X.; Wang, P. Inkjet printing for direct micropatterning of a superhydrophobic surface: Toward biomimetic fog harvesting surfaces. J. Mater. Chem A 2014, 3, 2844–2852. [CrossRef]
10. Wang, Y.; Zhang, L.; Wu, J.; Hedhili, M.N.; Wang, P. A facile strategy for the fabrication of a bioinspired hydrophilic-superhydrophobic patterned surface for highly efficient fog-harvesting. J. Mater. Chem. A 2015, 3, 18963–18969. [CrossRef]
11. Ju, J.; Bai, H.; Zheng, Y.; Zhao, T.; Fang, R.; Jiang, L. A multi-structural and multi-functional integrated fog collection system in cactus. Nat. Commun. 2012, 3, 1247. [CrossRef]
12. Zheng, Y.; Bai, H.; Huang, Z.; Tian, X.; Nie, F.Q.; Zhao, Y.; Zhai, J.; Jiang, L. Directional water collection on wetted spider silk. Nature 2010, 463, 640–643. [CrossRef] [PubMed]
13. Kim, G.; Gim, S.; Cho, S.; Koratkar, N.; Oh, I. Graphene films: Wetting-transparent graphene films for hydrophobic water-harvesting surfaces. Adv. Mater. 2014, 26, 5070. [CrossRef]
14. Olivier, J.; Rautenbach, C.J. The implementation of fog water collection systems in South Africa. Atmos. Res. 2002, 64, 227–238. [CrossRef]
15. Estrela, M.; Valiente, J.; Corell, D.; Millán, M. Fog collection in the Western Mediterranean Basin (Valencia region, Spain). Atmos. Res. 2008, 87, 324–337. [CrossRef]
16. Ji, J.G.; Wang, R.Z.; Li, L.X. New composite adsorbent for solar-driven fresh water production from the atmosphere. Desalination 2007, 212, 176–182. [CrossRef]
17. Kim, H.; Yang, S.; Rao, S.R.; Narayanan, S.; Kapustin, E.A.; Furukawa, H.; Umans, A.S.; Yaghı, O.M.; Wang, E.N. Water harvesting from air with metal-organic frameworks powered by natural sunlight. Science 2017, 356, 430–434. [CrossRef]
18. Li, R.; Shi, Y.; Shi, L.; Alsaedi, M.; Wang, P. Harvesting water from air: Using anhydrous salt with sunlight. Environ. Sci. Technol. 2018, 52, 5398–5406. [CrossRef] [PubMed]
19. Brahimi, T. Using artificial intelligence to predict wind speed for energy application in Saudi Arabia. Energies 2019, 12, 4669. [CrossRef]
20. 2019 Annual Report, Saline Water Conversion Corporation. Available online: https://www.swcc.gov.sa/Arabic/mediacenter/swccpublications/pages/default.aspx (accessed on 24 January 2021).
48. Wang, C.; Liu, X.; Demir, N.K.; Chen, J.P.; Li, K. Applications of water stable metal–organic frameworks. *Chem. Soc. Rev.* **2016**, *45*, 5107–5134. Available online: https://pubs.rsc.org/en/content/articlelanding/2016/cs/c6cs00362a#divAbstract (accessed on 24 January 2021). [CrossRef] [PubMed]

49. Donkers, P.A.J.; Beckert, S.; Pel, L.; Stallmach, F.; Steiger, M.; Adan, O.C.G. Water Transport in MgSO$_4$·7H$_2$O during Dehydration in View of Thermal Storage. *J. Phys. Chem. C* **2015**, *119*, 28711–28720. Available online: https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b08730 (accessed on 24 January 2021). [CrossRef]

50. Alsaedi, M.K. Atmospheric Water Harvesting by an Anhydrate Salt and Its Release by a Photothermal Process towards Sustainable Potable Water Production in Arid Regions. Master’s Thesis, KAUST, Thuwal, Saudi Arabia, 2018.

51. Cešek, B.; Milchovský, M.; Potucek, F. Kinetics of Vapour Diffusion and Condensation in Natural Porous Cellulosic Fibre Web. *ISRN Mater. Sci.* **2011**, *2011*, 794306. Available online: https://www.hindawi.com/journals/isrn/2011/794306/ (accessed on 24 January 2021). [CrossRef]