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Techno-Economic Analysis of Atmospheric Water Generation by Hybrid Nanofluids to Mitigate Global Water Scarcity

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Abstract: Globally, multiple efforts are being made to develop active atmospheric water generation (AWG) or atmospheric water extraction (AWE) systems, particularly using direct air-cooling technology to produce water from ambient air. However, this legacy technique is highly energy-intensive; it can only be operated when the local dew point is above the freezing point of water, and does not scale to create enough water to offer solutions for most industries, services, or agriculture. Liquid-desiccant-based AWG methods show promising performance advantages, and offer a versatile approach to help address the thermodynamics, health risks, and geographic constraints currently encountered by conventional active AWG systems. In this study, we performed a techno-economic analysis of a liquid-desiccant-based AWG system with a continuous operating style. An energy balance was performed on a single design point of the AWG system configuration while using a LiCl liquid desiccant loaded with multiwalled carbon nanotubes (MWCNTs). We showed that the MWCNTs can be doped in LiCl for effective heat transfer during water desorption, resulting in lowering of the sensible heat load by $\approx 49\%$ on the AWG system. We demonstrated that the specific energy consumption (SEC) can currently be obtained as low as 0.67 kWh per US gallon, while changing the inlet desiccant stream concentration of MWCNT-doped LiCl under the given conditions. While the production cost of water (COW) showed a significant regional dependency, economic analysis revealed that water can be produced at a minimum selling price of USD 0.085 per US gallon, based on the 2021 annual average wholesale electricity cost of USD 0.125 per kWh in the U.S.A., thereby providing a strong foundation for future research to meet desirable and competitive water costs by 2026, but before 2031.

Keywords: atmospheric water generation; liquid desiccant; carbon nanotubes; hygroscopicity; nanofluids



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1. Introduction

Access to clean, healthy drinking water has become a luxury in the current global environment. According to *UNESCO/UN-Water 2020*, half of the world's population will be living in water-stressed areas by 2050. It was reported that 1.2 billion people worldwide lack access to water, and a total of 2.7 billion experiences water scarcity for at least one month of the year [1–3]. The increasing burden on the land to feed 7.95 billion people (around 7% of the total sum of all humans who have ever lived) is causing increased strain on agricultural lands, leading to losses in productivity [4]. As traditional methods of agriculture are replaced with modern high-output industrial machines, soil fertility diminishes. Unreplenished soil typically requires 30% more water for irrigation. Thus, in the next 10 years, the world will be producing less food and using more water. In addition, water shortages are causing friction and tensions where the human dependency on water is the greatest. In many cases, water needs are being exploited to influence governments, and are even leading to conflict and war. Border closures and trade restrictions have limited free movement across continents, and have entirely isolated communities dependent on imports for their fragile existence. Ongoing issues with climate transformation and resource

mismanagement will further exacerbate global water stress and hugely impact an increasing number of residential, commercial, industrial, and agricultural water consumers around the world. Unsurprisingly, children are frequently among the most affected by the systematic destruction or contamination of potable water; this directly affects their “rights to life, to the enjoyment of the highest attainable standard of health, to an adequate standard of living, education, and dignity” [5,6].

Atmospheric water generation (AWG) is a nature-mimicking technology inspired by the hydrological cycle, which harvests fresh water from ambient air [7–9]. Water within the Earth’s dynamic atmosphere is continuously moving and changing its physical state. It is estimated that Earth’s ubiquitous atmosphere contains around 13 sextillion (10^{21}) liters of fresh water at any given time, 98% of which are in vapor form, making water production from the ambient air a promising pathway to solve global water scarcity [9]. Such water is generally equivalent to 75 times the fresh water contained in all of Earth’s lakes, rivers, and streams. Therefore, regions affected by severe drought, trade restrictions, border conflicts, and adverse climate-related challenges may consider sustainable AWG technologies that tap into this overhead reservoir of water in Earth’s atmosphere.

Previous studies have reported various AWG systems using both active and passive techniques, including fog harvesting, dewing [10], direct air-cooling [11], and desiccant-based methods [12,13]. Fog harvesting and dewing, despite being widely studied and practically implemented as conventional technologies over the decades [14], suffer from several limitations thermodynamically, climatically, and geographically. On the other hand, several efforts are being made to develop active AWG systems—particularly those using direct air-cooling technology to effectively produce water from ambient air. This method relies on the forced cooling of bulk ambient air through a refrigerated surface to below the dew point to provoke the water to condense and form liquid water. The associated technology is well-studied, and commercial systems are currently available from several vendors, but it is also limited by multiple factors. To name a few, direct air-cooling can only operate when the local dew point is above the freezing point of water, which is a caveat in relatively low-humidity conditions [11]. Moreover, direct air-cooling fails in arid regions such as the Southwestern United States, due to the high energy consumption required to produce a unit of water, which was estimated to be between 270 kWh/m³ and 460 kWh/m³. Although several attempts have been made to modify direct air-cooling AWG systems by introducing vapor separation techniques to reduce the energy requirements, they are still limited in terms of their feasibility on a global scale due to their constrained scalability. While solar-powered sustainable water production from the atmosphere looks promising, it is still in its initial stages [13,15,16]. Further investigation should be carried out to overcome some of the challenges associated with solar-powered technologies before they are potentially integrated with AWG units—particularly those that are operated at large scale in all-weather conditions. Studies on renewable energy resources, such as solar energy, often have discrepancies in testing conditions that are associated with light intensity and stability (indoor vs. outdoor), which could lead to differences in energy efficiency and unreliable data; thus, standardization of test conditions is sought.

Desiccant-based AWG systems [12,17]—particularly those using liquid desiccants [18,19]—have begun to attract significant interest owing to their potential for sustainability, system continuity, scalability, and freedom associated with system integration in a wide range of climatic conditions. Although multiple desiccant types—including solid desiccants [20,21] and composite desiccants [22,23]—have been commonly studied for AWG systems, they are limited by their hydrophobic nature, poor wettability, structural defects, and bacterial growth, which reduces dehumidification and water regeneration performance due to ineffective mass and heat transfer [24]. To date, several hygroscopic liquid desiccants—including ionic liquids (ILs), as well as organic and inorganic desiccants—have been utilized in various industrial and laboratory applications [25,26]. Organic desiccants such as diethylene glycol and triethylene glycol [27,28] are mostly used in air conditioning applications, but are limited by their volatility due to low surface vapor pressure, which

leads to desiccant losses and equipment contamination [28]. ILs, which are essentially organic salts, are often referred to as “target specific” solvents, and could serve a wide range of applications due to their structural diversity and highly tunable properties [29]. Inorganic liquid desiccants—including halide salts such as LiBr, LiCl, and CaCl_2 —are prominent for AWG system configurations due to their large water-uptake capacity, as governed by their low vapor pressure, low cost, inert toxicity, low viscosity, eco-friendliness, and ready availability; however, these gains frequently come with the penalty of corrosiveness [30,31].

While some commercial units of active AWG systems using liquid desiccants are already being developed, the performance of such systems is primarily dependent on the local atmospheric conditions and desiccant media. Particularly, liquid desiccants can be used to capture water from the ambient air, accounting for 20–65% in immediate energy savings due to vapor separation processes [32]. However, for AWG systems that are operated at a large scale, forced convection by blowers is typically used to move ambient air to the liquid desiccant, which contributes to the overall energy consumption to a small degree. The captured water can be actively regenerated with external electric and/or thermal energy input by heating the desiccant solution. Although 80–90% of the total energy is consumed for liquid desiccant regeneration, liquid desiccant technology allows for the recovery of both latent and sensible heat from the liquid desiccant between the scrubber and flash vessel, which generally occurs at different temperatures [33]. The minimum specific energy consumption (SEC) for AWG using desiccant technology, if energy recovery is not implemented, is equal to the enthalpy of vaporization of water (694 kWh/m^3), which is significantly higher when compared to other water production techniques—including seawater reverse osmosis (RO), which requires only $3\text{--}4 \text{ kWh/m}^3$ [33]. However, little has been reported to date on AWG system-level design with approaches to reduce this energy consumption, and the likely costs of water produced by AWG with liquid desiccants.

In this work, we provide a novel theoretical framework for AWG system configuration using hybrid nanofluids. We perform a techno-economic analysis with the intention of reducing the overall energy demand of AWG systems—with a special emphasis on the regeneration aspect, where most of the energy is invested—and enabling lower-cost water production from ambient air. The ability to produce low-cost water can help support the United Nations Sustainable Development Goals. In turn, advancements in this area of technology can uplift humanity by providing access to affordable water even in water-scarce regions or locations that are landlocked, or where water transportation infrastructure (i.e., aqueducts, pipelines, water trucks, etc.) may not be practical or cost-effective.

2. Methods

2.1. Description of the System

The proposed liquid-desiccant-based AWG system configuration was designed to operate continuously in a closed loop; the desiccant regeneration requires only low-grade thermal energy. The system configuration in Figure 1 consists of four major unit operations: (1) a scrubber column that absorbs water vapor from the ambient air, (2) a liquid–liquid heat exchanger (HE1), (3) a flash vessel that facilitates liquid desiccant regeneration by desorbing water, and (4) a two-phase heat exchanger that acts as a condenser (HE2).

The scrubber is an adiabatic packed-bed tower filled with a high-surface-area packing material onto which LiCl trickles to maximize the water absorption capacity. In operation, air—at ambient temperature and pressure—and LiCl enter the scrubber column in a counter-flow configuration. In general, liquid desiccants such as LiCl possess surface vapor pressure as low as 0.36 kPa [34]. As air contacts LiCl in the scrubber column, cooling-free water condensation with almost no energy input takes place due to a vapor pressure gradient [24], unlike direct air-cooling techniques, which require external energy input to provoke condensation [34]. In addition, liquid desiccants allow the molecules into the bulk volume, where an initial surface capture takes place, followed by a subsequent internal permeation process. This mass transfer caused by the vapor pressure gradient occurs until an equilibrium is reached between water in the air and LiCl. Ideally, 100% efficiency in the

scrubber column can be achieved when the vapor pressure of water in the air at the column outlet is equal to the vapor pressure of the LiCl at the column inlet. The concentration of LiCl drops and becomes diluted by the absorbed water until equilibrium is achieved. It should be noted that it is assumed that an air filter is placed upstream of the absorber column to avoid contamination of LiCl by any large dust particles in the atmosphere.

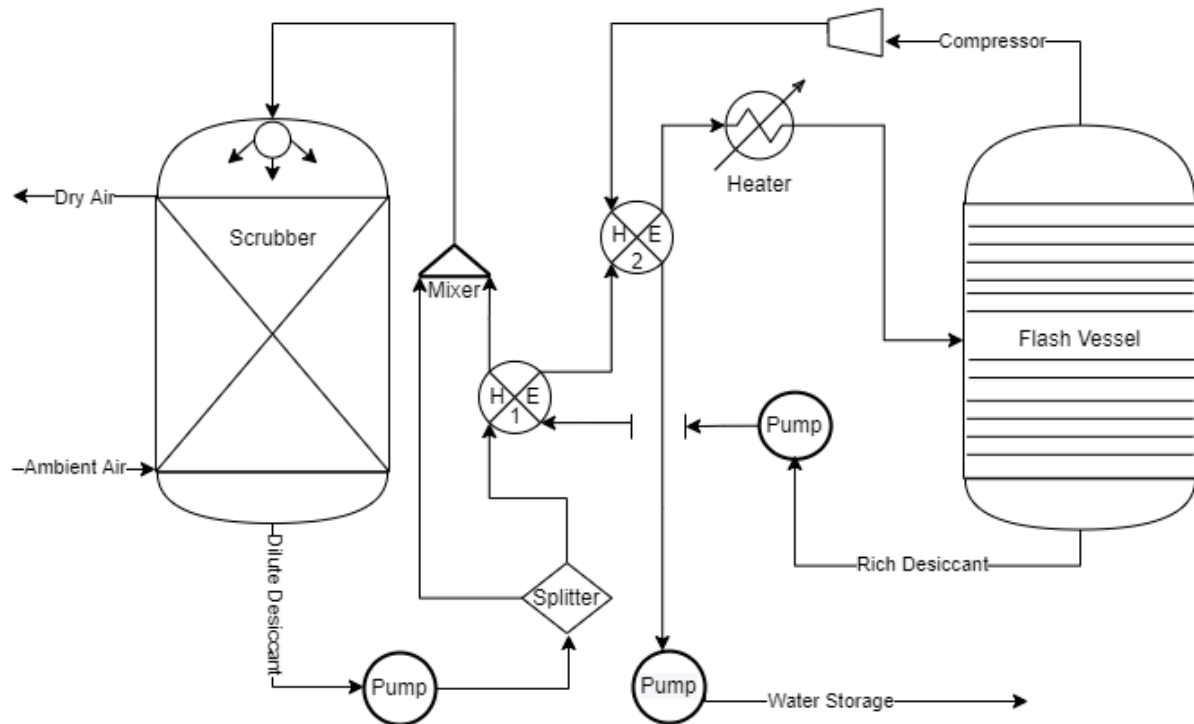


Figure 1. Schematic design of the generic liquid-desiccant-based AWG system configuration.

Diluted LiCl from the scrubber column that is operated adiabatically must be regenerated with external energy input, where the internal water molecules continue to diffuse toward the surface via the concentration gradient [34]. A fraction of the diluted LiCl is regenerated, allowing it to initially pass through HE1, where it is preheated by the returning hot regenerated (rich) LiCl to recover the sensible heat. In the second stage, LiCl from HE1 is passed through a two-phase heat exchanger (HE2) that functions as a condenser to recover the latent heat of condensation from the returning superheated vapor exiting the isobaric compressor at saturated pressure. The hot LiCl stream from HE2 enters the heater to further elevate the temperature, followed by a flash vessel where the LiCl regeneration takes place at sub-atmospheric pressure. Since LiCl has a very low vapor pressure at relatively high temperatures, it does not evaporate with the water, thereby mitigating the liquid desiccant carryover. A final concentration of LiCl is achieved at saturation temperature of water in the flash vessel when all of the water content is desorbed. The rich LiCl desiccant is then recirculated back to the scrubber column through HE1, where the majority of the sensible heat is recovered. The precooled LiCl from HE1 is mixed with a split diluted LiCl to help further reduce the temperature of the inlet LiCl desiccant stream to the scrubber column. In addition, the splitter enables us to maintain the desired flow rate of an inlet desiccant stream to the scrubber, allowing LiCl to regain its optimal moisture absorption capacity. Finally, the condensed water from HE2 is collected in a storage tank.

2.2. Thermodynamic Analysis

The AWG system configuration shown in Figure 1 was mathematically defined using an energy balance. To conduct the performance analysis, the following assumptions were made:

- All system components are operated under steady-state conditions;
- Kinetic and potential energy changes are negligible;
- Pumps' and blowers' energy requirements are negligible;
- The isothermal compressor is operated at an efficiency of 85%;
- The coefficient of performance is 2.5;
- LiCl leaves the scrubber and flash vessel in a saturation state.

2.3. Mathematical Modeling

To evaluate the comprehensive system performance, an energy balance was performed on AWG with continuous-style operation using a liquid LiCl desiccant, which has been studied previously, and the material properties of which have been well documented [35]. In addition to atmospheric conditions, SEC analysis is also a function of the material properties of the desiccant media, allowing the analysis of AWG system performance by introducing the new dimension of operational conditions. At a given dry-bulb temperature and water vapor pressure, it is assumed that the LiCl reaches the saturation state at equilibrium concentration due to the vapor pressure gradient, with no energy input during the absorption phase. The energy requirement of the blower for the air convection to the LiCl is negligible, although this is not always the case in real scenarios—particularly when the system is operated at large scale. During regeneration, the equilibrium LiCl concentration reaches its final desiccant concentration when all of the absorbed water has been desorbed to pure water vapor in a saturation state. Typically, regeneration temperatures range between 323.15 K and 533.15 K, making regeneration an energy-demanding operation [36]. However, to avoid the higher regeneration temperatures, in this design, the flash vessel was operated at sub-atmospheric pressure. While assuming that the energy contribution of the blower is negligible, the energy requirement of the system is primarily attributed to the desiccant regeneration. Thus, the total thermal energy requirement, Q_{total} , to operate the AWG system with no energy recovery is thermodynamically given by the sum of the sensible heat and the latent heat of vaporization:

$$Q_{total} \left[\frac{\text{kJ}}{\text{kg}_{\text{H}_2\text{O}}} \right] = q_s + q_l \quad (1)$$

$$q_s \left[\frac{\text{kJ}}{\text{kg}_{\text{H}_2\text{O}}} \right] = \frac{C_2}{C_2 - C_1} * c_{p,des} * (T_{Reg} - T_{amb}) \quad (2)$$

where q_s refers to the sensible heat, which is dependent on the regeneration temperature T_{Reg} , ambient temperature T_{amb} , and specific heat capacity $c_{p,des}$ of LiCl, while the inlet and outlet concentrations of the flash vessel are represented by C_1 , and C_2 , respectively; q_l corresponds to the latent heat of vaporization.

The difference between the mass of the LiCl solution entering and exiting the flash vessel is equal to the total mass of water $M_{\text{H}_2\text{O}}$ produced, based on the assumption that the composition of LiCl is unaffected by additives in the scrubber column, and the mass of LiCl is unchanged throughout the entirety of the AWG configuration, as given by Equations (3) and (4):

$$M_{\text{H}_2\text{O}} = M_{s1} - M_{s2} \quad (3)$$

$$C_1 = \frac{M_{des}}{M_{s1}}, C_2 = \frac{M_{des}}{M_{s2}} \quad (4)$$

Since the AWG system is operated continuously, and using liquid desiccants in general, both the latent and sensible heat can be recovered in HE2 and HE1, respectively. Then, the amount of total energy is expressed as follows:

$$Q_{total} \left[\frac{\text{kJ}}{\text{kg}_{\text{H}_2\text{O}}} \right] = \frac{(1 - \alpha)M_{s1}}{M_{\text{H}_2\text{O}}} * c_{p,des} * (T_{Reg} - T_{amb}) - \Delta h_{shv} - \Delta h_{scl} + W_C + W_{pdp} + (1 - \beta)q_l \quad (5)$$

$$W_C = \frac{c_{p,vap} * T_{Reg} (PR^{\frac{\gamma-1}{\gamma}} - 1)}{\eta_C} \quad (6)$$

$$PR = \frac{P_{comp}}{P_{reg}} \quad (7)$$

The saturated water vapor exiting the flash vessel is compressed from the regeneration pressure P_{reg} to the compressor pressure P_{comp} , resulting in a pressure ratio PR across the compressor; γ refers to the specific heat ratio. Thus, the work done by the compressor W_C with efficiency η_C is given in Equation (6), under the assumption that water may be approximated as an ideal gas at relatively low pressures. From Equations (5)–(7), the minimum specific energy consumption SEC_{AWG} to operate the comprehensive active AWG system is expressed as follows:

$$SEC_{AWG} \left[\frac{\text{kJ}}{\text{kg}_{\text{H}_2\text{O}}} \right] = \frac{\frac{(1-\alpha)M_{s1}}{M_{\text{H}_2\text{O}}} * c_{p,des} * (T_{Reg} - T_{amb}) - \Delta h_{shv} - \Delta h_{scl}}{COP} + \frac{c_{p,vap} * T_{Reg} (PR^{\frac{\gamma-1}{\gamma}} - 1)}{\eta_C} + W_{pdp} + \frac{(1-\beta)q_l}{COP} \quad (8)$$

where β and α correspond to the recovery factors of latent heat of condensation of superheated vapor, and sensible heat during diluted LiCl regeneration, respectively; Δh_{shv} and Δh_{scl} are the heat recovered from the sensible heat of superheated vapor and subcooled liquid leaving HE2, respectively; COP is the coefficient of performance; and W_{pdp} is the work done by the positive displacement pump to compress the condensate back to the atmospheric pressure, since the system is operated continuously at sub-atmospheric pressure and, therefore, must be pressurized prior to the water storage. However, in this case, the energy requirement of the pump is assumed to be negligible.

3. Results and Discussion

Using the previously described thermodynamic analysis, the minimum specific energy consumption SEC_{AWG} was analyzed for a continuous-style AWG operating system (Figure 1) using a LiCl liquid desiccant solution. The parameters stated in Table 1 were used to estimate the SEC_{AWG} values for a system operated at air inlet conditions of 299.81 K and 60% relative humidity (RH), with both sensible and latent energy recovery. The baseline conditions were chosen based on a rough industry standard for machine rating in AWG.

Table 1. List of parameter values considered for a single-design-point evaluation of the AWG system.

Parameters	Values	Parameters	Values
C_1	33 wt. %	Δh_{scl}	37.65 kJ kg ^{−1}
C_2	36.7 wt. %	α	0.7
$c_{p,des}$	2.69 kJ kg ^{−1} K ^{−1}	PR	4.0
T_{Reg}	349.15 K	$c_{p,vap}$	1.99 kJ kg ^{−1} K ^{−1}
T_{amb}	300.15 K	γ	1.4
Δh_{shv}	264.35 kJ kg ^{−1}	COP	2.5
β	0.7	W_{pdp}	negligible

To minimize the high-temperature swing in the flash vessel, LiCl regeneration was carried out at sub-atmospheric pressure while maintaining the saturation temperature in the vessel at 349.15 K. Initially, diluted LiCl at a concentration of 35.1 wt. % was sent to HE1 at 300.15 K, where 70% of the sensible heat was assumed to be recovered in exchange with incoming hot LiCl at 36.7 wt. % from the flash vessel. While 70% sensible heat recovery seems to be a reasonable approximation in theory [33], some practical issues related to heat exchangers must be dealt with in order to implement heat recapture. The resulting water vapor after water desorption, with a specific heat capacity of 1.99 kJ kg^{−1} K^{−1} in a saturation state, was sent to a compressor operating with a pressure ratio of 4.0 and 85% compressor efficiency. The increase in boiling point, as determined by the E-NRTL

thermodynamic model, was considered in this study to determine the desired operating pressure of the flash vessel. In addition, it should be noted that the compressor plays a key role in generating superheated steam for achieving greater energy recovery in the condenser, which reduces the energy charge through mechanical vapor recompression (heater). However, the compressor would likely have to be customized for practical implementation to sustain the high-temperature application described in this work. The enthalpies of superheated vapor Δh_{shv} and subcooled liquid Δh_{scl} were considered to be $264.35 \text{ kJ kg}^{-1}$ and 37.65 kJ kg^{-1} , respectively. The exiting LiCl stream from HE1 was sent to HE2, where the latent heat of condensation was assumed to be 70% recovered in exchange with the condensate, while assuming that the unit was operated non-adiabatically.

Although most of the energy consumption is attributed to water release, liquid desiccants provide the opportunity to recover significant latent and sensible heat through an internal loop, thereby minimizing the SEC_{AWG} [32,33]. Regardless, the current energy trends for liquid-desiccant-based AWG systems are relatively higher when compared with other technologies, including freshwater production from liquid water resources (i.e., desalination) [37]. However, this energy penalty can be mitigated through the controlled choice of liquid desiccants [32,34,37], while simultaneously introducing nanomaterial-doped hybrid nanofluids with improved thermal, mechanical, and physical properties [38–40]. Based on the classical and statistical mechanics, a detailed model was previously developed [41,42] to determine the specific heat capacity of a nanofluid $C_{p, hf}$ as a function of the nanomaterial volume fraction φ in the liquid desiccant. If we assume that the thermal equilibrium is established between the particles and the surrounding fluid, then the specific heat capacity of a hybrid nanofluid $C_{p, hf}$ is given as follows:

$$C_{p, hf} = \frac{\varphi(\rho C_p)_{np} + (1 - \varphi)(\rho C_p)_{des}}{\varphi \rho_{np} + (1 - \varphi) \rho_{des}} \quad (9)$$

Previous studies investigated the dependency of various nanoparticles—including carbon nanotubes, graphene nanoplatelets, and alumina nanospheres—and their loading concentrations on the specific heat capacities of nanofluids [40,43]. The results showed that the specific heat capacities decrease with an increase in the volume fraction of nanoparticles, due to reduced surface atomic contributions [40,43]. In this study, the influence of nanoparticles such as multiwalled carbon nanotubes (MWCNTs) and their loading concentrations in LiCl on the SEC_{AWG} of the system was modeled. The specific heat values of MWCNTs and LiCl were taken as $0.833 \text{ kJ kg}^{-1} \text{ K}^{-1}$ and $2.69 \text{ kJ kg}^{-1} \text{ K}^{-1}$, respectively, at the regeneration conditions [44,45]. Moreover, the density values of MWCNTs and LiCl were determined to be 1.35 g cm^{-3} and 1.23 g cm^{-3} , respectively [35]. By replacing the specific heat values of liquid desiccants with those of hybrid nanofluids, the SEC_{AWG} of a system operated by hybrid nanofluids can be determined as follows:

$$SEC_{AWG} \left[\frac{\text{kJ}}{\text{kg}_{\text{H}_2\text{O}}} \right] = \frac{\frac{(1-\alpha)M_{s1}}{M_{\text{H}_2\text{O}}} * c_{p, hf} * (T_{\text{Reg}} - T_{\text{amb}}) - \Delta h_{shv} - \Delta h_{scl}}{COP} + \frac{c_{p, vap} * T_{\text{Reg}} (PR^{\frac{\gamma-1}{\gamma}} - 1)}{\eta_C} + \frac{(1-\beta)q_l}{COP} \quad (10)$$

Using the parameters in Table 1 and Equation (10), we estimated the SEC_{AWG} values of a system configuration (Figure 1) while assuming that the composition and absorption rate of LiCl in the scrubber column were unaffected by the MWCNTs in the LiCl. Understanding the nature of LiCl doped with additives in the absorption column is worthy of future study. Table 2 shows the breakdown of AWG system performance under two different liquid desiccant conditions: (1) LiCl, and (2) LiCl loaded with MWCNTs. In the case of the LiCl desiccant solution, the sensible heat load was estimated to be $342 \text{ kJ kg}_{\text{H}_2\text{O}}^{-1}$, which significantly decreased by $\approx 49\%$ with the loading of 0.5 vol.% MWCNTs in the LiCl. Therefore, the sensible heat load required to heat the same amount of LiCl doped with MWCNTs was reduced during hybrid nanofluid regeneration. While the heat capacity of hybrid nanofluids showed a strong influence on SEC, it is worth noting that the SEC

also depends on the viscosity of the nanofluids—especially in the case of a turbulent flow region, which is typical in practical applications. Several studies previously investigated the rheological behavior of water-based nanofluids containing 1D nanotubes [46–48]. The results showed that the flow properties of nanofluids doped with MWCNTs are dependent on the temperature and the volume fraction of nanotubes [46,47]. At higher concentrations of nanotubes, the shear viscosity of nanofluids showed a pronounced shear-thinning behavior as a function of shear rate at 293.15 K. This could be attributed due to the alignment of the structural network of nanotubes under enough shear, along with their lubrication properties [46–49], resulting in a reduction in viscous force, which would greatly improve the performance of thermal management equipment such as heat exchangers in practical applications. In addition to the loading concentration of nanoparticles in base fluids, SEC also depends on the size, shape, and morphologies of the nanoparticles [46,47,49]. Regardless, the typical operating conditions of AWG at large scale produce a highly turbulent regime where the role of the thermophysical properties of the hybrid nanofluids is critical. Therefore, the selection of the operating temperature and loading concentrations of MWCNTs with controlled size and shape in a LiCl liquid desiccant plays a vital role, and should be rationalized by future research for comprehensive AWG system improvement.

Table 2. Performance of the AWG using 33 wt.% LiCl at sub-atmospheric regeneration pressure.

AWG Configuration	Desiccant Solution	Sensible Load (kJ/kg _{H2O})	Latent Load (kJ/kg _{H2O})	Compressor Load (kJ/kg _{H2O})	SEC _{AWG} (kWh/US gal)
AWG with latent + sensible recovery	LiCl	342	271	398	1.06
AWG with latent + sensible recovery	LiCl + 0.5 vol.% MWCNTs	175	271	398	0.88

To determine the optimal SEC_{AWG} values, the inlet stream concentration of LiCl to the flash vessel was varied from 30 wt.% to 35.1 wt.%. We compared the results for two cases (Figure 2a): (1) LiCl without MWCNTs, and (2) LiCl with MWCNTs at a concentration of 0.5 vol.%. For the case of LiCl alone, the results showed that the SEC_{AWG} values gradually increased up to a LiCl concentration of 33 wt.%, and then a significant increase in SEC_{AWG} values was observed as it approached the LiCl saturation concentration in the flash vessel. Meanwhile, in the case of LiCl loaded with 0.5 vol.% MWCNTs, a significant decrease in SEC_{AWG} values was observed—especially at higher inlet stream concentrations (≥ 33.3 wt.%) of LiCl—indicating that the presence of MWCNTs in LiCl played a key role in reducing the sensible heat load. An optimal SEC_{AWG} value of 0.67 kWh per US gallon was recorded at an inlet LiCl concentration of 30 wt.%, indicating that relatively low energy is required if hybrid nanofluids with a high water-carrying capacity and enhanced heat-transfer properties are used. Under optimal conditions, we also modeled the AWG system carrying LiCl with MWCNTs at varied concentrations between 0 and 0.5 vol.% (Figure 2b). A gradual decrease in SEC_{AWG} was observed with respect to the concentration of MWCNTs, leading to a maximum drop of $\approx 7.5\%$ at 0.5 vol.% MWCNTs in 30 wt.% LiCl solution. This behavior could be attributed to the constrained liquid desiccant layering at the surface of the nanoparticle-free boundary caused by the changes in the phonon vibration mode at the solid–liquid interface [50,51].

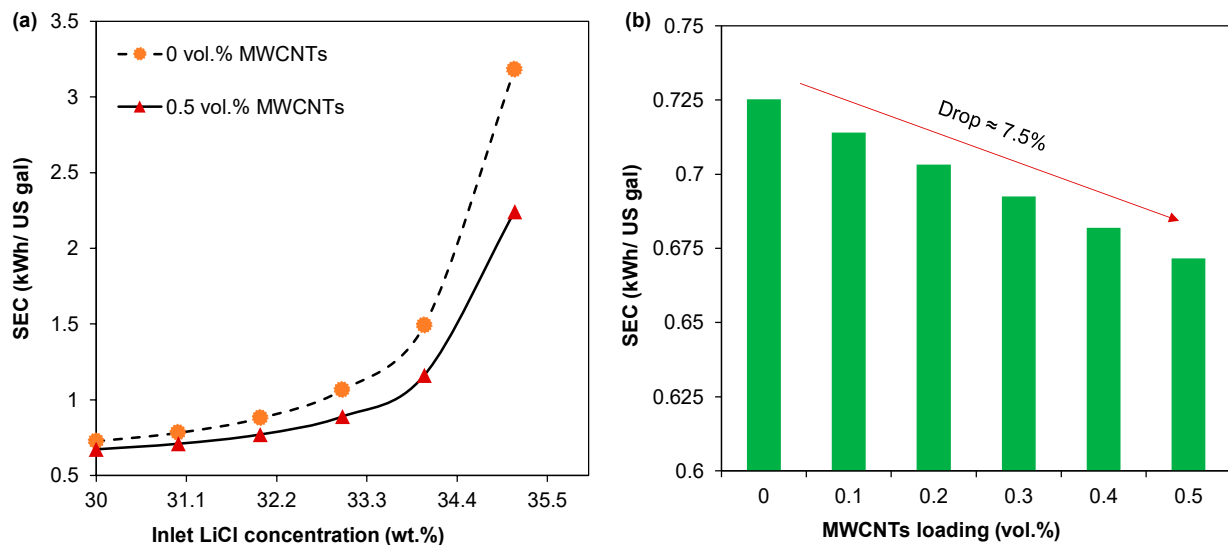


Figure 2. (a) The specific energy consumption (SEC) trend with varied inlet stream concentrations of multiwalled carbon nanotubes (MWCNT)-doped LiCl desiccant from 30 to 35.1 wt.%. (b) Histogram of the SEC values of the atmospheric water generation (AWG) system configuration with 30 wt.% LiCl loaded with MWCNTs at concentrations between 0 and 0.5 vol.%.

3.1. Economic Analysis

The SEC_{AWG} values associated with the sensible and compressor work were used to determine the cost of water COW_{AWG} produced over the whole region (Equation (11)). While the wholesale electricity cost is determined by various region-specific factors, the annual average wholesale electricity costs in 2021 (U.S. Energy Information Administration) were recorded over the region to determine the COW_{AWG} values at a given SEC_{AWG} value of 0.67 kWh per US gallon. Figure 3a shows that the U.S.A. recorded the lowest COW_{AWG} values, while Germany reported the highest. It is important to note that these costs are highly seasonal, due to variable heating and cooling needs; thus, significant changes can be observed in the COW_{AWG} values for different regions.

$$COW_{AWG} \left[\frac{\$}{\text{US gal}} \right] = SEC_{AWG} \left[\frac{\text{kWh}}{\text{US gal}} \right] \times \text{Average wholesale electricity cost} \left[\frac{\$}{\text{kWh}} \right] \quad (11)$$

The performances of the hybrid-nanofluid-based AWG systems and off-the-shelf direct air-cooling AWG systems are compared in Figure 3b. For direct air-cooling technology, the energy requirement is used almost entirely for the processing of bulk ambient air to provoke condensation, which is a major drawback in efforts to effectively scale up these systems. As a result, direct air-cooling AWG systems cannot fit global climatic conditions while meeting the expectations of low energy and cost requirements. Theoretically, liquid-desiccant-based AWG has the best SEC value relative to the other commercial AWG systems, due to the special advantages associated with the tunability of liquid desiccants, while also recovering sensible and latent heat. A second-law analysis [52,53] was performed on an air-to-water separation system to determine the theoretical minimum work of separation (process agnostic). At the baseline conditions of 299.81 K and 60% RH, the theoretical minimum work of separation required to remove a gallon of water from ambient air was determined under the assumption that the moisture in the air is captured completely. Based on the analysis performed via CHEMCAD™ modeling, the minimum work of separation was found to be ≈ 0.07 kWh per US gallon. Figure 3b shows the projection of SEC_{AWG} values towards the theoretical minimum value by 2031 if present research advancements continue, based on present trends observed between 2018 and 2022 (in liquid desiccant air-to-water capture simulations, proofs of concept, digital twins, and pilot plants). This efficiency trend suggests that more optimal system configurations and fluids can be designed and achieved by carefully considering both thermodynamic and economic modeling together.

Qualitatively, it is a reasonable hypothesis that the time period required to advance more rapidly than the current trend (toward the theoretical minimum SEC values as low as ≈ 0.07 kWh per US gallon) could be achieved with focused research and development informed by both thermodynamic and economic factors (Figure 3b, illustrated by the dashed line). It should be noted that majority of the literature including the energy ratings reported on commercially available system, does not account for the overall energy used by the complete systems. Thus, it is possible that reported energy uses in currently reported systems may be significantly higher, up to 100%, than actually reported.

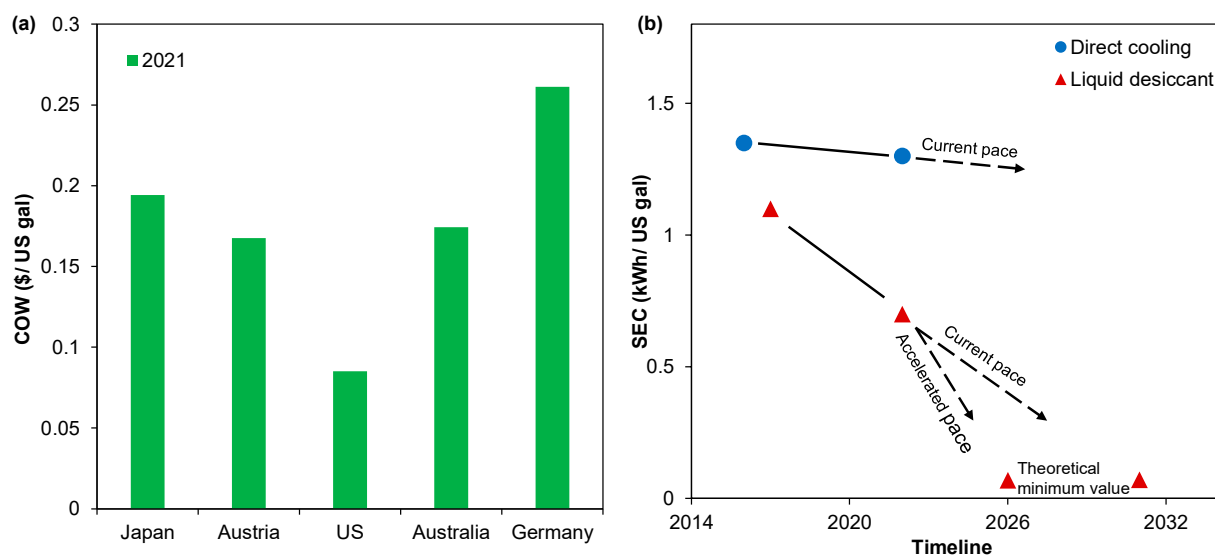


Figure 3. (a) The cost of water produced by region using the AWG system configuration with hybrid nanofluids in 2021. (b) The comparison of the SEC values of the AWG system operated by direct air-cooling and liquid desiccant technologies, and highlighting current and projected trends to meet the theoretical minimum value of SEC by 2031, or as early as 2026. The data points were obtained from the model results [32] and, off-the-shelf direct-cooling AWG systems (according to the manufacturers' specifications).

3.2. Directions for Future Research

It is evident that SEC_{AWG} is primarily dependent on the atmospheric conditions and liquid desiccant material properties. While the loading concentration of MWCNTs in LiCl showed a significant influence on SEC_{AWG} , it is worth noting that the nanotube concentration also influences the absorption rate in the scrubber. Previous studies [54,55] investigated the absorption rates of hybrid nanofluids containing nanoparticles such as CNTs and CuO. The results showed that the absorption rate of water vapor in air by hybrid nanofluids increases with the increase in the loading concentration of nanotubes at the given ambient air and desiccant mass flow rate conditions [54,55]. This could be attributed to the convective motion of nanotubes, such as Brownian motion. More specifically, by adding nanotubes to the desiccant fluid, the random collisions due to thermal fluctuations among the suspended nanotubes and solution molecules are intensified, resulting in an increase in turbulence within the fluid streams, which greatly improves the absorption rate. However, in this study, we assumed that the loading concentrations of MWCNTs have no influence on the absorption rate of water vapor by LiCl, although this is not always the case in real scenarios—particularly when the system is operated at a large scale. Under the given conditions, the selection of loading concentrations of nanomaterials with controlled sizes and shapes in LiCl liquid desiccant plays a vital role in the absorption rates and desiccant compositions in the fluid streams, and can be rationalized by future research on comprehensive AWG system improvement. In addition, it is worth testing different 1D and 2D nanomaterials as additives—including, but not limited to, boron nitride and graphene-based nanomaterials—to help further optimize the heat and mass transfer of

fluids in the AWG system configuration. Furthermore, understanding the flow behavior of hybrid nanofluids doped with nanomaterials in process streams, via CFD analysis and changes in fluid composition throughout the entirety of the AWG system design, is worthy of future study. The theoretical understanding based on this work, in conjunction with the proposed future work, could be integrated to achieve the holistic techno-economic analysis of a hybrid-nanofluid-based AWG system, while accounting for the operational and capital costs of equipment, in addition to the energy costs of the practical implementation of our existing design prototypes.

4. Conclusions

In summary, we conducted a techno-economic analysis of a liquid-desiccant-based atmospheric water generation system with a continuous closed-loop operating style. An energy balance was performed, with a major emphasis on theoretical understanding of regeneration, while using LiCl loaded with MWCNTs at single-design-point parameters of the AWG system configuration. Our results show that MWCNT-doped LiCl is an effective liquid desiccant, reducing the sensible heat load by $\approx 49\%$ and, thus, enabling new avenues to test a wide range of nanomaterials for efficient heat-transfer applications during water desorption. We showed that the specific energy requirements can be obtained as low as 0.67 kWh per US gallon, while changing the inlet desiccant stream concentration of MWCNT-doped LiCl under saturation conditions. While the production cost of water shows a significant regional dependency, economic analysis revealed that water can be produced at a minimum selling price of USD 0.085 per US gallon, based on the 2021 average annual wholesale electricity cost of USD 0.125 per kWh in the U.S.A., thereby providing a strong foundation for future work to meet the desired water production costs without being dependent on legacy water sources during or before the next decade.

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