



Evaluating the emerging adsorbents for water production potential and thermodynamic limits of adsorption-based atmospheric water harvesting systems

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ABSTRACT

In the context of global water scarcity, adsorption-based atmospheric water harvesting (AWH) is an emerging technology for providing potable water at anytime/anywhere. In this regard, the study evaluates silica-gel, zeolite, ionogel, polymer, membrane, and metal-organic framework based ten kinds of emerging adsorbents for the AWH systems. A thermodynamic modeling framework comprising of adsorption equilibrium models and governing steady-state equations is performed. Performance of AWH systems is always judged on water production potential (WPP), energy consumption (EC) whereas thermodynamic correctness can be measured by first (η_I) and second law (η_{II}) efficiencies. Thereby, the adsorbents are evaluated from perspectives of WPP, EC, η_I and η_{II} . As per results, ionogel based adsorbent enables maximum WPP ranging up to 1.55 kg/kg/cycle, EC of 4214.96 kJ/kg_w/cycle, η_I of 0.54, and η_{II} of 0.21. Whereas MIL-101(Cr) observe WPP ranging up to 0.87 kg/kg/cycle, EC of 4499.84 kJ/kg_w/cycle, η_I of 0.50, and η_{II} of 0.19. Parametric analyses results show that η_I of ionogel and MIL-101(Cr) can be increased up to 0.65 and 0.69 while η_{II} up to 0.23 and 0.25, respectively. Furthermore, η_I and η_{II} of dual-stage system can improve by 33% as compared to single-stage that can improve by 68-74% as compared to vapor compression system.

1. Introduction

Global freshwater scarcity is elevating due to climate-induced desertification and extensive groundwater resources depletion [1,2]. About two-thirds of the world's population is experiencing water scarcity as of 2020 which is mainly prevalent in remote and arid-regions [3,4]. Traditional freshwater resources rely on rivers, lakes and rainfall which has uneven distribution due to geography [5,6]. Other freshwater resources like glaciers, ice caps, and deep groundwater are constrained by limited access [5,7]. Due to scarcity of good quality

water worldwide, there are lots of water/wastewater treatments and strategies are employed in recent decades to mitigate the water scarcity challenges which are usually uneconomical [8,9]. Similarly, seawater desalination techniques used compressor based technologies that are responsible for greenhouse gases emissions, extensive energy consumption (EC), demand for brine disposal, and transportation cost particularly in landlocked areas [10–12]. In this context, renewable source of freshwater is in the atmosphere that holds over six times greater than all rivers present in the globe [13]. The potential of the atmospheric water is directly linked with air temperature and humidity; however, it can be slightly influenced by factors like atmospheric

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Nomenclature			
AWH	atmospheric water harvesting	2-3	desorption
C_p	specific heat capacity [kJ/kg-K]	3-4	isosteric cooling
COP	coefficient of performance [-]	4-1	isobaric adsorption
D-A	Dubinin–Astakhov	a	dry air
E	characteristic energy [kJ/kg]	ad	adsorbent
EC	energy consumption [kJ/kg]	ads	adsorption
e	specific flow exergy [kJ/kg]	a, i	intermediate state between isosteric heating and desorption
HS	heat source	cond	condenser
h	enthalpy [kJ/kg]	des	desorption
h_{fg}	latent heat of evaporation [kJ/kg]	DS	dual-stage
MOFs	metal organic frameworks	ha	humid air
ML	modified Langmuir	HS	heat source
m	mass [kg]	i	inlet
P	pressure [kPa]	o	outlet or thermodynamic dead state
Q	thermal energy [kJ]	pw	produced liquid water
$Q_{H,least}$	least thermal energy requirement [kJ]	sat	saturation
Q_{st}	isosteric heat of adsorption/desorption [kJ/kg]	v	vapor
RH	relative humidity [%]	w	liquid water
R_a	air gas constant [kJ/kg-K]		
R_o	specific gas constant [kJ/kg-K]		
SGs	silica gels		
S	entropy [kJ/kg-K]		
T	temperature [K/°C]		
VC	vapor compression		
WPP	water production potential [L/kg/day]		
w	adsorption uptake [kg/kg]		
W_{least}	least work requirement [kJ/kg]		
Subscripts		Superscripts	
1-2	isosteric heating	m_{ML}	heterogeneity factor of modified Langmuir [-]
		n	structural heterogeneity parameter or D-A fitting constant [-]
		0	zero coverage
		Greek letters	
		η_I	first law efficiency [-]
		η_{II}	second law efficiency [-]
		ω	humidity ratio [kg/kg]
		$\tilde{\omega}$	vapor mole fraction ratio [-]

density, rainfall, and likewise [14–16]. In order to access this plentiful freshwater source, there is a dire need of reliable atmospheric water harvesting (AWH) technology.

Current AWH technologies can be segregated into active and passive systems. The active AWH systems required an external source of energy for producing potable water. Some common types of active AWH systems may include vapor compression (VC), thermoelectric cooling, and membrane based system [17,18]. Such systems have significant water production potential (WPP) ranging between 15 and 2000 L/day from civil to industrial scales, however facing limitation of huge EC [19]. On the other hand, passive AWH systems are solely powered by solar energy without the need of any external energy source or other high-grade power. Some common types of passive systems may include fog, dew and adsorption-based AWH technology [17]. The fog and dew systems are constrained by climate dependency, less WPP and thermal efficiency [20,21]. In this regard, adsorption-based AWH technology getting huge interest because of its potential to operate with solar energy or low-grade heat source [22]. The adsorption based AWH technology is aims to collect water-vapors from ambient air by means of adsorbent material. Once the adsorbent achieves saturation condition, desorption energy is supplied that could be achieve by solar, wind and low-grade waste heat to release the water-vapors [23,24]. The extensive details of both active and passive systems can be found from [17,25].

Indeed, the adsorbent material is a key component for the success of adsorption-based AWH systems. In literature, different kinds of adsorbents have been explored including silica-gels (SGs) [26–28], zeolites [29,30], ionogels [31,32], polymer [33,34], membrane [35] and metal-organic frameworks (MOFs) [30,36] for producing potable water. Such adsorbents have been incorporated in both open and close cycle based systems to perform single adsorption/desorption and condensation cycle

[37,38]. For instance, Essa et al. [26] investigated SG based AWH system and results concluded that SG has water production potential (WPP) of 0.4 L/kg/day at adsorption temperature (T_{ads}) between 28 and 39 °C, adsorption relative humidity (RH_{ads}) of 62%, desorption temperature (T_{des}) of 72.5 °C, and condenser temperature (T_{cond}) between 38 and 45 °C. Sleiti et al. [39] investigated orange SG based system and concluded that the SG has WPP of 0.8 L/kg/day at T_{ads} of 22 °C, RH_{ads} between 30 and 60% and T_{cond} of 35 °C. LaPotin et al. [29] investigated AQSOA-Z01 (zeolite) based AWH system and concluded that the AQSOA-Z01 has WPP of ~0.65 L/m²/day at T_{ads} of 20 °C, RH_{ads} of 68% and T_{des} of 78 °C. Qi et al. [31] evaluated iongel based AWH system and results concluded that the ionogel has WPP of 2.8 L/m²/day at T_{ads} of 25 °C, and RH_{ads} of 80%. Guo et al. [33] hygroscopic polymer films and concluded that the polymer has WPP of ~5.5 L/kg/day at RH_{ads} between 11 and 42%. Kim et al. [35] evaluated nanofibrous membrane based AWH system and concluded that the membrane observed adsorption capacity of 0.96 kg/kg at RH_{ads} of 30%. Similarly, recent study [30] summarized MOF-based AWH systems and concluded that WPP by mostly MOFs ranging from 0.25 L/kg/day to ~6 L/kg/day. On the other hand, LaPotin et al. [29] introduced dual-stage configuration that aims to utilize two adsorbent beds and recover condensation heat for desorption process, thereby increase WPP from 0.65 L/m²/day to 0.77 L/m²/day and overall thermal efficiency [29]. Despite the advancements in material science, the AWH systems are facing significant challenges from viewpoints of their key performance metrics including low WPP, high EC up to 23,000 kJ/kg and low first (η_I) and second law (η_{II}) efficiencies [40–42]. The main reasons for low WPP, high EC, low η_I and η_{II} may include discrepancies between design and practical conditions and poor-designed operational parameters like T_{ads} , T_{des} and T_{cond} [37]. Additionally, the adsorption equilibrium and kinetics are critical

for performance evaluation of hydrophilic adsorbents in AWH application which is different mechanism when compared to conventional heavy metals adsorption and wastewater treatment [43–45]. This motivates the need for robust understanding of thermodynamic limits of adsorbents and system's operational parameters.

Thermodynamic analysis plays a crucial role to identify thermodynamic limits and optimal operational parameters to optimize the WPP, EC η_I and η_{II} . In this perspective, different methodological concepts have been investigated including Monte Carlo simulation [46,47] and thermodynamic modeling [42,48–50] framework for the performance evaluation of both open and close cycle based AWH system. It has been observed that the thermodynamic modeling framework based on the first and second law of thermodynamics, given and developed by Kim et al. [48] showed extraordinary results due to its simplicity and efficiency. The modeling framework assumes a close cycle AWH system in which internal recirculation of saturated air from condenser can be used to achieve desired desorption RH. The authors validated their developed modeling framework with experiments and concluded that the framework increases thermal efficiency of the system by 2–3 folds as compared to experiments. The authors stated that the thermodynamic modeling framework could be used as a benchmark for different adsorbents materials to evaluate or optimize the performance of AWH systems. Recently, Rao et al. [42] investigated the performance of different

adsorbents by assuming open cycle AWH system in which ambient air is used for acquiring desorption RH and validated their results with [48].

In this regard, the study utilizes similar thermodynamic modeling framework given by Kim et al. [48] to evaluate performance of silica-gel, zeolite, ionogel, polymer, membrane and MOF based ten kinds of emerging adsorbents for the AWH systems. The modeling framework comprises of Dubinin–Astakhov (D-A) and Modified Langmuir (ML) models and governing steady state equations. Performance of each adsorbent is evaluated from perspectives of water production potential (WPP), (EC), first (η_I) and second law (η_{II}) efficiencies. After that, the study performs parametric analyses to evaluate performance variability among each studied adsorbent with respect to different operational parameters including T_{ads} , RH_{ads} , T_{des} , RH_{des} , and T_{cond} . Furthermore, both η_I and η_{II} for the VC and dual-stage AWH systems are evaluated and compared with single-stage system.

2. Adsorption-based atmospheric water harvesting (AWH) systems

Single-stage adsorption-based AWH system comprises of an adsorption and desorption beds, a heat source (HS) and a condenser which executes the adsorption of water-vapors from air with closed loop desorption and water generation processes, respectively. A generalized

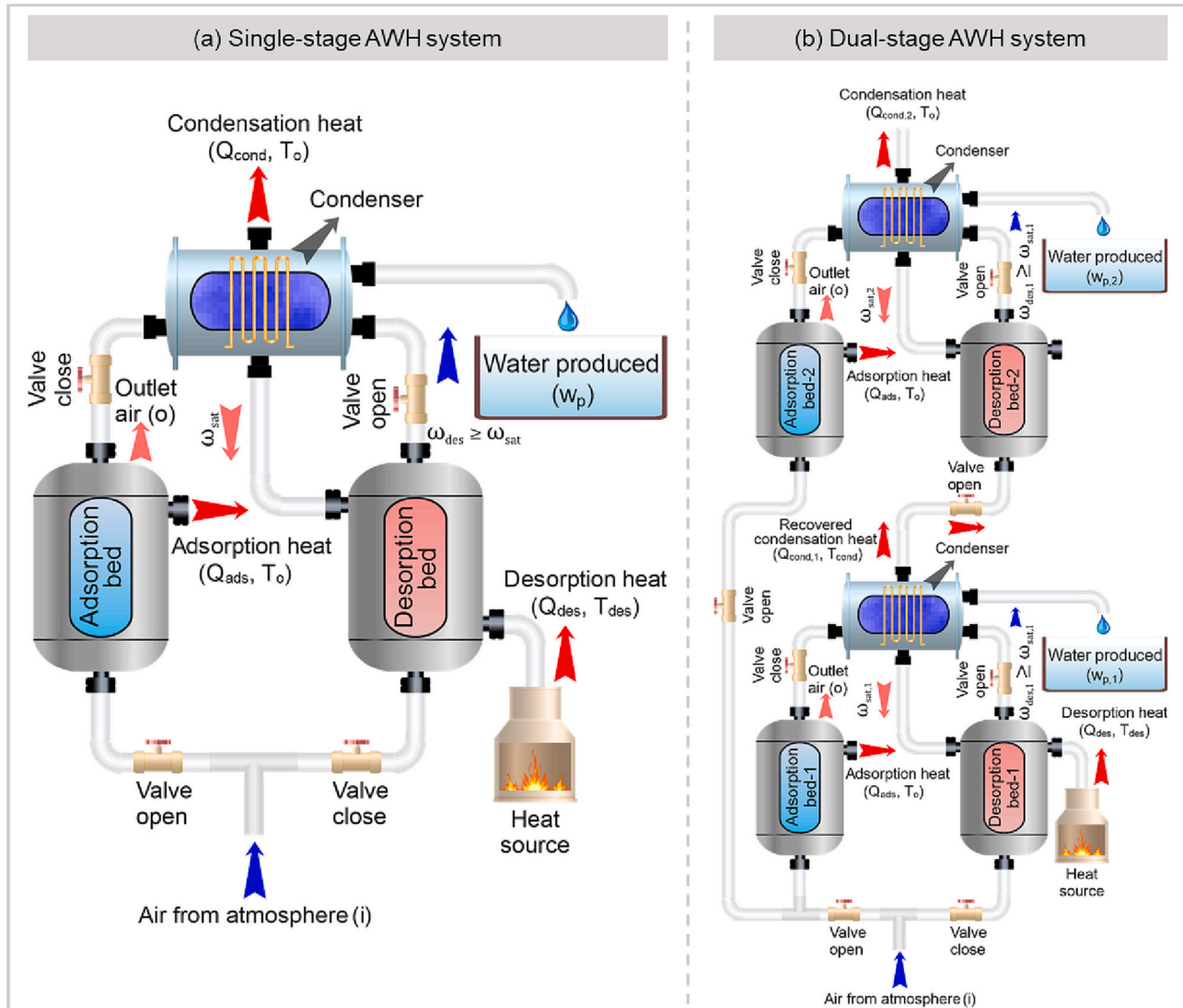


Fig. 1. Working schematic of single-stage (left) and dual-stage (right) adsorption-based AWH system.

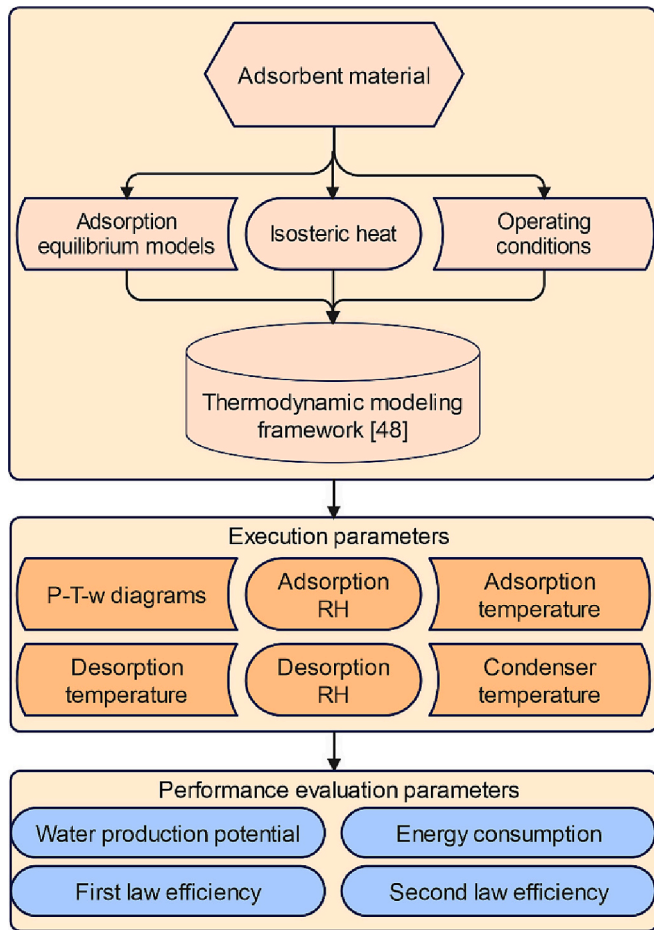


Fig. 2. A flow chart representing the summary of research methodology executed in this study.

working schematic of the single-stage AWH system is shown in Fig. 1(a). Adsorbent is a key component of the AWH system which can perform both adsorption and desorption process under certain sets of operating conditions including temperatures and pressures. High temperatures and pressures are typically favorable for the desorption while low are suitable for the adsorption. During adsorption process, the adsorbent captures water-vapors from atmospheric air because of its high affinity towards water-vapors and presence of strong hydrogen bonding during chemisorption and weak van der Waals forces during physisorption, thereby adsorption heat (Q_{ads}) is released owing to exothermic process. It is worth mentioning that the amount of water-vapors adsorbed by the adsorbent depends on its adsorption equilibrium, thermophysical properties, and operating conditions. During desorption process, saturated adsorbent is subjected to desired T_{des} powered by the HS for breaking the hydrogen bonding and van der Waals forces. In the end, desorb water-vapors are subjected to the condenser to condense water-vapors by capturing desorption heat (Q_{des}) and rejecting condensation heat (Q_{cond}) for production of liquid water.

The primary purpose of dual-stage configuration of the AWH system is to increase water production and efficiency of the system by reducing thermal energy input per generated cooling load. In literature, the cascaded or dual-stage configuration with two or more adsorbent beds has been studied for heat pump applications [51,52]. In such configuration, thermal energy rejected during the adsorption process from bed-1 is recovered and employed for the desorption of bed-2 to increase system's thermal efficiency. On the other hand, the AWH system entails adsorption of water-vapors under ambient conditions specifically with low T_{ads} and humidities, making it challenging to recover the Q_{ads} .

However, if the condensation and water production is eventuated at higher temperature the Q_{cond} can be harvested and recovered for the desorption of bed-2 owing to availability of high T_{des} . Fig. 1(b) shows working schematic of dual-stage configuration of the AWH system with adsorption, desorption, water production, and condensation heat recovery processes. It is worth mentioning that the mass of bed-2 should be smaller than bed-1 which can be operated at low T_{des} and enthalpy of adsorption for the feasibility of Q_{cond} recovery.

3. Materials and methods

Fig. 2 shows a flow chart representing the summary of research methodology executed in this study. The research methodology consists of two processes namely: water-vapor adsorption equilibrium and thermodynamic modeling framework. The extensive details of each process can be found in following sub-sections.

3.1. Adsorbent materials

In this study, silica-gel, zeolite, ionogel, polymer, membrane and MOF based ten kinds of adsorbents are studied for adsorption-based AWH systems. The studied adsorbents include (1), RD SG [53], (2) AQSOA-Z01 [54], (3) Syloid 72FP + 57 wt% EMIM-Ac [32], (4) PS-II [34] (5) GO-SSNF [35] (6) MOF-801 [55], (7) alum fumarate [55], (8) NH_2 -UiO-66 [56] (9) MIL-100(Fe) [55], and (10) MIL-101(Cr) [57]. The thermophysical properties, SEM images and crystal structures of studied adsorbents are listed in Table 1. It has been reported that about two-thirds of the world experiencing $RH \leq 50\%$ [58]. The studied adsorbents can achieve most of the water vapors at $RH \leq 50\%$ followed by different shapes of isotherms as shown in Fig. 3.

3.2. Water-vapor adsorption equilibrium

The well-known Dubinin–Astakhov (D-A) model given by Eq. (1) [70] was used for the evaluation of adsorption equilibrium data for RD SG [53], AQSOA-Z01 [54], Syloid 72FP + 57 wt% EMIM-Ac [32], PS-II [34], and GO-SSNF [35].

$$w = w_{max} \exp \left[- \left(\frac{R_o T}{E} \ln \left(\frac{P_{sat}}{P} \right) \right)^n \right] \quad (1)$$

where, w , w_{max} , R_o , T , E , P_{sat} , P , and n represents adsorption equilibrium [kg/kg], maximum adsorption uptake [kg/kg], specific gas constant [kJ/kg/K], temperature [K], characteristic energy [kJ/kg], saturation pressure [kPa], vapor pressure [kPa], and D-A surface heterogeneity constant [-], respectively.

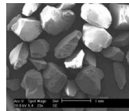
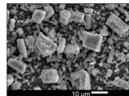
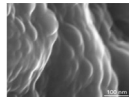
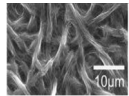
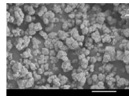
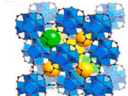
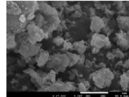
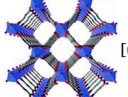
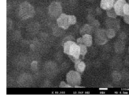
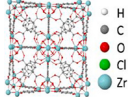
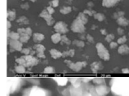
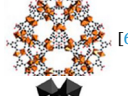
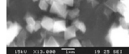
The Modified Langmuir (ML) model given by Eq. (2) [55] was used for the evaluation of adsorption equilibrium data for MOF-801 [55], alum fumarate [55], NH_2 -UiO-66 [56], MIL-100(Fe) [55], and MIL-101(Cr) [57].

$$w = w_{max} \frac{\left[\alpha \exp \left(\frac{m_{ML} (Q_{at}^0 - h_{fg})}{R_o T} \right) \right] \left(\frac{P}{P_{sat}} \right)^{m_{ML}}}{1 + \left[\alpha \exp \left(\frac{m_{ML} (Q_{at}^0 - h_{fg})}{R_o T} \right) - 1 \right] \left(\frac{P}{P_{sat}} \right)^{m_{ML}}} \quad (2)$$

where, α , m_{ML} , Q_{at}^0 , and h_{fg} represents pre-exponential coefficient of ML [-], heterogeneity factor of ML [-], isosteric heat of adsorption/desorption at zero coverage [kJ/kg], and enthalpy of evaporation [kJ/kg], respectively. The associated fitting parameters of both models are obtained from the cited literature and furnished in Table 2. It is worth mentioning that the study calculates the fitting parameters of GO-SSNF by using curve fit function from SciPy Python library. Due to unavailability of the adsorption equilibrium data at higher temperatures for GO-SSNF, the study utilizes available data for the D-A modeling at higher temperatures. Similar approach was also adopted in literature [59].

The Clausius–Clapeyron relationship given by Eq. (3) [71,72] is used

Table 1
Thermophysical properties, SEM image, and crystal structure of studied adsorbents.

Sr #	Adsorbents*	Thermophysical properties						SEM image	Crystal structure	Reference
		Pore size [nm]	Pore volume [cm ³ /g]	Surface area [m ² /g]	Average pore diameter [nm]	Bulk density [g/cm ³]	Thermal conductivity [W/m K]			
Silica-gel										
1	RD SG	6	0.345	686.3	3.19	1	0.14	 [59]	–	[53,60]
Zeolite										
2	AQSOA-Z01	0.74	0.087	132	1.2	–	0.2	 [29]	–	[54,61]
Ionogel										
3	Syloid 72FP + 57 wt% EMIM-Ac	10-15	1.2	–	13	–	0.221	 [32]	–	[32,62]
Polymer										
4	PS-II	–	–	–	19,316	0.82-0.85	–	–	–	[34]
Nanofibrous membrane										
5	GO–SSNF	–	–	–	1000	–	–	 [35]	–	[35]
Metal-organic frameworks (MOFs)										
6	MOF-801	500	0.45	1100	0.48-0.74	–	–	 [41]	 [63]	[55,64]
7	Alum fumarate	1.091	0.93	792.3	–	–	0.13	 [65]	 [66]	[65,66]
8	NH ₂ -UiO-66	–	0.44	979.2	1.9	–	0.93	 [56]	 [56]	[67]
9	MIL-100(Fe)	2.5-2.9	1.0	1917	0.55-0.88	0.16-0.35	0.207	 [59]	 [68]	[55]
10	MIL-101(Cr)	2.312	1.59	3402.69	–	–	–	 [57]	 [57]	[69]

* Adsorption equilibrium isotherm details of the studied adsorbents are provided in Fig. 3.

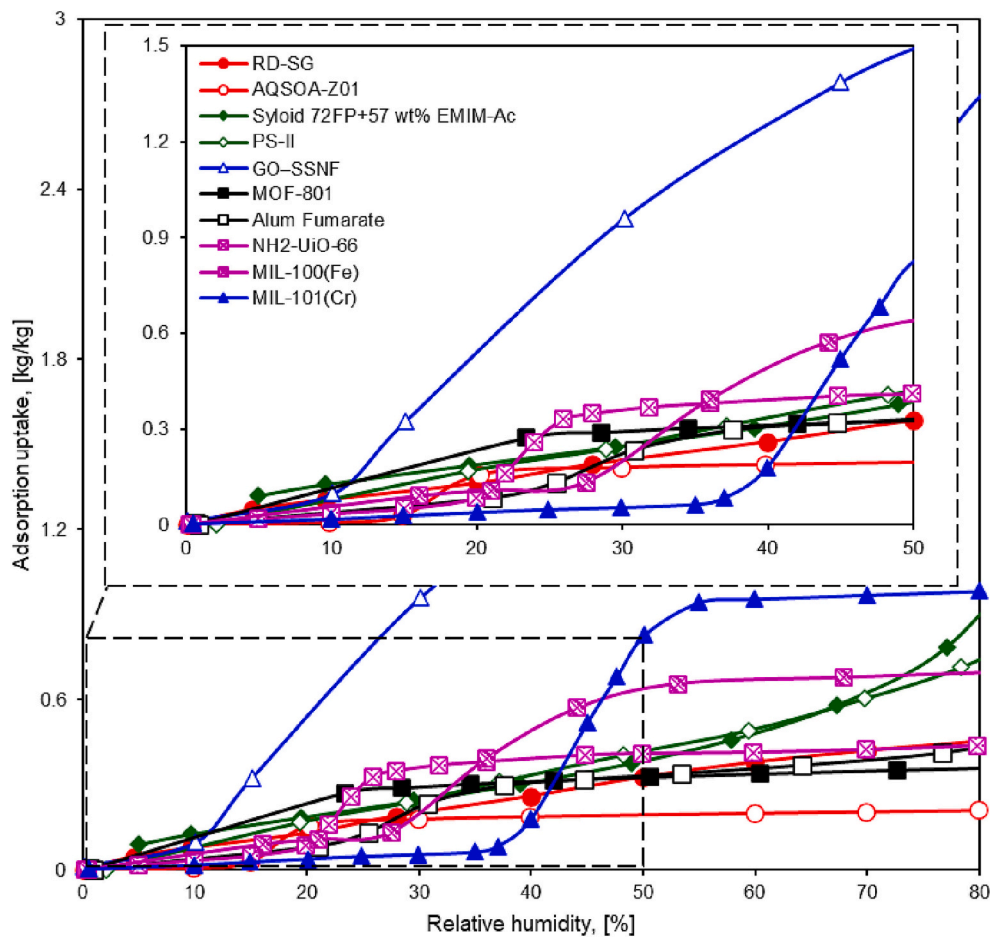


Fig. 3. Adsorption isotherm profiles of the studied RD SG [53], AQSOA-Z01 [54], Syloid 72FP + 57 wt% EMIM-Ac [32], PS-II [34], GO-SSNF [35] and MOFs [55–57]. The isotherm data are obtained from the cited literature at 25 °C, however, at 30 °C in case of PS-II, MOF-801, alum fumarate, and MIL-100(Fe), as per availability.

Table 2

D-A and ML fitting parameters for studied adsorbents taken from cited literature.

Sr #	Adsorbents	D-A parameters			ML parameters				Reference
		w _{max} [kJ/kg]	E [kJ/kg]	n [-]	w _{max} [kJ/kg]	Q _{st} ⁰ [kJ/kg]	α [-]	m [-]	
Silica-gel (SG)									
1	RD-SG	0.5046	185.18	1.21	–	–	–	–	[53]
Zeolite									
2	AQSOA-Z01	0.21	222.1	5.0	–	–	–	–	[54]
Ionogel									
3	Syloid 72FP + 57 wt% EMIM-Ac	32.20	1.04	0.20	–	–	–	–	[32]
Polymer									
4	PS-II	1.76	41.84	0.50	–	–	–	–	[34]
Nanofibrous membrane									
5	GO-SSNF	3.10	132.42	1.25	–	–	–	–	[35]
Metal-organic frameworks (MOFs)									
6	MOF-801	–	–	–	0.35	2906.63	3 × 10 ⁻²	2.27	[55]
7	Alum fumarate	–	–	–	0.47	2794.30	4 × 10 ⁻²	1.98	[55]
8	NH ₂ -UiO-66	–	–	–	0.41	2601.8	9.49 × 10 ⁻¹	6.30	[56]
9	MIL-100(Fe)	–	–	–	0.71	2734.83	1 × 10 ⁻²	4.65	[55]
10	MIL-101(Cr)	–	–	–	1.00	2670	6.75 × 10 ⁻⁴	9.55	[57]

for estimating isosteric heat of adsorption/desorption.

$$Q_{st} = -R_o \left[\frac{\partial \ln(P)}{\partial \left(\frac{1}{T}\right)} \right]_w \quad (3)$$

3.3. Thermodynamic modeling framework

The study uses the dedicated thermodynamic modeling framework developed by Kim et al. [48] due to its simplicity and correctness. The modeling framework is based on the first and second law of thermodynamics to be used for the evaluation of AWH adsorbents. The study executes the thermodynamic modeling framework in Python programming language. Psychrometric properties of the adsorbate water are obtained from the Python library CoolProp [73] validated by [74] with ASHRAE standards. Four processes of isosteric heating (process 1-2) given by Eq. 4(a), desorption (process 2-3) given by Eq. (4b), isosteric cooling (process 3-4) given by Eq. (4c), and isobaric adsorption (process 4-1) given by Eq. (4d) are involved for executing AWH cycle [48].

$$\frac{Q_{1-2}}{m_{pw}} = \left[\frac{1}{W} (C_{p,ad}) + C_{p,w} \right] \int_{T_1}^{T_2} dT \quad (4a)$$

$$\frac{Q_{2-3}}{m_{pw}} = \left[\frac{1}{W} (C_{p,ad}) + C_{p,w} \right] \int_{T_2}^{T_3} dT + \frac{1}{\omega_{sat}} \int_{\omega_{sat}}^{\omega_{des}} (C_{p,a} + \omega_{sat} C_{p,v}) d\omega + \int_{T_{cond}}^{T_3} dT + h_{ads} \quad (4b)$$

$$\frac{Q_{3-4}}{m_{pw}} = \left[\frac{1}{W} (C_{p,ad}) \right] \int_{T_4}^{T_3} dT \quad (4c)$$

$$\frac{Q_{4-1}}{m_{pw}} = \left[\frac{1}{W} (C_{p,ad}) + C_{p,w} \right] \int_{T_1}^{T_4} dT + h_{ads} \quad (4d)$$

where, subscripts pw, ad, w, des, sat, a, v, cond, and ads indicate produced water, adsorbent, water, desorption, saturation, air, condenser, and adsorption respectively. Q/m_{pw} indicates thermal energy input per mass of produced water [kJ/kg], W adsorbent uptake [kg/kg], C_p is specific heat capacity [kJ/kg-K], T is temperature [K], ω is humidity ratio [kg/kg], and h refers to enthalpy [kJ/kg], respectively. For simplicity, C_p of studied adsorbents is taken as unity.

It is worth mentioning that an integral method given by Eq. (5) [48] is used for evaluation of desorption outlet humidity ratio (ω_{des}) during desorption process.

$$\omega_{des} = \frac{\int_{T_{a,i}}^{T_{des}} \omega(RH_{des}, T) dT}{T_{des} - T_{a,i}} \quad (5)$$

where, subscripts des, and a, i denote desorption and intermediate state between isosteric heating and desorption processes. RH denotes relative humidity [%]. The ω_{des} is estimated by integrating along constant line of RH and divided by difference between desorption and intermediate state temperatures. More details about the integral method are presented in Appendix A (Fig. A1). Ultimately, the integral method provides reasonable average ω_{des} . Similar approach has been utilized in literature [42,48].

Consequently, the study investigates four performance parameters for the adsorption-based AWH system namely (i) water production potential (WPP) per cycle and its geospatial context using above mentioned adsorption equilibrium models (see Eq. (1-2)), (ii) energy consumption (EC) given by Eq. (6) [48], (iii) first law efficiency (η_I) given by Eq. (7a) [48], and (iv) second law efficiency (η_{II}) given by Eq. (7b) [48], respectively [48].

$$EC = \frac{Q_{1-2}}{m_{pw}} + \frac{Q_{2-3}}{m_{pw}} \quad (6)$$

$$\eta_I = \frac{h_{fg}}{EC} \quad (7a)$$

$$\eta_{II} = \frac{Q_{H,least}}{EC} \quad (7b)$$

where, EC, η_I , h_{fg} , η_{II} , and $Q_{H,least}$ denote energy consumption [kJ/kg], first law efficiency [-], latent heat of vaporization [kJ/kg], second law efficiency [-], and least energy requirements [kJ/kg], respectively. For geospatial context of WPP, 10 cycles/day is assumed for each studied adsorbent. It is worth mentioning that the modeling framework used in this study does not involve thermal conductivity, diffusivity, parasitic heat loss and fan power to circulate the air vapor mixtures towards the absorption/desorption beds for the evaluation of the EC. The $Q_{H,least}$ given by Eq. (8) [48] is evaluated for the adsorption-based AWH system.

$$\frac{Q_{H,least}}{m_{pw}} = \left[\frac{1}{\omega_i - \omega_o} (e_o - e_i) + e_{pw} \right] \left(1 - \frac{T_o}{T_{HS}} \right)^{-1} \quad (8)$$

where, subscripts i, o, and HS indicate inlet, outlet or dead state, and heat source, respectively. e represents specific flow exergy [kJ/kg]. The term $(1 - T_o/T_{HS})^{-1}$ represents the carnot efficiency while the term under brackets represents least work requirements (W_{least}) per kg of water. In order to evaluate the $Q_{H,least}$, specific flow exergy of humid air (e_{ha}) given by Eq. (9a) [75] and produced liquid water (e_{pw}) given by Eq. (9b) [75] should be considered.

$$e_{ha} = (C_{p,a} + \omega C_{p,v}) T_o \left[\frac{T}{T_o} - 1 - \ln \left(\frac{T}{T_o} \right) \right] + (1 + 1.608\omega) R_a T_o \ln \left(\frac{P}{P_o} \right) + R_a T_o \left[\ln \left(\frac{1 + 1.608\omega_o}{1 + 1.608\omega} \right) + 1.608\omega \ln \left(\frac{1.608\omega(1 + 1.608\omega_o)}{1.608\omega_o(1 + 1.608\omega)} \right) \right] \quad (9a)$$

$$e_{pw} = (h - h_o)_{pw} - T_o (S - S_o)_{pw} \quad (9b)$$

where R_a , P , h , and S refer to air gas constant [0.287 kJ/kg-K], pressure, enthalpy [kJ/kg], and entropy [kJ/kg-K], respectively. For comparison point of view the study evaluates first law efficiency given by Eq. (10a) [48], and second law efficiency given by Eq. (10b) [48] for VC based AWH system.

$$\eta_{I,vc} = \frac{h_{fg}}{Q_{vc}} \quad (10a)$$

$$\eta_{II,vc} = \frac{Q_{H,least}}{Q_{vc}} \quad (10b)$$

where, Q_{vc} indicate thermal energy input per kg of water by vapor compression system [kJ/kg]. In case of VC system, the study assumes endo reversible heat engine to supply heat energy that operate between T_{HS} and ambient temperatures to produce liquid water. Coefficient of performance (COP) of such system can be taken as 5 as reported by [76]. Consequently, the Q_{vc} can be calculated Eq. (11) [48].

$$\frac{Q_{vc}}{m_{pw}} = \left[\frac{1}{\omega_i - \omega_o} (C_{p,a} + \omega_i C_{p,v}) (T_i - T_o) + h_{fg} \right] COP^{-1} \left[\left(1 - \frac{T_o}{T_{HS}} \right)^{0.5} \right]^{-1} \quad (11)$$

Additionally, the study evaluates both first and second law efficiencies of studied adsorbents for dual-stage configuration of adsorption-based AWH system and compared with the single-stage system. The dual-stage first ($\eta_{I,DS}$) and second ($\eta_{II,DS}$) law efficiencies are evaluated by Eq. (12a-12b) [48], respectively.

$$\eta_{I,DS} = \left(1 + \frac{m_{pw,2}}{m_{pw,1}}\right) \eta_I \quad (12a)$$

$$\eta_{II,DS} = \left(1 + \frac{m_{pw,2}}{m_{pw,1}}\right) \eta_{II} \quad (12b)$$

where, subscript DS indicate dual-stage. The $m_{pw,2}/m_{pw,1}$ represents mass ratio of produced water by adsorbent bed-1 and bed-2. It is worth mentioning that due to difference in h_{ads} and h_{fg} the mass of adsorbent bed-2 should be less than the bed-1 which can be computed by Eq. (13) [48].

$$\frac{m_{pw,2}}{m_{pw,1}} = \frac{Q_{cond}}{m_{pw,1}} \bigg/ \frac{Q_{des,2}}{m_{pw,2}} \quad (13)$$

where, subscripts 1 and 2 indicate bed-1 and bed-2, respectively. $Q_{cond}/m_{pw,1}$ represents condensation heat rejected per kg of water by the bed-1 [kJ/kg] and $Q_{des,2}/m_{pw,2}$ represents desorption energy consumption per kg of water by the bed-2 [kJ/kg]. The condensation heat rejected and EC by the bed-1 and bed-2 can be evaluated by Eq. (14) and Eq. (15), respectively.

$$\frac{Q_{cond}}{m_{pw,1}} = \frac{1}{\int_{\omega_{sat}}^{\omega_{des}} d\omega} (C_{p,a} + \omega_{des} C_{p,v}) \int_{T_{cond}}^{T_3} dT + h_{fg} \quad (14)$$

$$\frac{Q_{des,2}}{m_{pw,2}} = \left[\frac{1}{W} (C_{p,ad}) + C_{p,w} + \frac{1}{\int_{\omega_{sat,2}}^{\omega_{des,2}} d\omega} (C_{p,a} + \omega_{sat,2} C_{p,v}) \right] \times \int_{T_{1,2}}^{T_{3,2}} dT + h_{ads} \quad (15)$$

4. Results and discussions

SG, zeolite, ionogel, polymer, membrane, and MOF based ten kinds of adsorbents (Table 1) are evaluated by means of thermodynamic modeling framework (heading 3.3) for the AWH systems. The study aims to evaluate water production potential (WPP), energy consumption (EC), first (η_I) and second law (η_{II}) efficiencies. After that, parametric analyses are discussed from viewpoints of key operational parameters including adsorption temperature (T_{ads}), adsorption relative humidity (RH_{ads}), desorption temperature (T_{des}), desorption relative humidity (RH_{des}), and condenser temperature (T_{cond}), respectively in order to highlight the performance variability among studied adsorbents. For comparison point of views, both η_I and η_{II} for vapor-compression (VC) based AWH system are evaluated and compared with the single-stage system. Additionally, both η_I and η_{II} for dual-stage system are evaluated and compared with the single-stage system. Following are detailed analyses of each category.

4.1. P-T-w diagrams

Fig. 4 presents the thermodynamic cycle on P-T-w diagram for each studied adsorbent using ideal cycle concepts of single-stage adsorption-based AWH system at T_{ads} of 25 °C, RH_{ads} of 50%, T_{des} of 100 °C, and RH_{des} of 10%. Among studied adsorbents, Syloid 72FP + 57 wt% EMIM-Ac, GO-SSNF and MIL-101(Cr) exhibit w_{max} of 2.73 kg/kg/cycle, 1.60 kg/kg/cycle and 0.87 kg/kg/cycle, respectively.

On the other hand, w_{min} is observed of 1.18 kg/kg/cycle, 0.06 kg/kg/cycle, and 0.001 kg/kg/cycle, respectively. The w_{max} and w_{min} for other studied adsorbents ranging from 0.21 to 0.63 kg/kg/cycle and 0.001 to 0.08 kg/kg/cycle, respectively. A quick overview of pressure ranges during the thermodynamic cycle of the AWH system corresponds to the operating conditions at different T_{ads} up to 100 °C are presented in Appendix A (Fig. A2).

4.2. Water production potential

The WPP is evaluated for studied adsorbents using Eq. (1) and Eq. (2)

with respect to T_{ads} of 25 °C, RH_{ads} of 50%, T_{des} of 100 °C, and RH_{des} of 10%. The results are presented in Fig. 5. The Syloid 72FP + 57 wt% EMIM-Ac, GO-SSNF, and MIL-101(Cr) enables maximum WPP of 1.55 kg/kg/cycle, 1.53 kg/kg/cycle, and 0.87 kg/kg/cycle which is 2.4 to 7.4 folds higher as compared to other studied adsorbents. Thereby, geo-spatial context of WPP on monthly basis is evaluated for these adsorbents by assuming passive device that can provide T_{des} of 100 °C to perform multiple adsorption/desorption cycles per day. Herein, the study assumes 72 min for adsorption and 72 min for desorption cycle to perform 10 cycles per day [77]. Ambient temperature and relative humidity data on monthly basis for 2021 is obtained from [78]. The results of WPP for Syloid 72FP + 57 wt% EMIM-Ac, GO-SSNF, and MIL-101(Cr) are presented in Fig. 6, Fig. 7, and Fig. 8). It can be noticed that partially humid to foggy regions ($RH = 40$ -100%) as well as ships over the Ocean are highly conducive in the WPP in whole year. On the other hand, relatively less WPP is observed in the extremely arid ($RH \leq 20\%$) to semi-arid regions ($RH = 20$ -30%). The WPP of Syloid 72FP + 57 wt% EMIM-Ac, GO-SSNF, and MIL-101(Cr) is ranging from 12 to 150 L/kg/day, 11 to 31 L/kg/day, and 4.5 to 9.9 L/kg/day, respectively in partially humid to foggy regions throughout the year. However, the WPP is ranging from 5.3 to 12 L/kg/day, 4 to 11 L/kg/day and 0.01 to 4.5 L/kg/day in extremely arid to semi-arid regions, respectively.

4.3. Energy consumption

The EC by each studied adsorbent is evaluated using Eq. (6) and the results are presented in Fig. 9. Among studied adsorbents, minimum EC of 4214.96 kJ/kg_w/cycle is observed by the Syloid 72FP + 57 wt% EMIM-Ac as compared to GO-SSNF (4348.06 kJ/kg_w/cycle), and MIL-101(Cr) (4499.84 kJ/kg_w/cycle). On the other hand, MOF-801 possesses maximum EC of 4874.89 kJ/kg_w/cycle which is ~1.6 folds higher as compared to the Syloid 72FP + 57 wt% EMIM-Ac. It is because higher values of mass of produced water results in higher denominator values, thereby decreasing the overall EC. Furthermore, high enthalpy of adsorption results in higher EC and vice versa. In order to evaluate most influencing parameters on the EC, sensitivity analysis is also performed with the choice of Syloid 72FP + 57 wt% EMIM-Ac and results are presented in Appendix A (Fig. A3). It has been observed that besides enthalpy of adsorption, decrease in RH_{des} , and T_{cond} results in lower EC.

4.4. First and second law efficiencies

The first (η_I) and second law (η_{II}) efficiencies of single-stage adsorption-based AWH system for each studied adsorbent are evaluated using Eq. (7a) and Eq. 7(b). The results are provided in Fig. 10. Among studied adsorbents, the Syloid 72FP + 57 wt% EMIM-Ac, GO-SSNF, MIL-101(Cr) is capable to achieve maximum η_I of 0.54, 0.52 and 0.50, respectively while η_{II} of 0.21, 0.20, and 0.19, respectively because of maximum WPP and minimum EC. On the other hand, the MOF-801 achieves minimum η_I and η_{II} of 0.46 and 0.18, respectively. The AQSOA-Z01 observed η_I and η_{II} of 0.49 and 0.19, respectively. However, Kim et al. [48] reported both η_I and η_{II} of 0.32 and 0.17, respectively for MOF-801 at T_{des} of 100 °C. Similarly, Feng et al. [58] reported η_I of 0.25 and 0.41 for MOF-801 and AQSOA-Z01, respectively at T_{des} of 120 °C. The deviations in both η_I and η_{II} of the studied adsorbents is observed due to their different adsorption equilibrium nature and thermophysical properties. Since the results of both η_I and η_{II} are based on same operating conditions for each studied adsorbent, therefore small variations are observed. In this regard, the study performs parametric analyses in order to evaluate most influencing operational parameters on the performance of the AWH systems. Following are the detailed parametric analyses for each studied adsorbent.

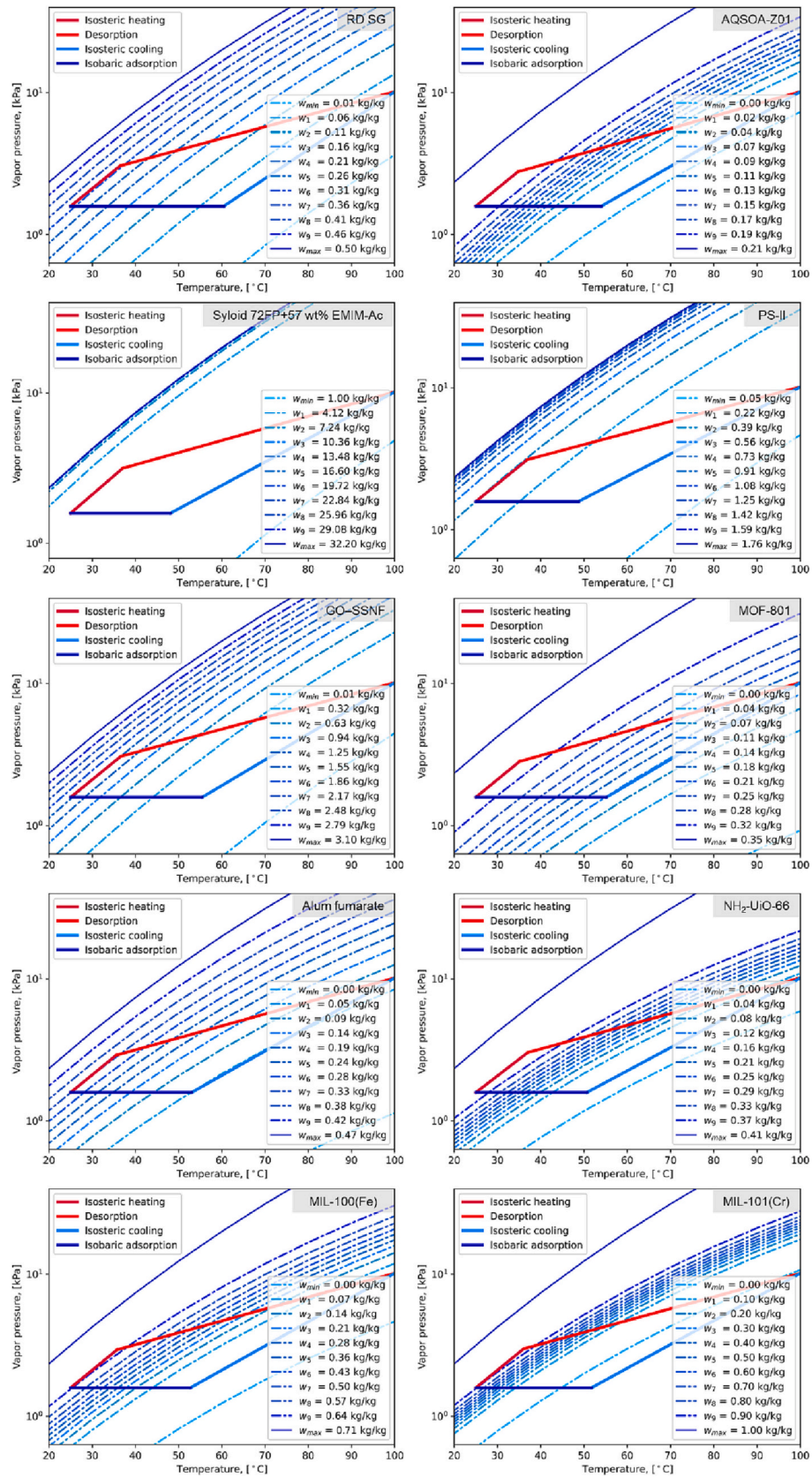


Fig. 4. P-T-w diagrams of studied adsorbents at T_{ads} of 25 °C, RH_{ads} of 50%, T_{des} of 100 °C, and RH_{des} of 10%.

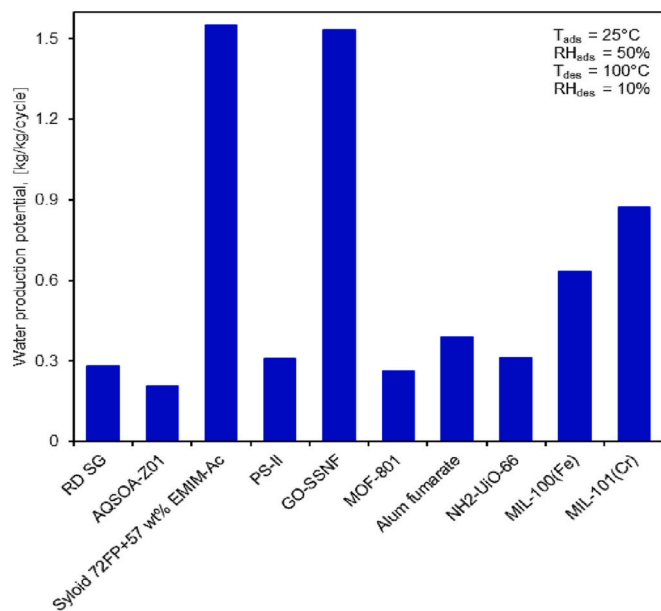


Fig. 5. Comparison of water production potential per cycle among each studied adsorbent.

4.5. Parametric analyses

4.5.1. Effects of adsorption conditions

Effects of T_{ads} and RH_{ads} on the WPP and EC for each studied adsorbent are evaluated. The results are presented in Fig. 11 and Fig. 12. It can be noticed that the WPP by each studied adsorbent shows decreasing trend with the increase in T_{ads} while increasing trend with the increase in RH_{ads} . For instance, the WPP by the Syloid 72FP + 57 wt% EMIM-Ac decreases from 0.58 to 0.48 kg/kg/cycle with respect to T_{ads} increasing from 10 °C to 40 °C while maintaining RH_{ads} of 20%. Similarly, the WPP increases from 0.58 to 3.38 kg/kg/cycle corresponds to varying in RH_{ads} between 20 and 80% while maintaining T_{ads} of 10 °C. Similar trends of the WPP are observed in case of other studied adsorbents. It is important to mention here that the trends of WPP may also depends on type of an adsorption isotherm. For instance, in case of S-shaped isotherm (MIL-101(Cr)), the WPP becomes nearly constant at $RH_{ads} > 50\%$.

Consequently, the EC by each studied adsorbent follows increasing trend with the increase in T_{ads} while it follows decreasing trend with the increase in RH_{ads} . For instance, the EC by the Syloid 72FP + 57 wt% EMIM-Ac increases from 6512.26 to 6548.86 kJ/kg_w/cycle corresponds to increase in T_{ads} from 10 to 40 °C while maintaining RH_{ads} of 20%. Similarly, the EC decreases from 6512.26 to 6449.57 kJ/kg_w/cycle corresponds to increase in RH_{ads} from 20 to 80% while maintaining T_{ads} of 10 °C. Similar trends are observed in case of other studied adsorbents. It is noticeable that the EC remains constant $RH_{ads} > 50\%$ for most of the studied adsorbents, thereby concluding that the EC is not significantly influenced by higher adsorption uptake.

Additionally, the effect of T_{ads} and RH_{ads} on the η_I and η_{II} for each studied adsorbent is evaluated and results are presented in the Fig. 13 and Fig. 14. It is observable that the η_I for each studied adsorbent follows decreasing trend with the increase in T_{ads} whereas it follows increasing trend with the increase in RH_{ads} . For instance, in case of MOF-801, the η_I decreases from 0.30 to 0.28 with respect to T_{ads} of 10 °C to 40 °C while maintaining RH_{ads} of 20%. Similarly, the η_I increases from 0.28 to 0.30 corresponds to increase in RH_{ads} from 20 to 80% while maintaining T_{ads} of 10 °C. Similar trends of the η_I are observed in case of other studied adsorbents. However, very small variations in η_I are observed at higher RH_{ads} in case of S-shaped adsorbents because of constant adsorption uptake. On the other hand, η_{II} for each studied adsorbent follows increasing trend with the increase in T_{ads} while it follows decreasing

trend with the increase in RH_{ads} . For instance, in case of MOF-801, the η_{II} increases from 0.14 to 0.21 with respect to increase in T_{ads} from 10 to 40 °C while maintaining RH_{ads} of 20%. Similarly, the η_{II} decreases from 0.14 to 0.07 corresponds to varying in RH_{ads} from 20% to 80% while maintaining T_{ads} of 10 °C. Similar trends are observed in case of other studied adsorbents. It implies that the η_{II} for each studied adsorbent is observed maximum in extremely arid to semi-arid regions as compared to humid regions because least work and energy requirements are lower in humid regions. The extended details of least work and energy requirements with respect to T_{ads} and RH_{ads} are presented in Appendix A (Fig. A4).

4.5.2. Effects of desorption conditions

Effects of T_{des} and RH_{des} on the WPP and EC for each studied adsorbent are evaluated and the results are presented in Fig. 15. It is observable that the WPP by each studied adsorbent follows increasing trend with increase in T_{des} while it follows decreasing trend with the increase in RH_{des} . For instance, the WPP by the Syloid 72FP + 57 wt% EMIM-Ac increases from 1.45 to 1.52 kg/kg/cycle with increase in T_{des} from 50 to 100 °C while maintaining RH_{des} of 10%. This is because higher T_{des} desorb more water-vapors from adsorbent bed and are subjected towards condenser. Similarly, the WPP decreases from 1.52 to 1.07 kg/kg/cycle corresponds to increase in RH_{des} from 10 to 25% while maintaining T_{des} of 100 °C. Similar trends of the WPP are observed in case of other studied adsorbents. In case of adsorbents following S-shape isotherms (e.g., AQSOA-Z01 and MOFs except MOF-801), higher RH_{des} does not significantly affect the WPP. In this regard, such type of adsorbents can be regenerated at higher RH_{des} . Consequently, the EC by each studied adsorbent follows decreasing trend with the increase T_{des} , and RH_{des} . For instance, the EC by the Syloid 72FP + 57 wt% EMIM-Ac decreases from 20,710.21 to 4214.96 kJ/kg_w/cycle with the increase in T_{des} from 50 to 100 °C while maintaining RH_{des} of 10%. Similarly, the EC decreases from 4214.96 to 3032.85 kJ/kg_w/cycle corresponds to increase in RH_{des} from 10 to 25% while maintaining T_{des} of 100 °C. Similar trends are observed in case of other studied adsorbents. It implies that higher T_{des} and RH_{des} significantly affect the WPP and overall EC by the AWH system. It is worth mentioning that the WPP and EC trends for each studied adsorbents are plotted with respect to $T_{a,i}$ which varies with RH_{des} for better comparison. The $T_{a,i}$ is the point where RH of heated air equals to RH_{des} of the adsorbent. Furthermore, the overall EC by the AWH system during desorption process involve adsorbent sensible energy, air vapor sensible energy and adsorption enthalpy. In this regard, overall EC is evaluated for each studied adsorbent with respect to the T_{des} and results are presented in Fig. 16. The adsorbent and air vapor sensible energy followed increasing and decreasing trends, respectively with the increase in T_{des} and later stabilize at higher T_{des} results in declining trend of overall EC. For instance, the minimum adsorbent sensible EC by the Syloid 72FP + 57 wt% EMIM-Ac is 54.18 kJ/kg_w/cycle at T_{des} of ~61 °C while the maximum is ~185.90 kJ/kg_w/cycle at T_{des} of 100 °C. Additionally, effect of RH_{des} with respect to RH_{ads} on WPP, and EC for each studied adsorbent are presented in Appendix A (Fig. A5).

Conversally, the maximum air vapor sensible EC is 10,602.60 kJ/kg_w/cycle at T_{des} of 61 °C while the minimum is 885.72 kJ/kg_w/cycle at T_{des} of 100 °C. Consequently, overall EC is 13,068.80 kJ/kg_w/cycle at T_{des} of 61 °C while minimum 3483.62 kJ/kg_w/cycle at T_{des} of 100 °C. Similar trends of EC are identified by other studied adsorbents. It has been observed that the most influencing parameter affecting the EC during one cycle are T_{des} and RH_{des} . Maximum RH_{des} required by an adsorbent consumes minimum EC e.g., RH_{des} of 25% in case of MIL-101 (Cr). Since desorption outlet humidity ratio is evaluated based on integral method (Eq. 5). Due to this method even small increase in RH_{des} causes considerable rise of outlet humidity ratio, thereby resulted in higher T_{cond} which significantly reduce the air vapor sensible energy and overall EC by the system. Although, the EC by the system decreases but

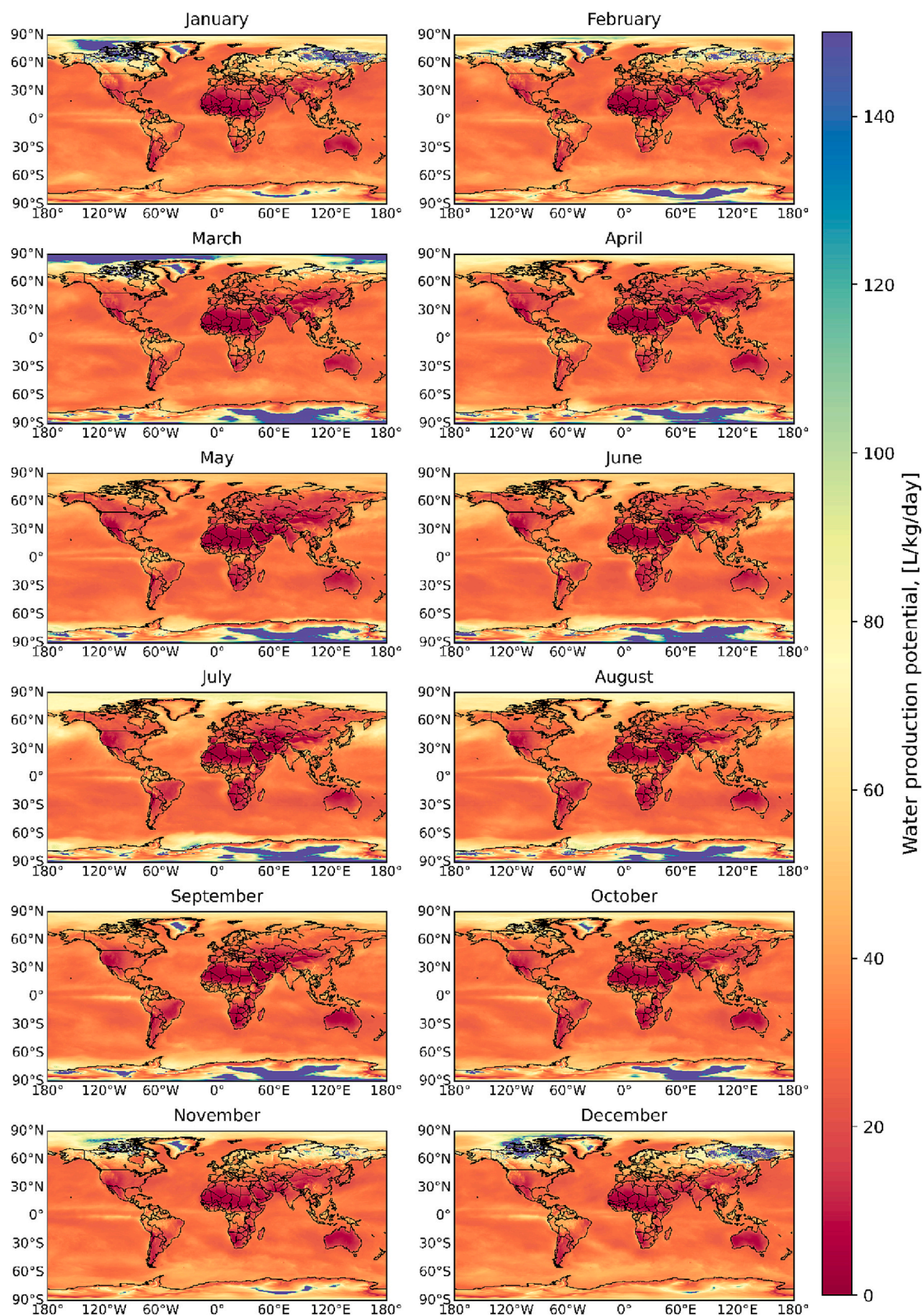


Fig. 6. Geospatial context of water production potential on monthly basis for ionogel-based adsorbent (Syloid 72FP + 57 wt% EMIM-Ac).

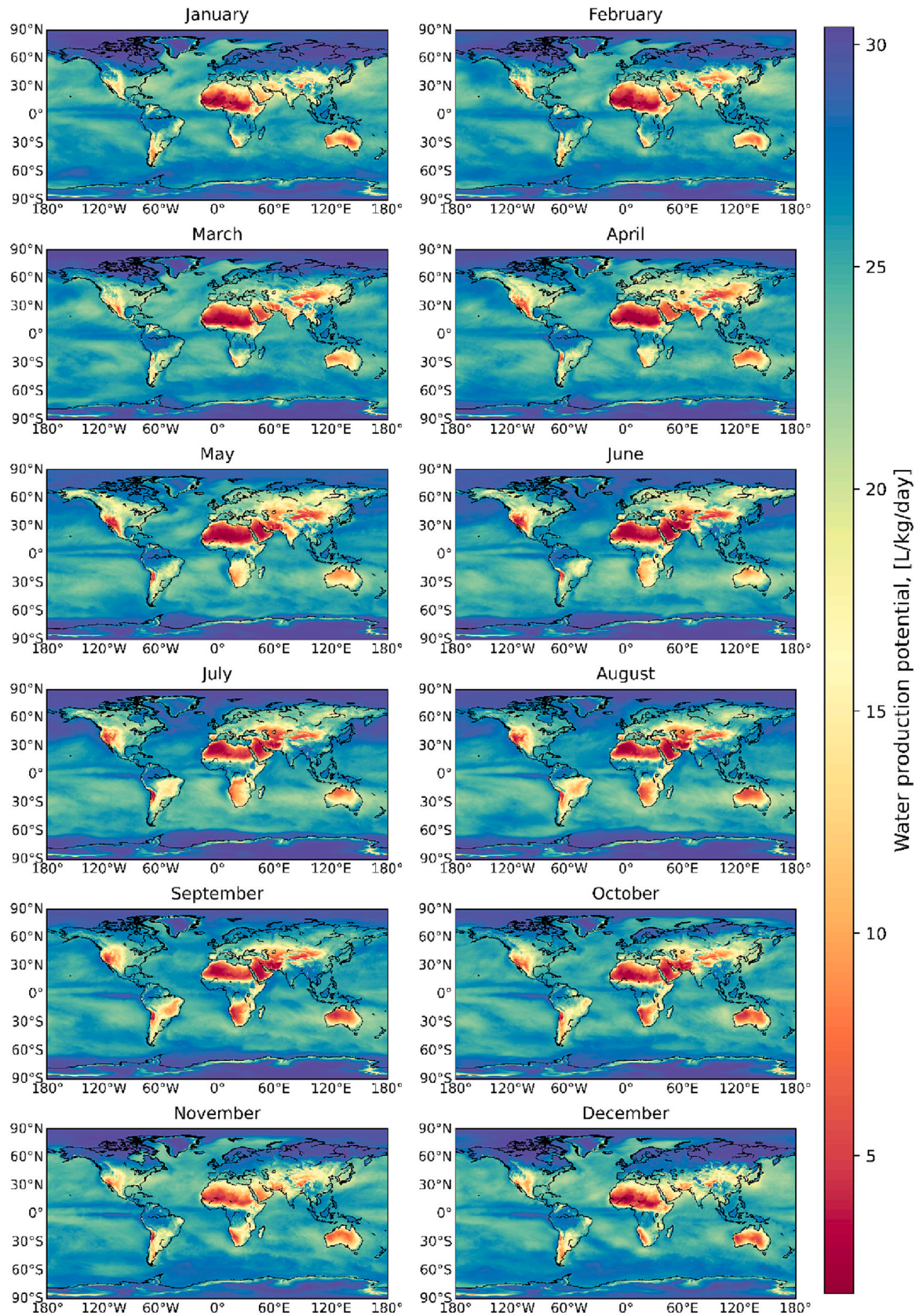


Fig. 7. Geospatial context of water production potential on monthly basis for membrane-based adsorbent (GO-SSNF).

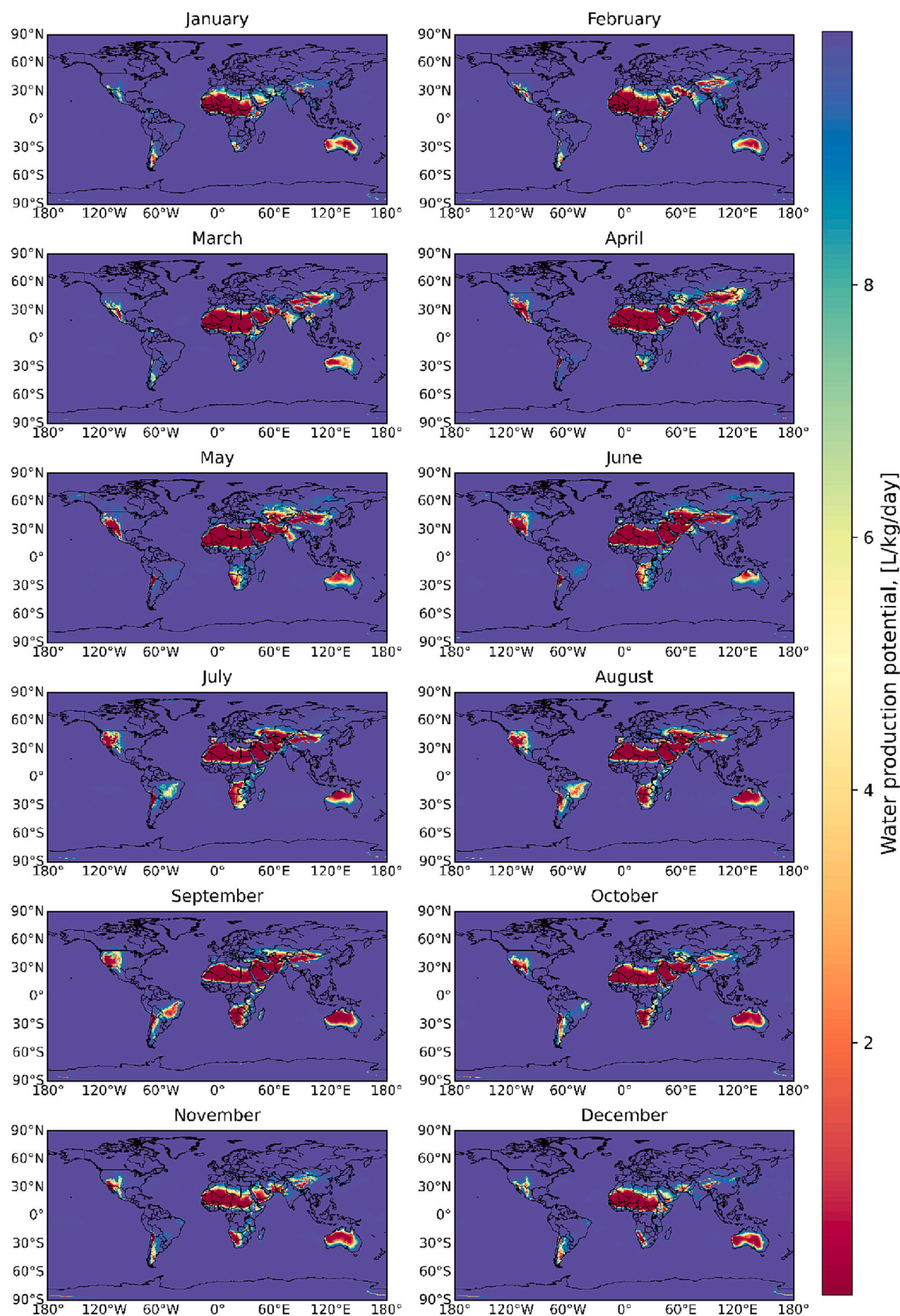


Fig. 8. Geospatial context of water production potential on monthly basis for MOF-based adsorbent (MIL-101(Cr)).

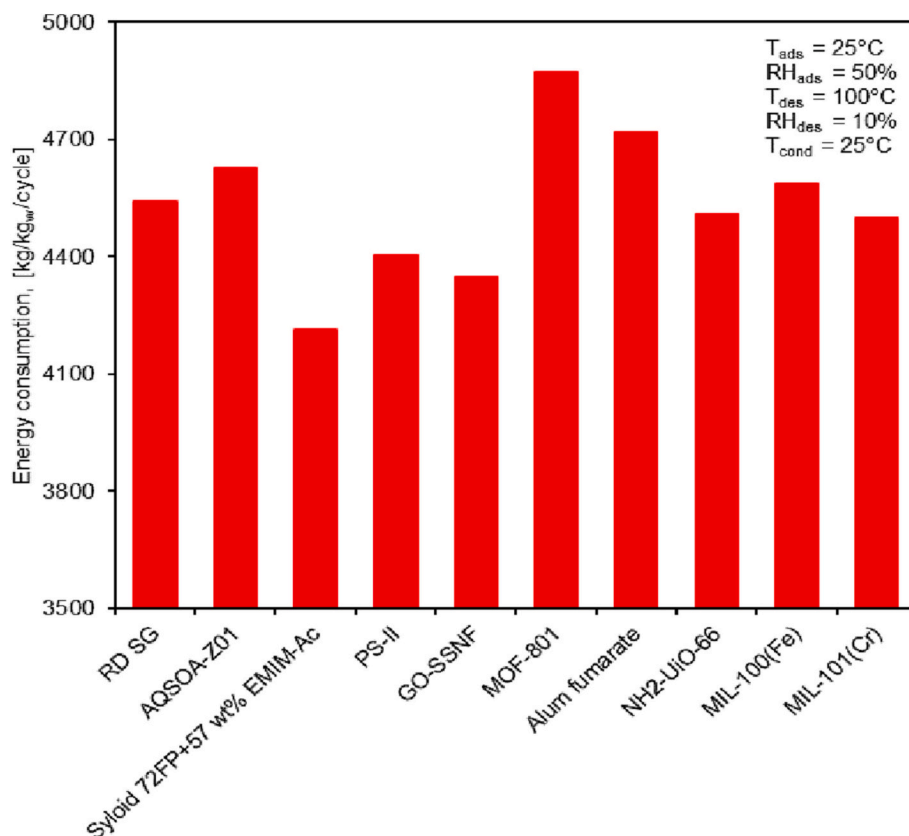


Fig. 9. Comparison of energy consumption per cycle among each studied adsorbent.

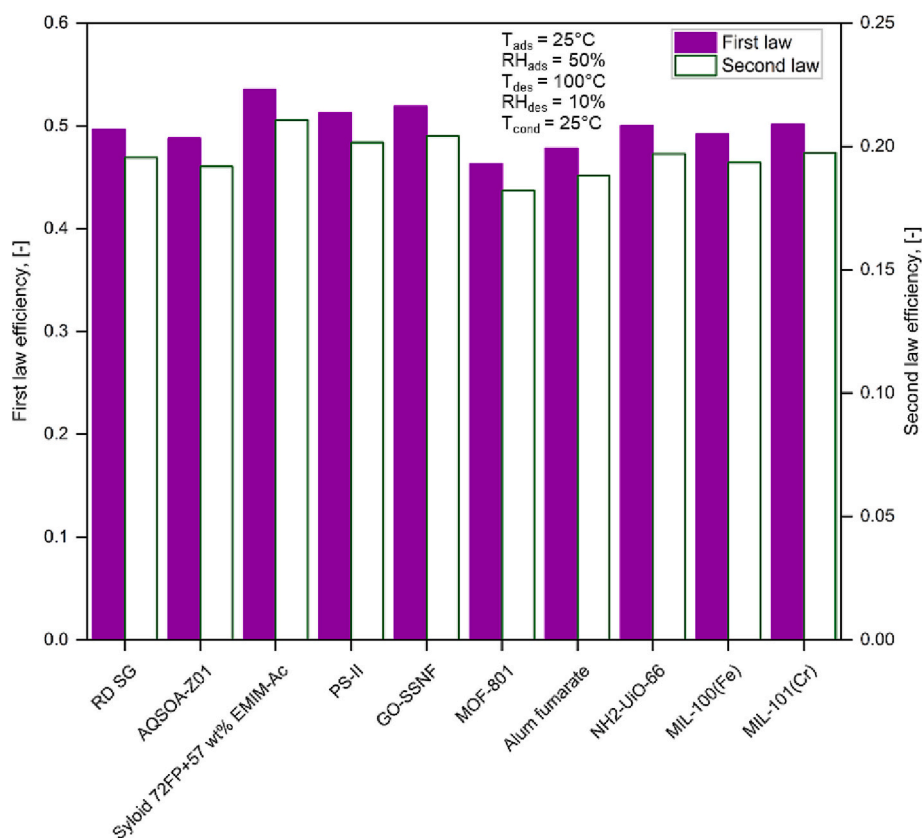


Fig. 10. Comparison of first and second law efficiencies among each studied adsorbent.

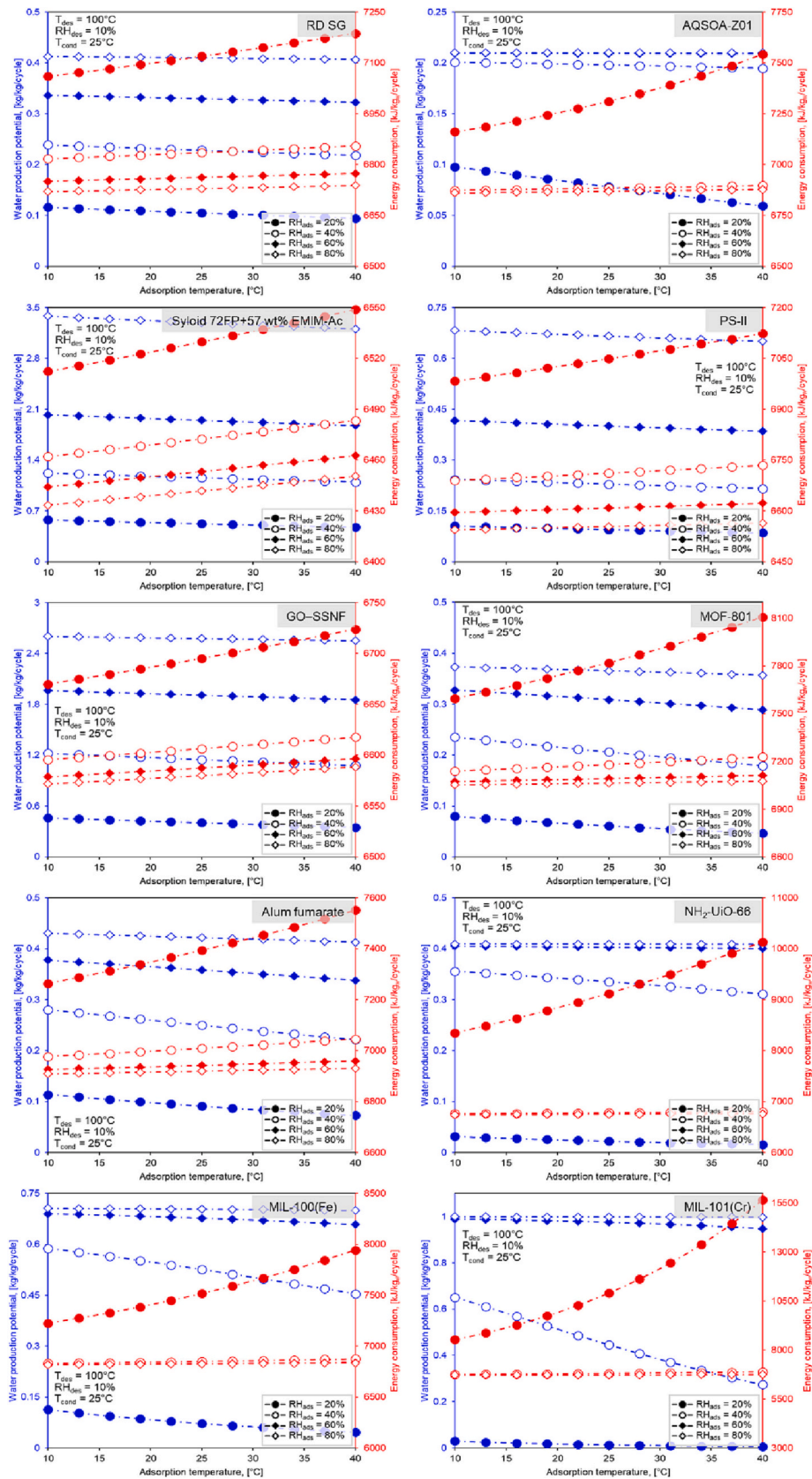


Fig. 11. Effect of adsorption temperature on water production potential and energy consumption for each studied adsorbent at T_{des} of 100 °C, RH_{des} of 10%, and T_{cond} of 25 °C.

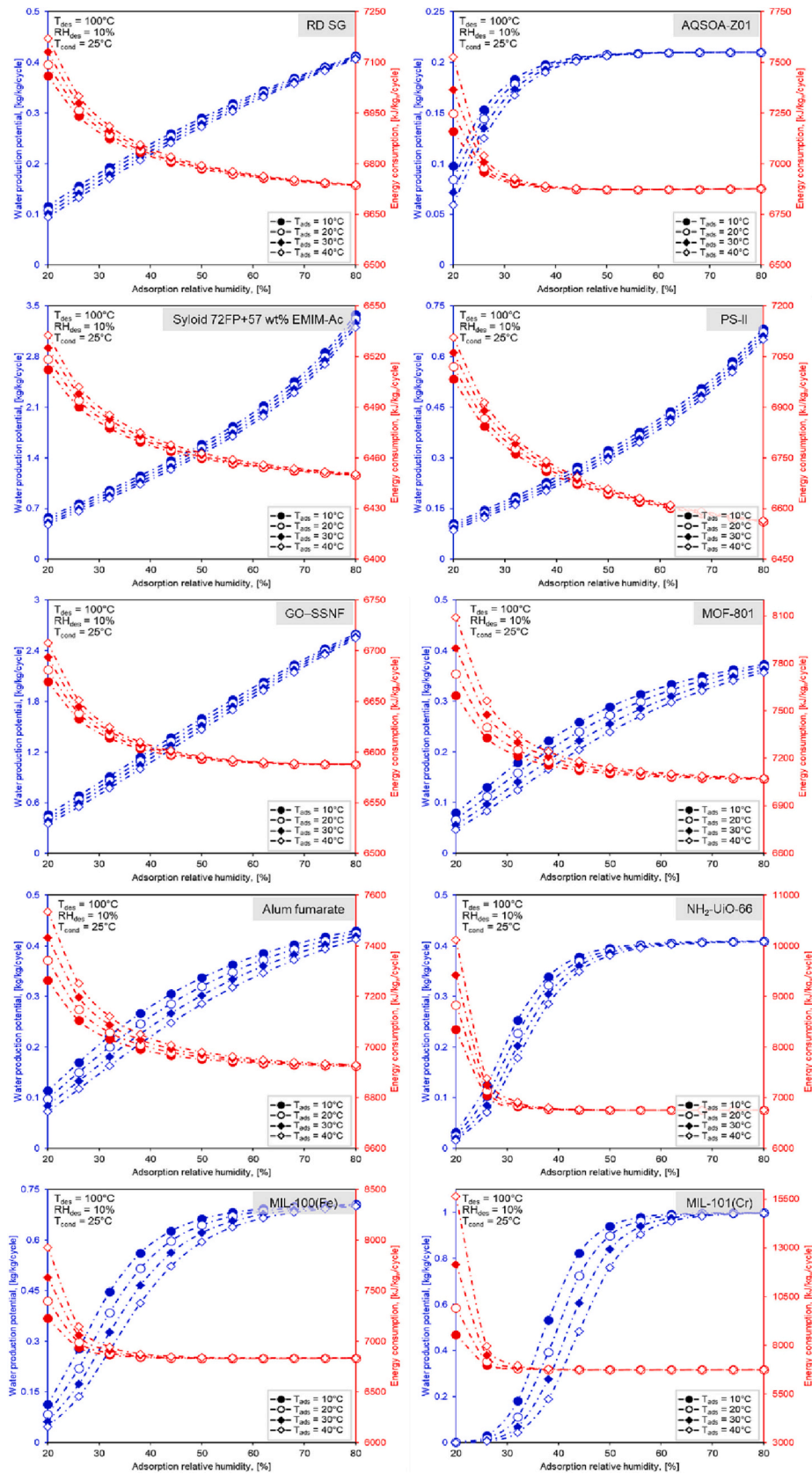


Fig. 12. Effect of adsorption relative humidity on water production potential and energy consumption for each studied adsorbent at T_{des} of 100°C , RH_{des} of 10%, and T_{cond} of 25°C .

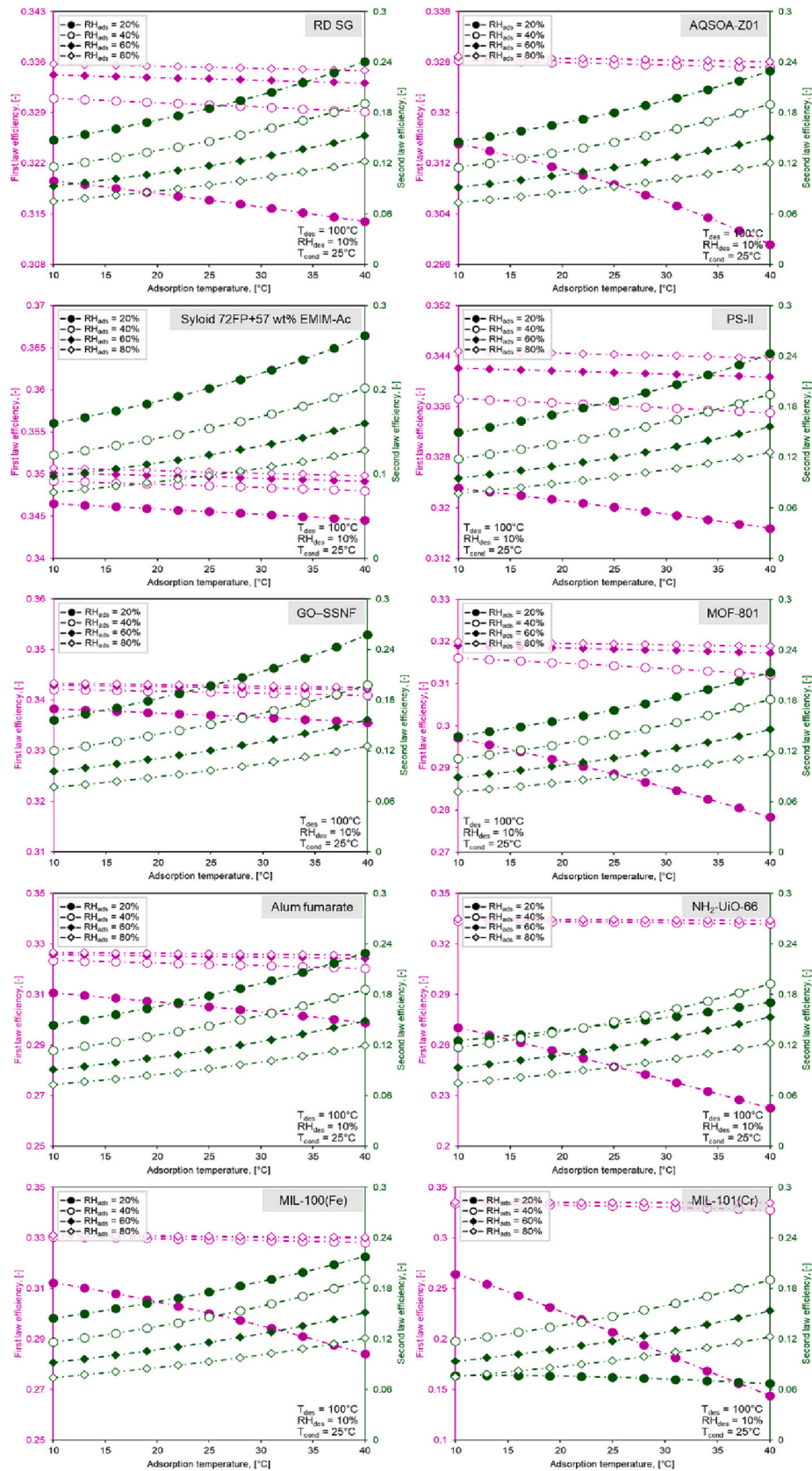


Fig. 13. Effect of adsorption temperature on first and second law efficiencies for each studied adsorbent at T_{des} of 100 °C, RH_{des} of 10%, and T_{cond} of 25 °C.

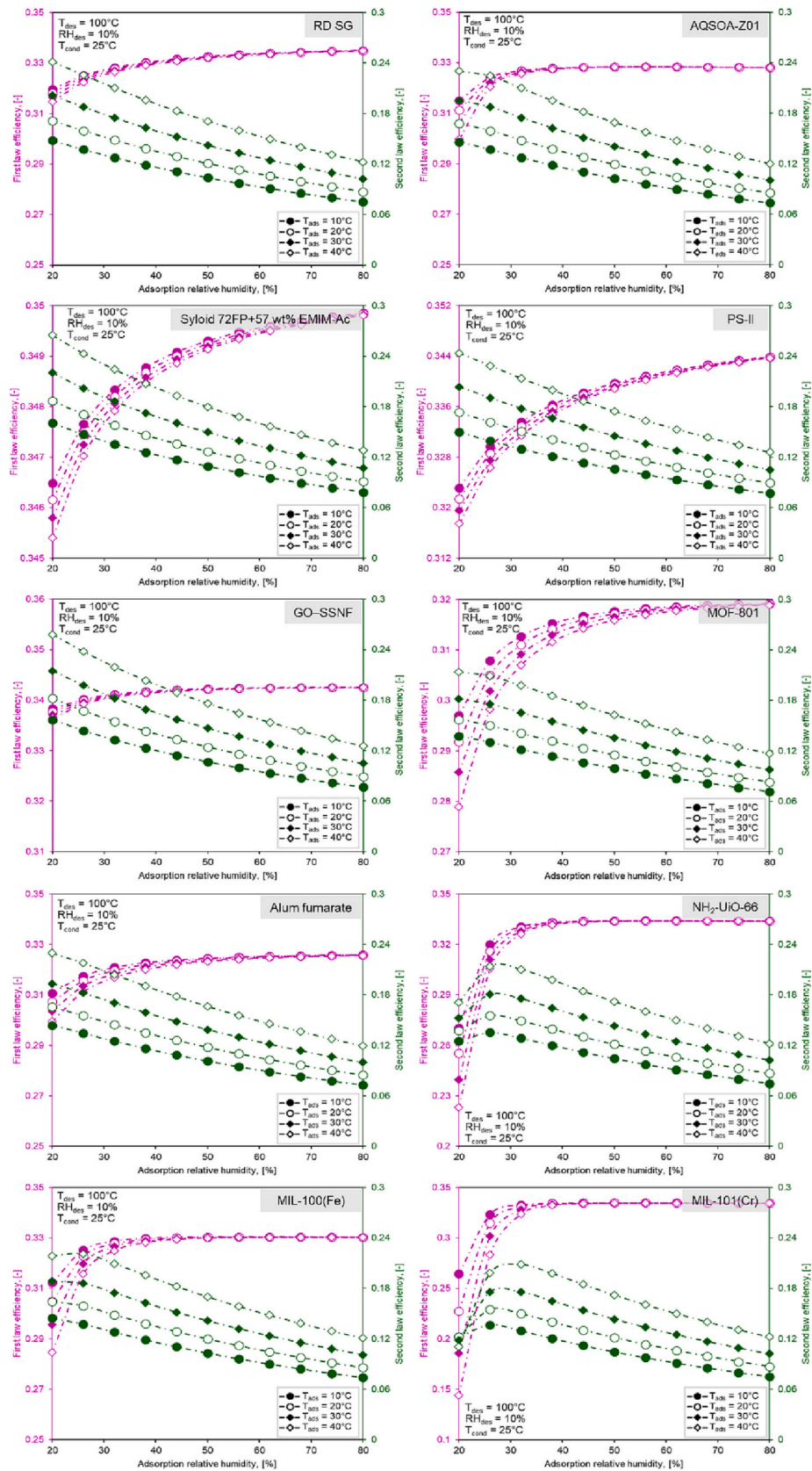


Fig. 14. Effect of adsorption relative humidity on first and second law efficiencies for each studied adsorbent at T_{des} of 100 °C, RH_{des} of 10%, and T_{cond} of 25 °C.

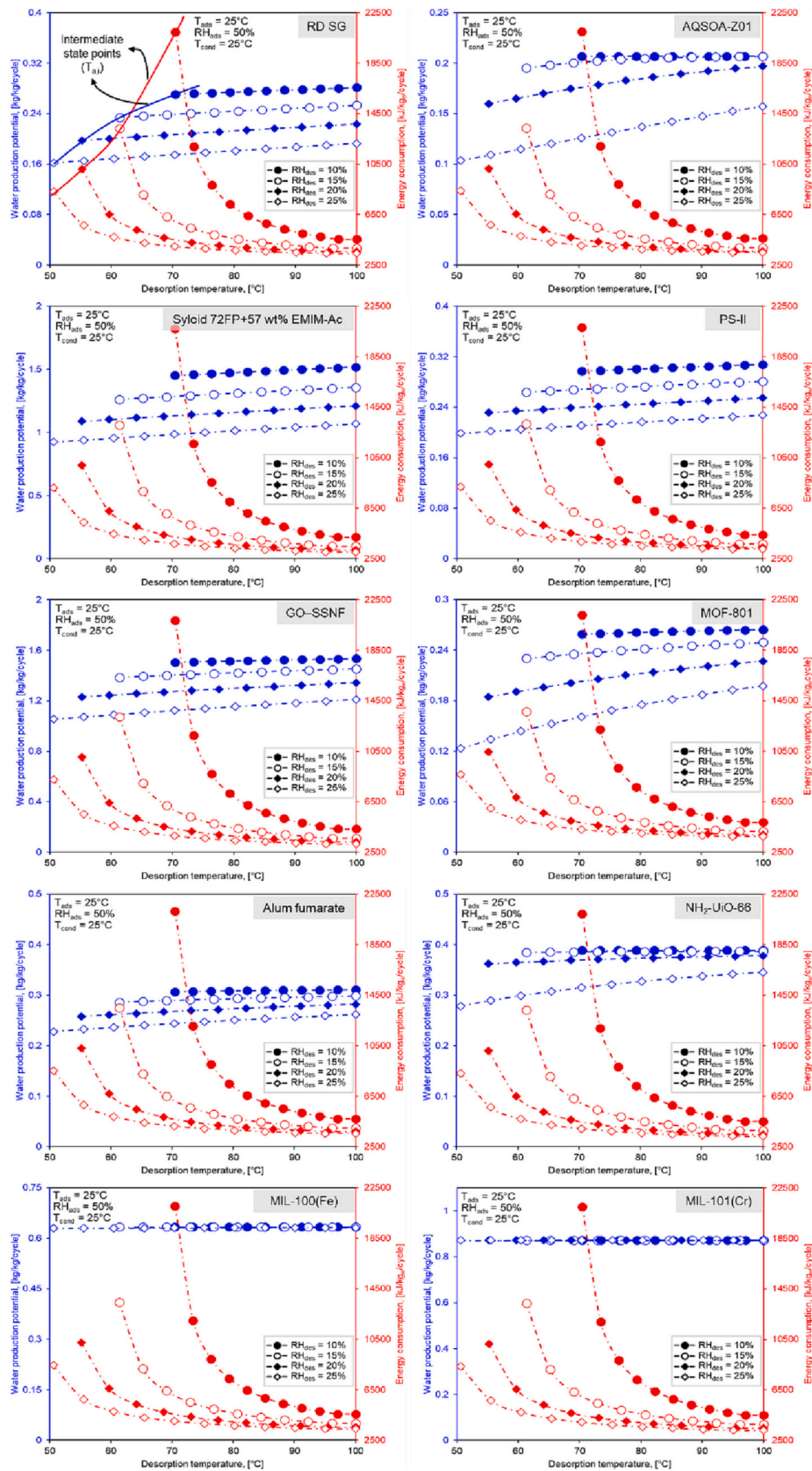


Fig. 15. Effect of desorption temperature on water production potential (WPP) and energy consumption (EC) for each studied adsorbent at T_{ads} of 25 °C, RH_{ads} of 50%, and T_{cond} of 25 °C. The intermediate state temperatures correspond to RH_{des} are indicated by the blue and red solid line joining initial points of WPP and EC. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

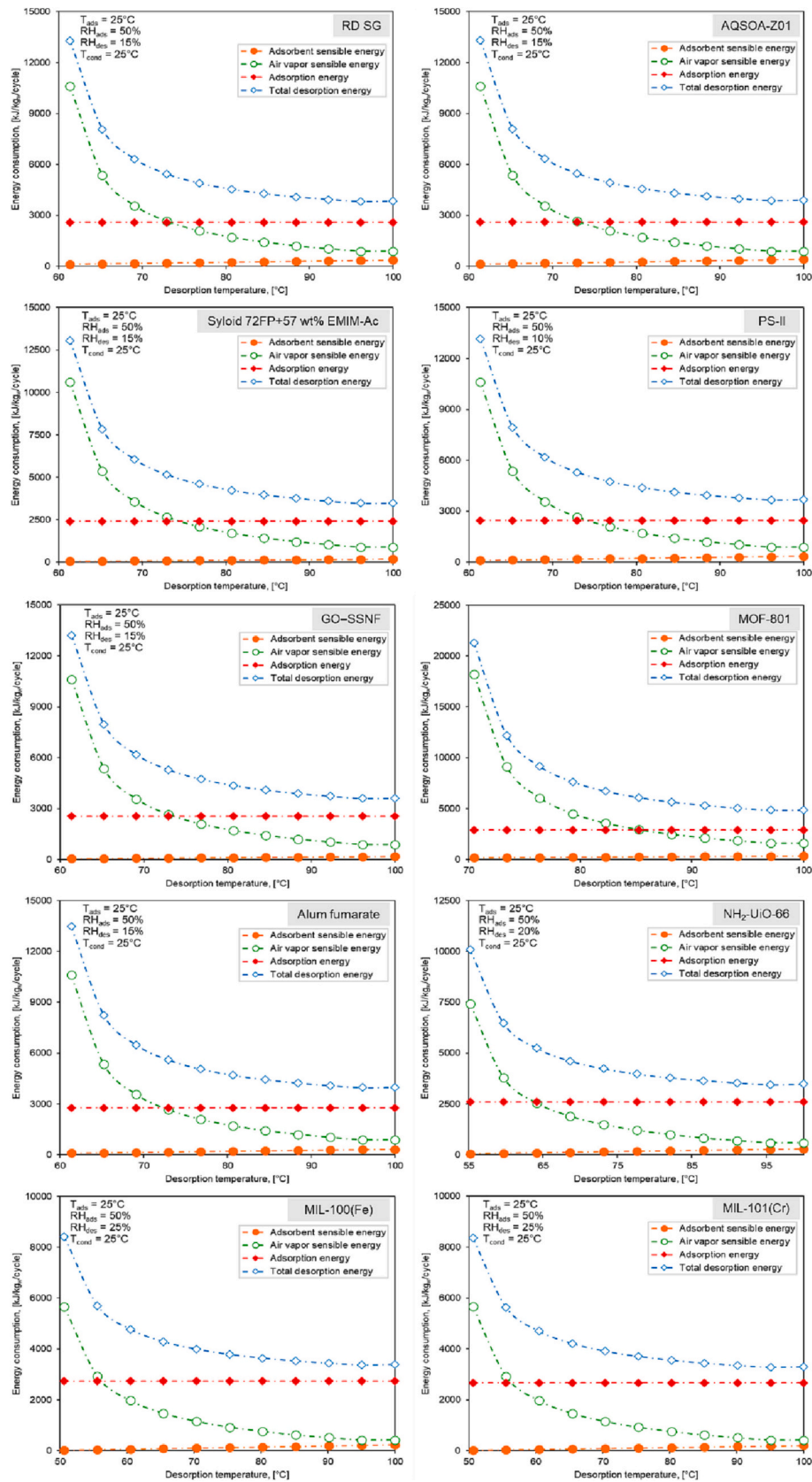


Fig. 16. Effect of desorption temperature on energy consumption for each studied adsorbent at T_{ads} of 25°C , RH_{ads} of 50% , and T_{cond} of 25°C and different RH_{des} for adsorption-based AWH system.

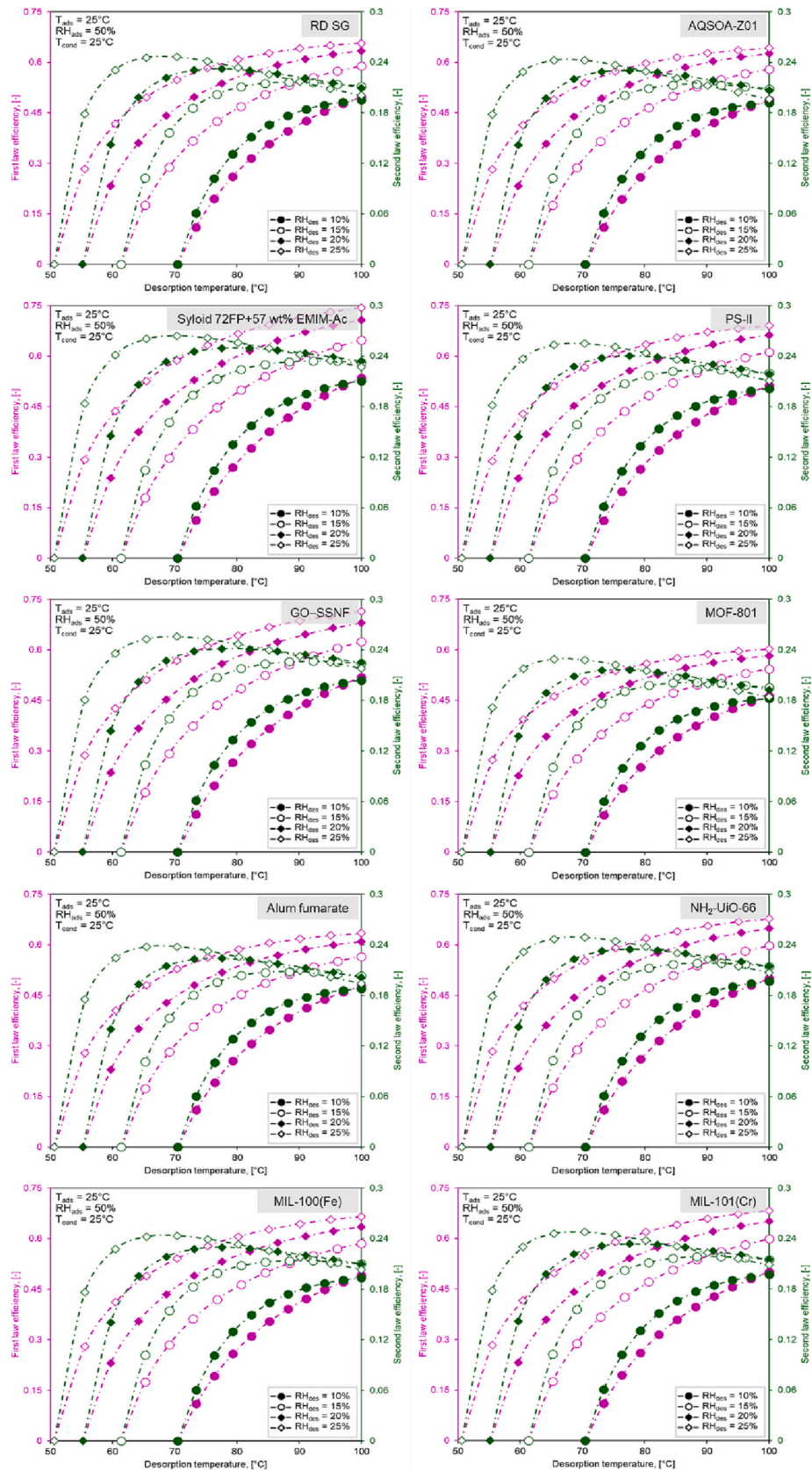


Fig. 17. Effect of desorption temperature and desorption relative humidity on first and second law efficiencies for each studied adsorbent at T_{ads} of 25 °C, RH_{ads} of 50%, and T_{cond} of 25 °C.

stabilize at a non-zero minimum. In this regard, more water is generated and consequently denominator of the EC during desorption process increases while the absolute amount of energy required to desorb that humidity increases the numerator, justifying this tradeoff.

The effect of T_{des} and RH_{des} on the η_I and η_{II} for each studied adsorbent are evaluated and results are presented in Fig. 17. It is observable that the η_I by each studied adsorbent follows increasing trend with respect to increase in T_{des} and RH_{des} while equivalent to zero at $T_{a,i}$. In case of adsorption heat pump systems, once the T_{des} becomes greater than $T_{a,i}$, η_I remains nearly constant [51,79] while in case of AWH system, the η_I follows increasing trend. This is because the system employed air vapor mixture as a working substance, therefore humidity ratio from $T_{a,i}$ to T_{des} follows increasing trend. As a result, total amount of air per mass of produced liquid water requisite to travel through adsorbent bed decreases, thereby enhancing the η_I . For instance, the η_I by the Syloid 72FP + 57 wt% EMIM-Ac increases from 0.20 to 0.54 with increase in T_{des} of 80 to 100 °C while maintaining RH_{des} of 10% resulting in increase of 2.7 folds at 100 °C. Similarly, the η_I increases from 0.54 to 0.74 with the increase in RH_{des} from 10 to 25% while maintaining T_{des} of 100 °C. The η_{II} increases from 0.14 to 0.21 with increase in T_{des} from 80 to 100 °C while maintaining RH_{des} of 10%. Similarly, the η_{II} increases from 0.21 to 0.23 with increase in RH_{des} from 10 to 25% while maintaining T_{des} of 100 °C while maximum of 0.26 at RH_{des} of 25% and T_{des} of ~71 °C. It is worth mentioning that the η_{II} after achieving peak value at certain T_{des} follows declining trend corresponds to higher RH_{des} . It is because $Q_{H,least}$ at higher RH_{des} and at certain T_{des} starts decreasing, thereby resulting in declining trend of the η_{II} . Additionally, effect of RH_{des} with respect to RH_{ads} on η_I and η_{II} for each studied adsorbent are presented in Appendix A (Fig. A6).

4.5.3. Significance of condenser temperature

Effects of T_{cond} on the WPP, EC, η_I , and η_{II} with respect to RH_{ads} are evaluated with the choice of Syloid 72FP + 57 wt% EMIM-Ac. The results are presented in Fig. 18. It can be noticed that the WPP, η_I , and η_{II} follows decreasing trend while EC follows increasing trend with the increase in T_{cond} . For instance, the WPP by the Syloid 72FP + 57 wt% EMIM-Ac decreases from 1.86 to 1.62 kg/kg/cycle with increase in T_{cond} from 20 to 35 °C while maintaining RH_{ads} of 50%. This is because more heat transfer potential is available at low T_{cond} which take over more latent heat of desorption, thereby support the water-vapors for phase transition. Similarly, the η_I and η_{II} decreases from 0.35 to 0.32 and 0.12 to 0.10 while EC increases from 6422.50 to 7056.38 kJ/kg_w/cycle, respectively.

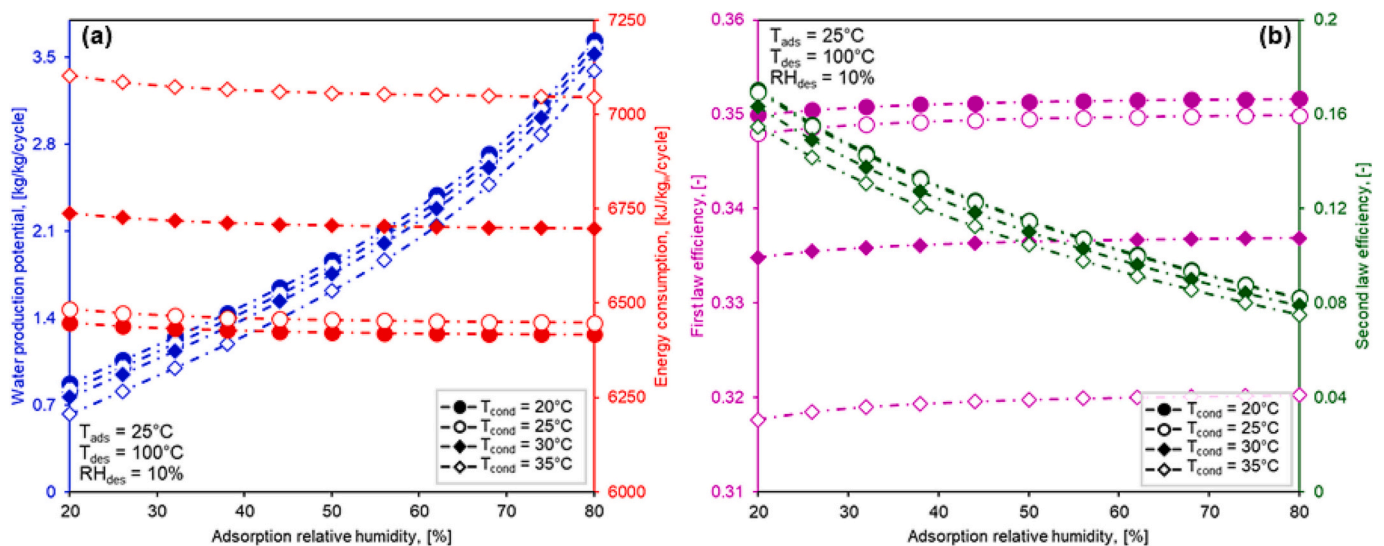


Fig. 18. Effect of condenser temperature on (a) water production potential and energy consumption, (b) first and second law efficiencies in case of Syloid 72FP + 57 wt% EMIM-Ac at T_{ads} of 25 °C, T_{des} of 100 °C, and RH_{des} of 10%.

Table 3

The final resulted water production potential and energy consumption by each studied adsorbent at T_{ads} of 25 °C, RH_{ads} of 50%, T_{des} of 100 °C and T_{cond} of 25 °C.

Sr #	Adsorbents	RH_{des}^*	WPP	EC
		[%]	[kg/kg/cycle]	[kJ/kg _w /cycle]
1	RD SG	15	0.26	3830.12
2	AQSOA-Z01	15	0.21	3890.92
3	Syloid 72FP + 57 wt% EMIM-Ac	15	1.40	3483.62
4	PS-II	15	0.34	3685.37
5	GO-SSNF	15	1.45	3614.43
6	MOF-801	10	0.26	4874.89
7	Alum fumarate	15	0.30	3990.79
8	NH ₂ -UiO-66	20	0.38	3479.11
9	MIL-100(Fe)	25	0.63	3390.20
10	MIL-101(Cr)	25	0.87	3302.46

* Selected based on the parametric analyses without significant effect on the WPP.

Overall, the parametric analyses of the study have provided valuable insights on the effect of different operational parameters for the performance evaluation of the adsorbents. It is concluded that T_{des} and RH_{des} are found to be most influential operational parameters among studied adsorbents. The resulted WPP and EC for each studied adsorbent at optimized RH_{des} are furnished in Table 3. It can be seen that, the EC for each adsorbent decreases without significant effect on the WPP as compared to EC at fixed RH_{des} (see Fig. 9). For instance, the EC for MIL-101(Cr) decreases from 4499.84 to 3302.46 kJ/kg_w/cycle. It implies that about 1.4 folds decrease in the EC is observed at optimized value of RH_{des} . Consequently, both η_I and η_{II} at optimized RH_{des} values are evaluated for single-stage AWH system and the results are presented in Fig. 19(a). It is observable that optimized RH_{des} for each studied adsorbent increases both η_I and η_{II} . For instance, in case of MIL-101(Cr), maximum η_I and η_{II} is 0.68 and 0.25 at RH_{des} of 25% which are 1.4 and 1.2 folds higher, respectively at RH_{des} of 10%.

In order to compare both η_I and η_{II} of single-stage AWH system with VC system, the study assumes T_{ads} , RH_{ads} , and T_{des} of 25 °C, 50% and 100 °C that are similar to the operating conditions of MIL-101(Cr). The outlet conditions are evaluated using saturation conditions. The VC system observed maximum η_I of ~0.18 and nearly constant η_{II} of ~0.08 which is ~3.8 and 3.1 folds less as compared to MIL-101(Cr). Additionally, the dual-stage configuration is evaluated for each studied adsorbent in terms of both η_I and η_{II} by fixing MIL-101(Cr) as bed-2

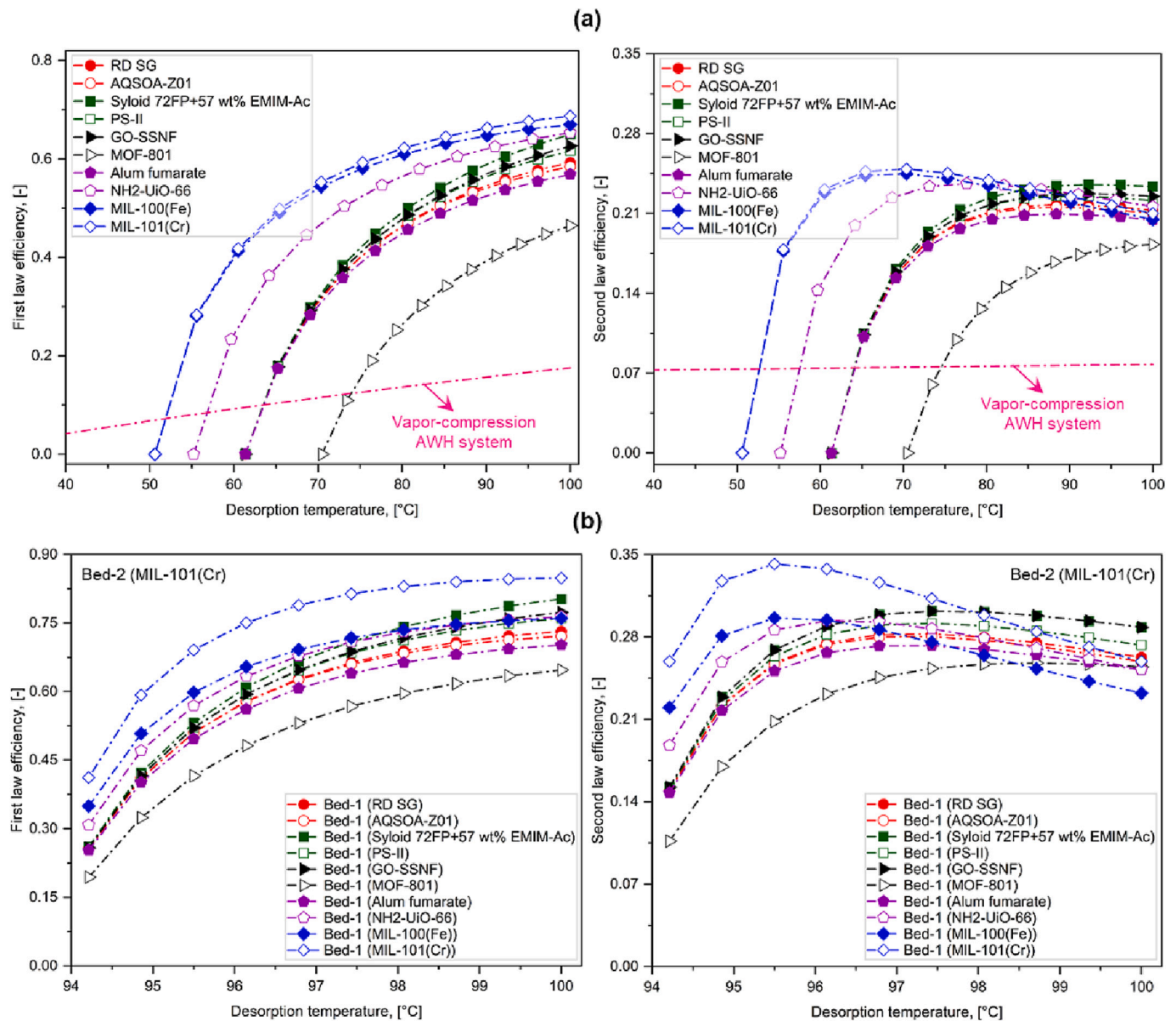


Fig. 19. The final resulted first (η_I) and second (η_{II}) law efficiencies of (a) single-stage AWH system for each studied adsorbent. For comparison purpose, the η_I and η_{II} of vapor-compression system are superimposed with dotted line. (b) The η_I and η_{II} of dual-stage system are also evaluated for comparison point of view with the single-stage.

(operating at T_{cond} of 60°C) and other adsorbent as bed-1. The P-T-w diagrams of the dual-stage system can be found from Fig. A7. The results of both η_I and η_{II} for the dual-stage are presented in Fig. 19(b). It has been observed that, both $\eta_{I,DS}$ and $\eta_{II,DS}$ increases from single-stage at T_{des} of 94°C . The maximum $\eta_{I,DS}$ and $\eta_{II,DS}$ is observed of 0.9 and 0.34 in case of fixing MIL-101(Cr) as both bed-1 and bed-2. It implies that dual-stage system can improve both η_I and η_{II} by 33% as compared to the single-stage.

5. Conclusions

The present study aims to evaluate silica-gel, zeolite, ionogel, polymer, membrane and metal-organic framework (MOF) based ten kinds of emerging adsorbents for atmospheric water harvesting (AWH) systems. A thermodynamic modeling framework enabling well-known Dubinin-Astakhov and Modified Langmuir models and steady-state equations is executed. The studied adsorbents are evaluated from viewpoints of

water production potential (WPP), energy consumption (EC), first (η_I) and second law (η_{II}) efficiencies. After that, parametric analyses are performed to evaluate performance variability among studied adsorbents corresponds to different adsorption and desorption conditions. Furthermore, the study evaluates both η_I and η_{II} for vapor-compression (VC) and dual-stage systems to compare with the single-stage system.

Results showed that Syloid 72FP + 57 wt% EMIM-Ac possess maximum WPP ranging from 0.55 to 1.55 kg/kg/cycle in extremely arid to partially humid regions, EC of 4214.96 kJ/kg_w/cycle, η_I of 0.54, and η_{II} of 0.21. Whereas MIL-101(Cr) observed maximum WPP up to 0.87 kg/kg/cycle in partially humid regions, EC of 4499.84 kJ/kg_w/cycle, η_I of 0.50, and η_{II} of 0.19. As per results of the parametric analyses, desorption temperature and desorption relative humidity are found to be most influencing parameters which significantly reduce the EC and increase both η_I and η_{II} without considerable change in the WPP. Based on the optimized conditions, the EC is observed of 3483.62 kJ/kg_w/cycle, η_I of 0.65, and η_{II} of 0.24 by the Syloid 72FP + 57 wt% EMIM-Ac.

Similarly, the EC is observed of 3302.46 kJ/kg_w/cycle η_I of 0.69, and η_{II} of 0.25 by the and MIL-101(Cr). Furthermore, single-stage system can improve both η_I and η_{II} between 68% to 74% as compared to the VC based system. Whereas dual-stage system can improve both η_I and η_{II} by 33% as compared to the single-stage system.

The study concludes that the Syloid 72FP + 57 wt% EMIM-Ac (ionogel) and MIL-101(Cr) (MOF) could be potential adsorbents for the AWH systems. However, the performance of real systems may vary due to adsorption kinetics, thermal conductivity, diffusivity and parasitic heat loss. Therefore, there is a dire need of simulation-based research on real AWH systems.

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CRediT authorship contribution statement

Muhammad Aleem: Conceptualization, Methodology, Software, Formal analysis, Investigation, Writing – original draft. **Muhammad Sultan:** Conceptualization, Methodology, Validation, Resources, Writing – original draft, Visualization, Supervision, Project administration, Funding acquisition. **Muhammad Farooq:** Writing – review & editing, Visualization. **Fahid Riaz:** Writing – review & editing, Visualization. **Sobhy M. Yakout:** Writing – review & editing, Visualization,

Project administration, Funding acquisition. **Md Shamim Ahamed:** Writing – review & editing, Visualization. **Hafiz M. Asfahan:** Methodology, Software. **Uzair Sajjad:** Writing – review & editing, Visualization. **Muhammad Imran:** Formal analysis, Validation, Writing – review & editing, Visualization. **Muhammad W. Shahzad:** Validation, Writing – review & editing, Visualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix

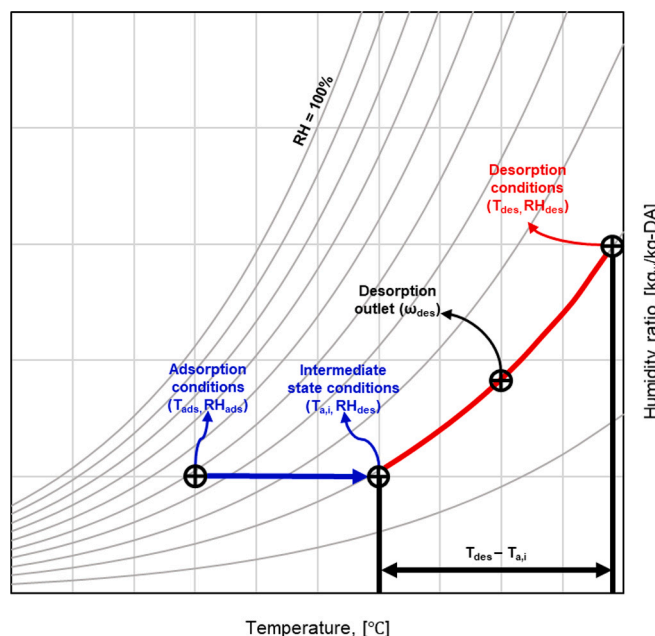


Fig. A1. Psychrometric representation of an integral method to evaluate desorption outlet humidity.

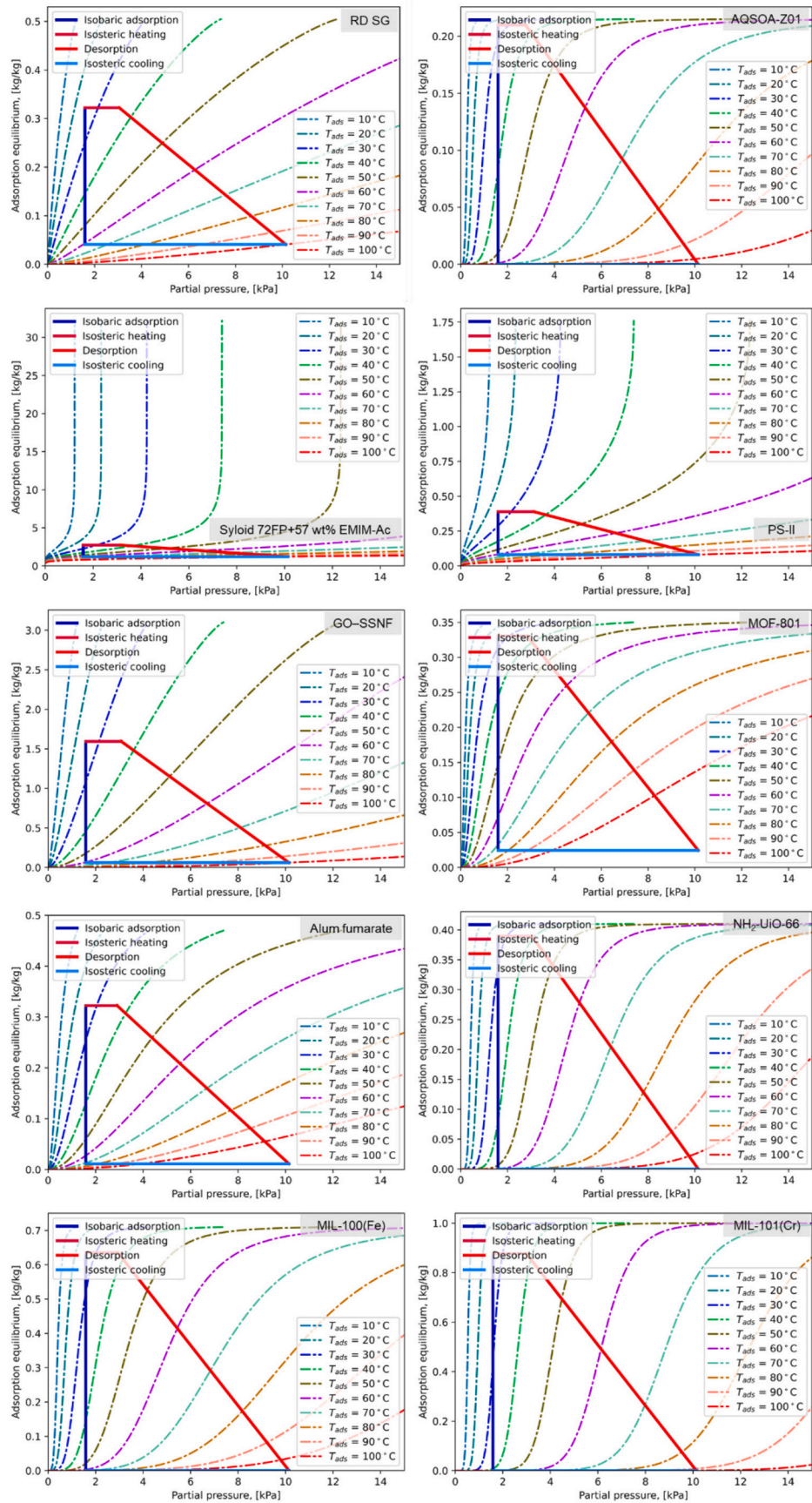


Fig. A2. Pressure ranges of ideal AWH cycle (superimposed with solid lines) for studied adsorbents with predicted adsorption equilibrium profiles (dash dotted lines) at T_{ads} of 10 °C to 100 °C.

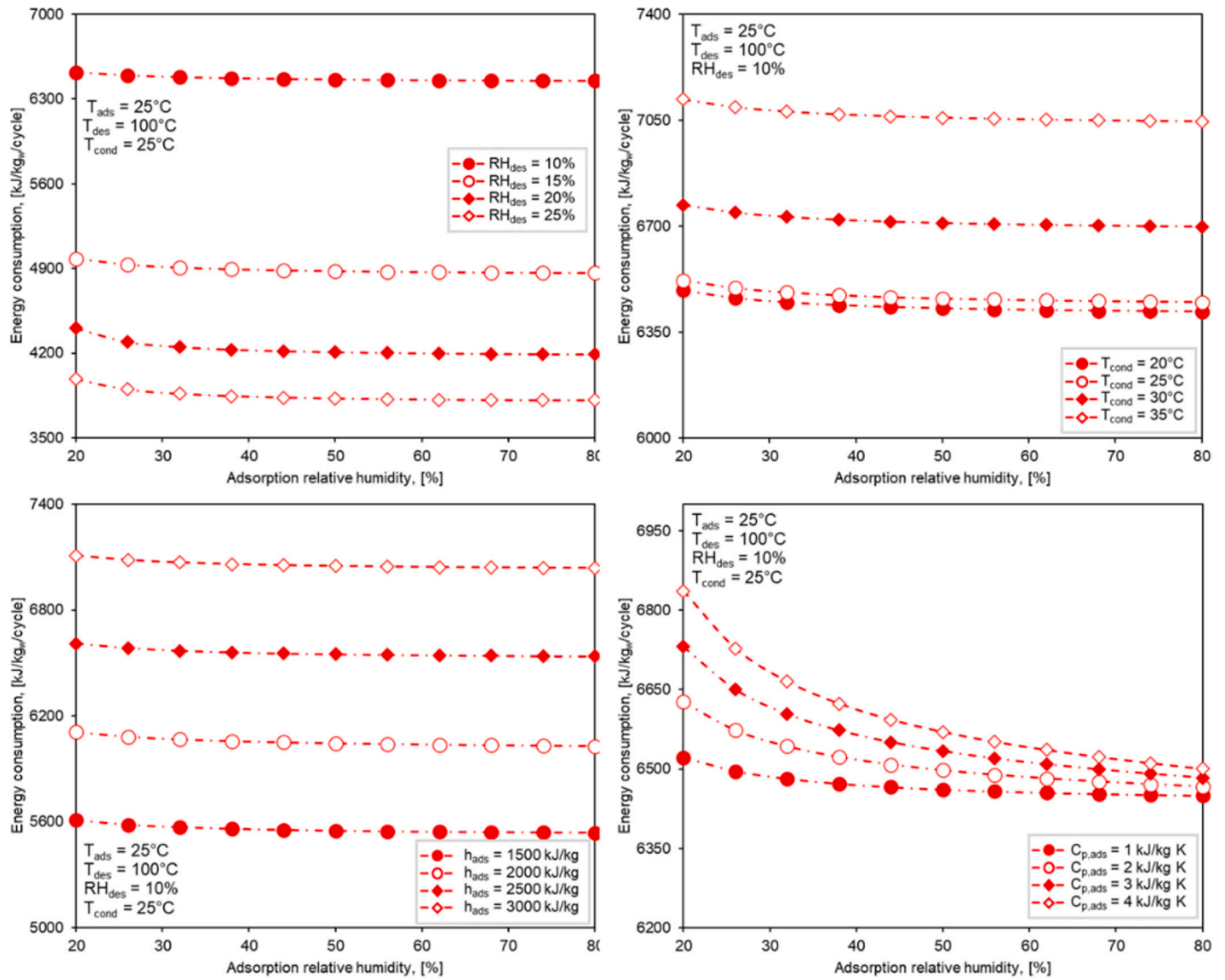


Fig. A3. Sensitivity analysis of energy consumption to evaluate most influencing parameter on the energy consumption by Syloid 72FP + 57 wt% EMIM-Ac for adsorption-based AWH system.

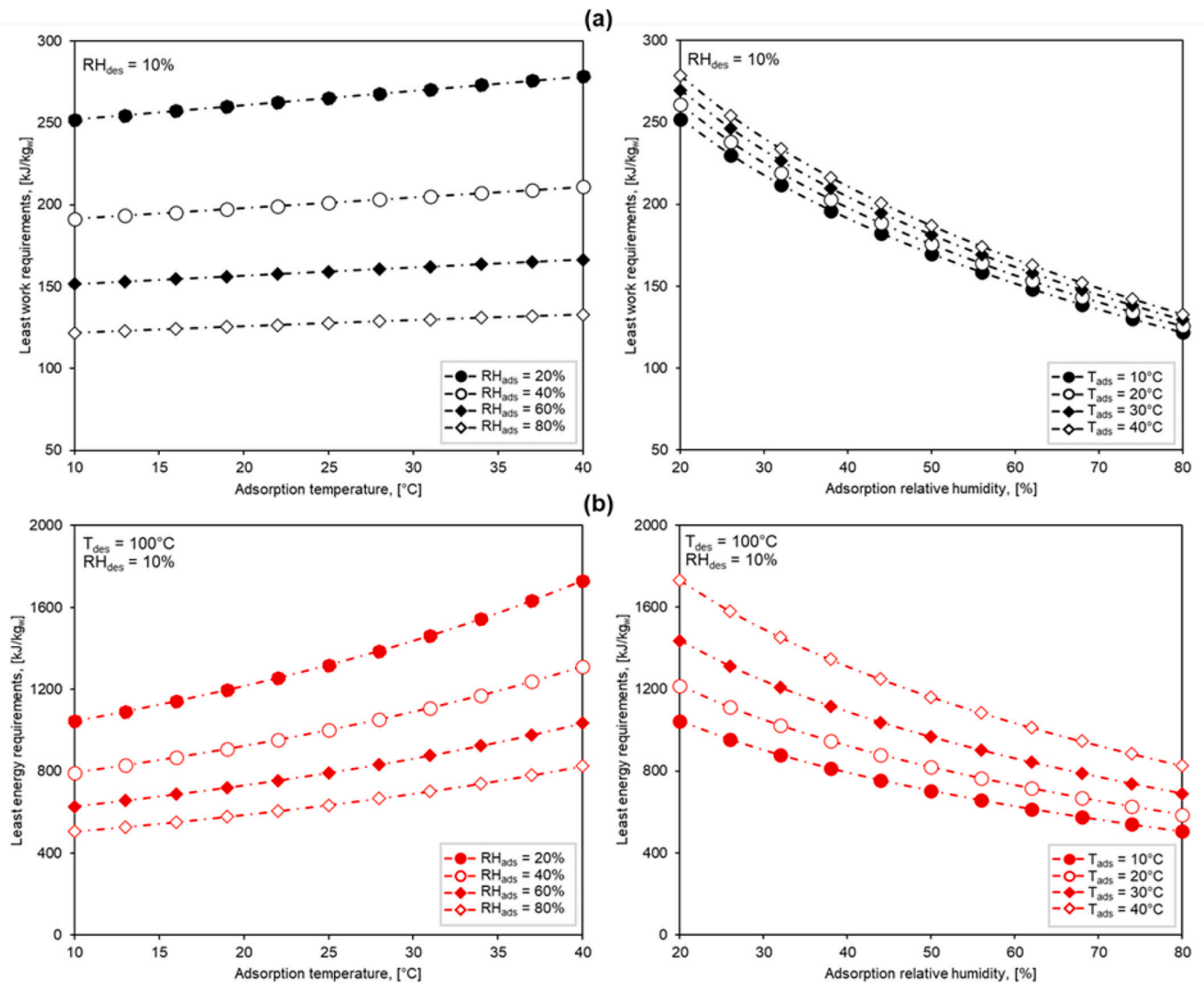


Fig. A4. Effect of adsorption temperature and relative humidity on (a) least work requirements, (b) least energy requirements.

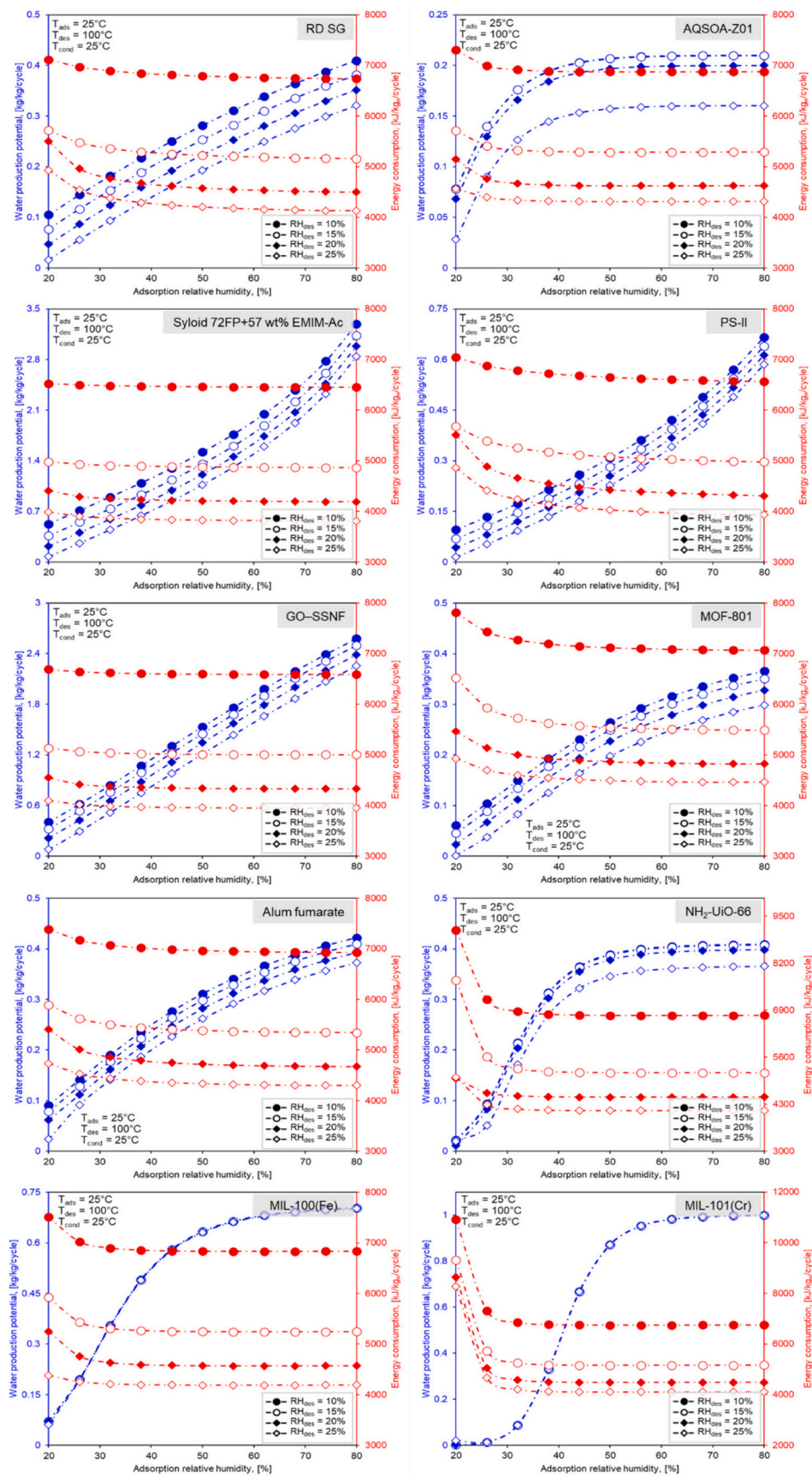


Fig. A5. Effect of desorption relative humidity on water production potential and energy consumption for each studied adsorbent.

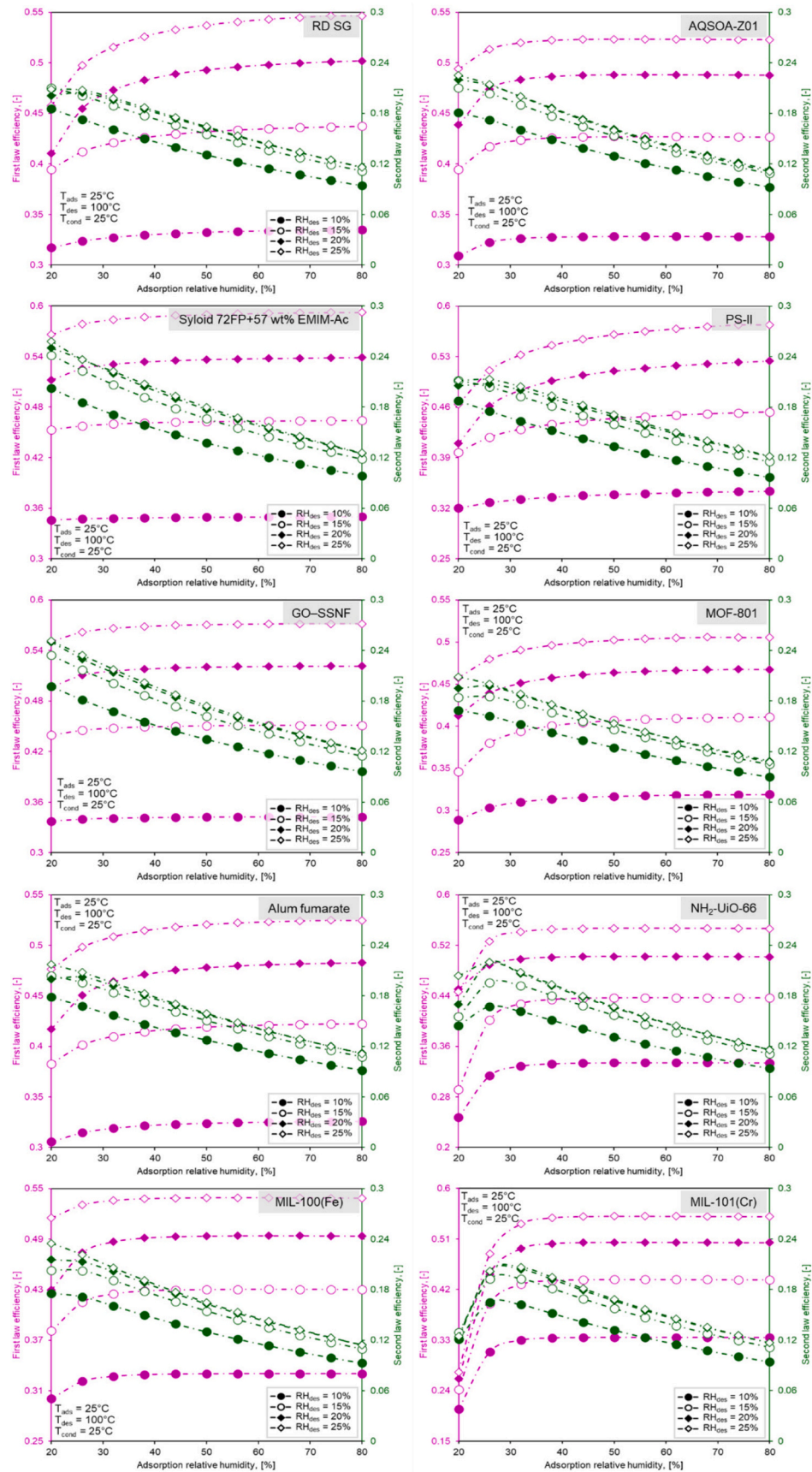


Fig. A6. Effect of desorption relative humidity on first and second law efficiencies for each studied adsorbent.

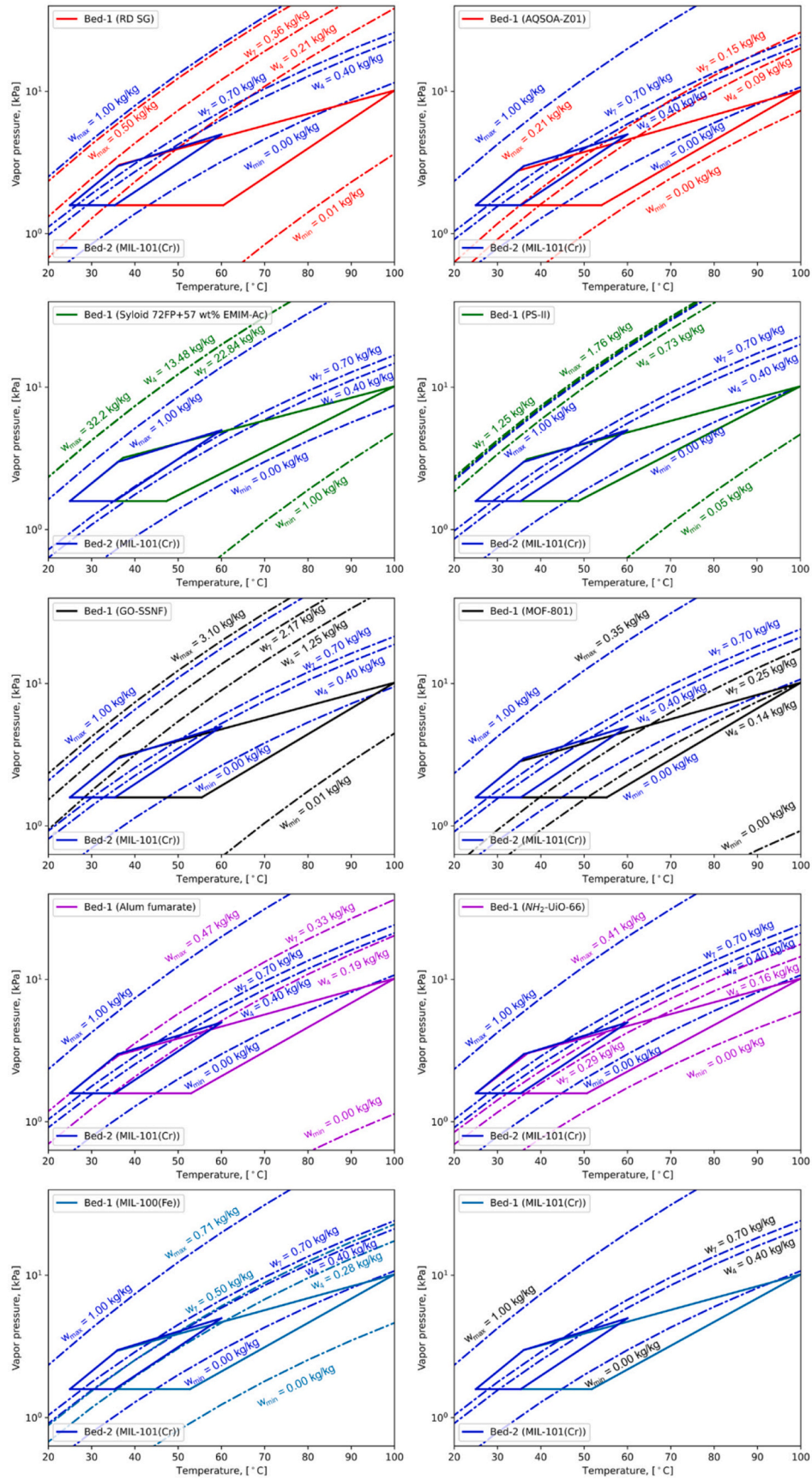


Fig. A7. Thermodynamic cycle or P-T-w diagrams of dual-stage configuration for each studied adsorbent (bed-1) by fixing MIL-101(Cr) as bed-2 at T_{ads} of 25 °C, RH_{ads} of 50%, T_{des} of 60 °C, and RH_{des} of 25%.

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