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# NUMERICAL EVALUATION OF THE INFLUENCE OF OPERATIONAL PARAMETERS ON THE ADSORPTION DESALINATION SYSTEM PERFORMANCE

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***Abstract.*** *Desalination processes based on adsorption cycles (AD/ADC) is attracting increasing attention due to their ability to co-generate two useful effects, the production of drinking water and cooling from the use of low-intensity thermal sources (solar). This work presents the results of a numerical and thermodynamic study of a simple bed adsorption desalination system using thermal energy from flat solar collectors. The evaluated system consists of three main components, the reactor with adsorptive bed loaded with silica gel, evaporator and a condenser that can be configured for desalination or desalination with refrigeration. In the simulation the configuration adopted was of the system in desalination with refrigeration, using a bed with 7 Kg of Fuji Davidson RD 2560 silica gel and the parameters evaluated with their respective impacts on the performance indexes were; the cycle time varying from 0-1500 s, the temperature of the thermal source from 55-85 °C and the cooling system varying from 15-30 °C. The maximum values obtained for COP, SWP (Specific Water Production) and SCP (Specific Cooling Power), were 0.45, 4.1 kg/kg silica gel, 245.3 W/kg silica gel respectively. The results obtained indicate that this technology presents a cycle compatible with other technologies.*

***Keywords:*** *adsorption, desalination, silica gel, solar desalination*

## 1. INTRODUCTION

Drinking water is an essential resource for the development of agriculture, industry and for consumption in domestic activities. The growth of the world population pressures the demand for the supply of food, goods and services and, consequently, consumption. It is estimated that by the year 2030 the demand for drinking water will have an increase of 2%, raising the demand to the level of 6,900 billion m³ (Bnm³) per year while the sustainable supply from the natural water cycle on the planet is of 4200 (Bnm³) (Ng et al. 2013a). In addition to the pressure of economic activities on the consumption of drinking water, climate change alters the balance in the rainfall regime, subjecting regions to extreme events such as floods and prolonged droughts. It is estimated that 80% of the planet's population is already, in some way, being subjected to situations of water stress, being more severe in desert and semiarid climate regions.

A practical solution to mitigate the effects of global water scarcity lies in the development of environmentally and economically sustainable technologies for converting marine or brackish water sources into potable water. Desalination is a process of separating excess salt and other minerals from marine or brackish water. The main widely used desalination technologies and their percentages of participation in relation to the global installed capacity are: thermally activated processes multi-stage-flashing (MSF) 27%, multi-effect-distillation (MED) 9%, and triggered processes by electrical energy such as reverse osmosis (RO) 59%, vapor compression (VC) 1% and electro-dialysis (ED) 4% (International desalination association (IDA) 2019). All these existing desalination technologies have limitations regarding their use, such as high energy consumption in the range of 3.5 to 12 kWh/m³, high maintenance costs, corrosion, application problems in sources with a high load of chemical contaminants and biological. It is observed that, in general, regions with problems of drinking water scarcity also have problems with the supply of electricity, therefore a challenge is posed to scientists and engineers to seek an alternative desalting process or system(s) that can operate with alternative energies sources, low operating cost and low environmental impact. One of the processes that meets these mentioned characteristics is the adsorption desalination process activated by solar energy.

Thermally activated adsorption desalination is an emerging process (Ng et al. 2013b) that has proven to be energy efficient and low environmental impact. This process is based on the physical adsorption properties of vapors on the surfaces of some porous materials (adsorbents) such as silica gel and zeolites. In addition to providing another effect, that of cooling, adsorption desalination has other competitive advantages when compared to other conventional processes: (a) low maintenance costs due to the lack of moving parts, (b) environmentally sustainable due to the non-use of chemical products, (c) lower incidence of evaporator scale due to operation at low evaporating temperature, (d) can be activated by low intensity heat sources such as solar or waste heat sources.

The topic of desalination by adsorption process has received increasing attention in the literature in recent years. Wang (Wang and Ng 2005) conducted some experiments in a desalination system with four adsorptive beds, monitoring the value of specific water production (SWP) from the control of several parameters. The optimum value for the specific water production observed was 4.7 kg per kilogram of silica gel. In this work it was observed that the SWP is sensitive to temperature variation of the cooling baths. In works by Thu (Thu et al. 2009) evaluated the performance of an adsorption desalination system with two adsorptive beds with internal heat regeneration between the condenser and the evaporator. In an experimental work and numerical simulation carried out by NG (Ng et al. 2012) the author investigates the performance of an adsorption desalination system with four adsorptive beds activated by residual heat using the refrigeration effect. The results presented demonstrated that the SWP (specific water production) and SCP (specific cooling power) can reach 8 kg and 0.18 kW per kilogram of silica gel, per day, respectively, when the system is configured for potable water production. Alsaman et al. (Alsaman et al. 2017) presented theoretical and experimental studies on performance evaluation of a 2-bed solar-driven adsorption desalination-cooling system based on an adsorption cycle. The results showed that the SWP and SCP were about 4.0 kg and 0.112 kW per kilogram of silica gel, per day respectively with a COP of 0.45. Other authors in the bibliography have theoretically and experimentally evaluated adsorption desalination systems (Wu, Hu, and Biggs 2012),(Wu, Biggs, et al. 2012),(Olkis, Brandani, and Santori 2019).

This work presents a numerical model for the thermodynamic processes of a theoretical adsorption cycle applied to a single bed small-scale desalination system and also evaluates the influence of cycle time variation on performance coefficients SWP, SCP and COP.

## 2. THE ADSORPTION DESALINATION SYSTEM

The Figure 1 schematically shows a thermally activated single bed desalination from a flat solar collector of evacuated pipes (ETC). This system is basically composed of three main components: The absorptive bed (loaded with silica gel), the condenser and the evaporator. In this configuration, the system operates intermittently, but the installation of other reactors allows the system to operate semi-continuously with increased capacity.

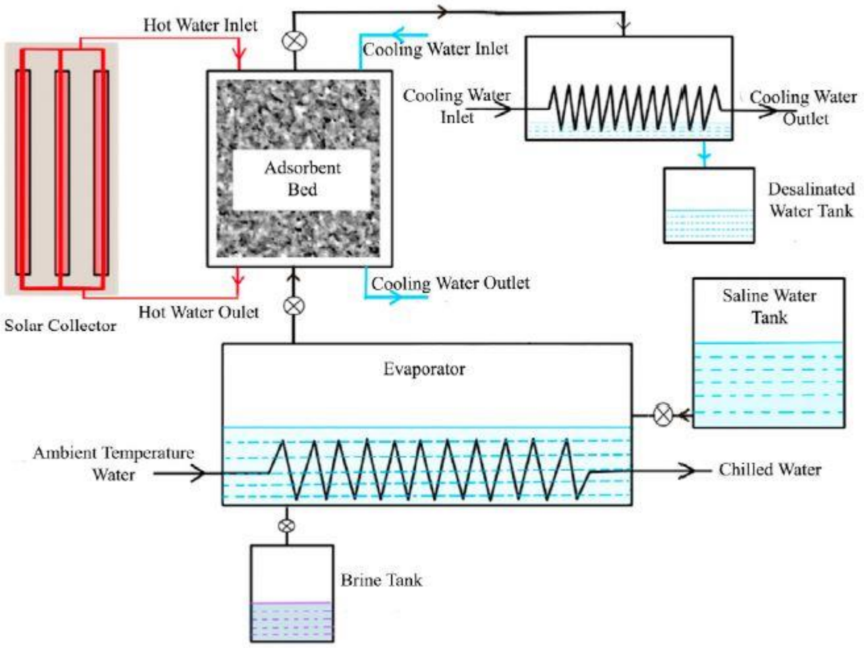

Figure1. Schematic diagram of an adsorption desalination system (Raj and Baiju 2019)

After the entire system has been evacuated and the saline water tank has been loaded, the valve between the saline water tank and the evaporator is opened. The saline water is then evaporated and its vapor is transferred to the adsorptive reactor with the valve opening between the evaporator and the reactor. Water steam is adsorbed by silica gel bed, and heat generated by the adsorptive process is removed through the circulation of cooling water through the reactor. Once saturated the adsorptive bed, the valve between the reactor and the evaporator is closed and at the same time the valve between the reactor and the condenser is opened. At the same time, the cooling water recirculation system is replaced by the hot water recirculation system from the solar panel. Increasing the temperature in the adsorptive bed extracts steam from adsorbed water, regenerating the silica gel. Steam extracted from the bed is removed from the reactor and sent to the condenser through the valve opening between the reactor and the condenser, where it will condense and collect fresh water. As soon as the temperature of the adsorptive bed reaches its maximum peak due to the recirculation of hot water, the silica gel regeneration process is complete and the system is ready to start another cycle.

It can be noted that in this cycle saline or brackish water is distilled twice, while the cooling effect formed in the evaporator can be used in air conditioning systems, or even employed in the condenser and adsorptive reactor cooling system. Another advantage of the adsorption desalination system is that it can be configured to obtain bi-distilled drinking water or can be configured with both bi-distilled water and chiller simultaneously.

Figure 2 presents the P-T-X diagram of a theoretical adsorption cycle, where the coordinates are ln P per ln (-1 / T), and X represents the amount of adsorbed by the adsorbent under equilibrium conditions (kg / kg). It can be verified that this theoretical cycle presents 4 processes, being two isosteric processes and two isobaric processes:

- **Process 1-2 -** Starting the process at point 1, the valve between the bed and the evaporator is closed, the cooling water recirculation is interrupted and the hot water recirculation in the adsorptive reactor is increased, increasing its temperature and pressure along the constant concentration line $X_{max}$= $X_1 = X_2$ This process continues until point 2 is reached whose pressure is $P_2$ determined by the water saturation pressure at the condenser temperature.
- **Process 2-3 -** At point 2, the valve between the adsorptive reactor and the condenser is opened and the desorbed vapor from the silica gel bed due to recirculation of hot water is transferred to the condenser. As cooling water recirculates through the condenser, water vapor is condensed. The pressure in the condenser and adsorptive reactor is constant until the adsorption bed reaches its maximum temperature and the concentration $X_{min} = X_3$=$X_4$
- **Process 3-4 -** At point 3, the adsorptive bed reaches its highest temperature and is $X_{min}$. At this point, the reactor is isolated to the condenser and evaporator by closing the valves and initiates the water recirculation process until the bed temperature decreased along the constant concentration line $X_{min}$ to point 4 where the pressure $P_4$ is a pressure water saturation temperature at evaporator temperature.
- **Process 4-1-** In state 4, the valve between the adsorptive reactor and the evaporator is opened while the cooling water recirculates through the adsorptive bed. The amount of saline water charged into the evaporator begins to evaporate and this water vapor is transferred to the adsorptive reactor through the valve opening. During this process the pressure remains constant $P_4 = P_1$, but the silica gel bed temperature continues to decrease until $T_1$ which is determined by the temperature of the cooling water. At point 1 the water concentration in the silica gel bed is maximum $X_1$=$X_{max}$ .

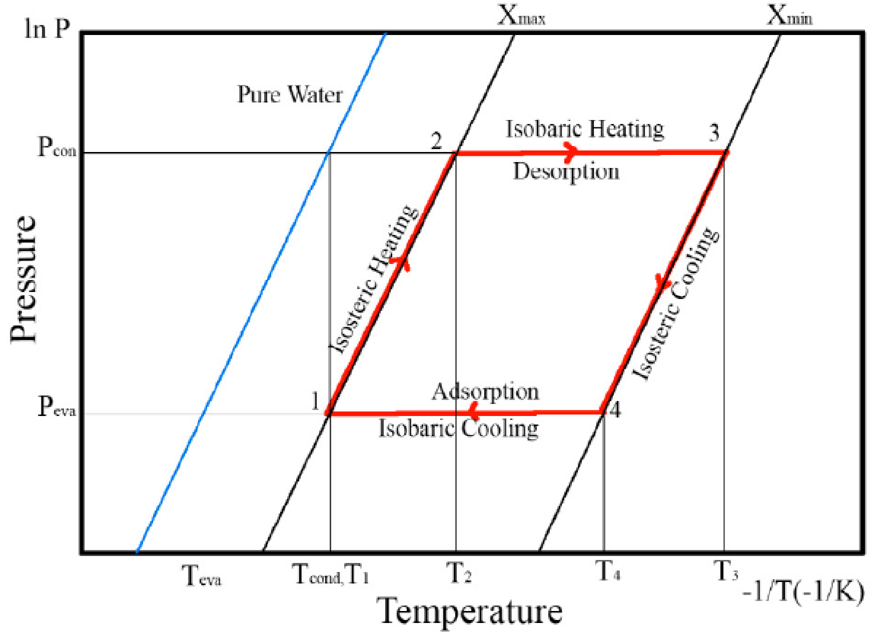

Figure 2. Adsorption desalination cycle

## 2.1 Assumptions made in mathematical modeling

This section describes the development of a mathematical model applied to a desalination system based on an adsorption cycle (ADC) carried out by an apparatus composed of single adsorptive bed reactors loaded with silica gel coupled to an evaporator and condenser. The model is based on isotherms and on the kinetics of the adsorptive processes as well as on the energy and mass balances applied to each of the components of the system. The purpose of the mathematical model is its use in the simulation and optimization of the operating parameters of the system under different conditions. In order to simplify the mathematical study, the following assumptions are considered for the development of the model: (i) the adsorptive reactors, the evaporator and the condenser are evaluated as a compact set, not considering variations in temperature and pressure between them; (ii) pressure, temperature and amount of adsorbate (water vapor) are considered uniform throughout the adsorptive reactors; (iii) it is assumed that water in the adsorbed phase behaves as a liquid, so the specific heat and density of the adsorbed phase are considered in the condition of water in the liquid phase; (iv) the loss of head due to steam and water flows in the circuit are disregarded; (v) due to good thermal insulation, heat losses through the surfaces of adsorptive reactors, evaporator, condenser and piping are disregarded; (saw). The thermal baths, hot and cold reservoirs are considered large and are not modeled; (vii) vapor density is significantly lower than silica gel and water, therefore its thermal capacity is not taken into account. (viii) both the gas phase adsorbate (water vapor) and the adsorbent (silica gel) are in equilibrium condition.

### 2.1.1 Mathematical modeling

In order to estimate the amount of steam adsorbed at different values of temperature and pressure, the adsorption isotherms must be initially determined. In an equilibrium condition, the uptake (C*) of water vapor by silica gel at a certain pressure (P) and temperature (T) can be estimated by the Tóth isotherm ratio (Chua et al. 2002) below:

$$C^* = \frac{K_0 . exp\left(\frac{\Delta h_{isos,ads}}{RT}\right) . P}{\left[1 + \left\{\left(\frac{K_0}{C_m}\right) exp\left(\frac{\Delta h_{isos,ads}}{RT}\right) . P\right\}^x\right]^{\frac{1}{x}}} \tag{1}$$

Where C* is the amount of adsorbate adsorbed by the mass of adsorbent in the equilibrium condition and on the right side of the equation; ; $K_0$ the pre-exponential constant, $\Delta_{isos,ads}$ is the variation of the isosteric enthalpy of the adsorption process, x is the dimensionless Tóth parameter, $C_m$ represents the maximum amount captured, R is the universal gas constant , T and P denote temperature and pressure respectively in the equilibrium condition. The vapor capture transient at a given pressure and temperature, that is, the adsorption and desorption kinetics is obtained using the equation of the LDF (Linear Driving Force), (Saha and Kashiwagi 1997) model given by:

$$\frac{dC(t)}{dt} = K_s a_v . (C^* - C(t)) \tag{2}$$

Where $K_s a_v$ the mass transfer coefficient that for operating regimes at low pressures (2 to10 kPa) is expressed in terms of the parameters $R_p$ and $D_{so}$ (Chihara and Suzuki 1983).

$$K_s a_v = 15 . \frac{D_s}{{R_p}^2} \tag{3}$$

$$D_s = D_{so} exp\left(-\frac{E_a}{RT}\right) \tag{4}$$

The parameters indicated in expressions (3) and (4) denote; $R_p$ the mean radius of the silica gel grain, $D_{so}$ the kinetic constant of the silica gel and water system and $E_a$ the activation energy. The evaluation of the mass balance taken in the evaporator of an ADC cycle takes into account the quantities referring to the mass flow of the saline water feed; marine or brackish, the mass production of drinking water extracted from the condenser and the disposal rate of the tailings concentrated in the form of brine. This mass balance, therefore, is represented by the following equation:

$$\frac{dM_{sw,evap}}{dt} = \dot{m}_{sw,i} - \dot{m}_{pw,cond} - \dot{m}_b \tag{5}$$

Where $dM_{sw,evap}$ is the amount of brackish or marine water contained in the evaporator, $\dot{m}_{sw,i}$ is the mass flow of saline water feeding into the evaporator, $\dot{m}_{pw,cond}$ a mass production and potable water extracted from the condenser, $\dot{m}_b$ is the concentrated tailings disposal rate. The pumping of feed saline water to the evaporator is done intermittently depending on the volume and level adjustment. Waste disposal occurs when the saline concentration of the internal volume in the evaporator reaches preset values. The mass balance equation (5) in the evaporator can be rewritten in terms of the salt concentration balance in the ADC system as:

$$M_{sw,evap}\frac{d\chi_{sw,evap}}{dt} = \theta.\chi_{sw,i}.\dot{m}_{sw,i} - n.\chi_v.\left(\frac{dC}{dt}\right).M_{sg} - \gamma.\chi_{sw,evap}.\dot{m}_b \tag{6}$$

In this equation $\chi_{sw,i}$ denotes the saline concentration of the feed water pumped to the evaporator $\chi_v$ the vapor concentration in the evaporator at equilibrium condition and $\chi_{sw,evap}$ the predetermined saline concentration for the brine disposal . The parameters θ (0,1), n (1,2), γ (0,1) are the parameters used to adjust the expression according to the mode of operation of the adsorptive cycle. The energy balance evaluated in the evaporator can be written as:

$$\begin{aligned}\left[M_{s,evap}.C_{p,s}\left(T_{evap},\chi_{s,evap}\right) + M_{hx,evap}.C_{p,hx,evap}\right]\frac{dT_{evap}}{dt} \\ = \theta.h_{f,sw}\left(T_{evap},\chi_{s,evap}\right).\dot{m}_{sw} - \gamma.h_{f,b}\left(T_{evap},\chi_{s,evap}\right).\dot{m}_b \\ - n.h_{fg}\left(T_{evap}\right)\frac{dC_{ads}}{dt}.M_{sg} + \dot{m}_{chil\,w}.C_{p,chil\,w}.\left(T_{chil,in} - T_{chil,out}\right)\end{aligned} \tag{7}$$

Where $\boldsymbol{M_{hx,evap}}$ is the total evaporator mass, $\boldsymbol{M_{sg}}$ is the total mass of the silica gel adsorbent, $\boldsymbol{\dot{m}_b}$ is the brine tailings discharge mass flow rate, $\boldsymbol{dC_{ads}}$ denotes the amount of vapor captured by the adsorbent during the adsorption process. The first term on the right side of equation (7) represents the amount of sensible heat due to the supply of saline water to the evaporator, in the second term there is the amount of sensible heat due to brine discharge, the third term denotes the amount of heat removed in the adsorption process, the fourth term represents the amount of heat provided by the cooling water stream feed. The parameters $\boldsymbol{C_{p,s}}$, sensible heat and $\boldsymbol{h_{f,b}}$, of saline water are calculated through correlations as a function of temperature and pressure (Nayar et al. 2016).

The outlet temperature of the cooling water in the evaporator $T_{(chil,out)}$ is estimated using the logarithmic mean temperature difference (LMTD) method given by:

$$T_{chil,out} = T_{evap} + \left(T_{chil,in} - T_{evap}\right)exp\left\{\frac{-U.A_{evap}}{\dot{m}_{chil\,w}.C_{p,chil\,w}}\right\} \tag{8}$$

Where the term $U.A_{evap}$ is the global heat transfer coefficient of the evaporator and, disregarding the thermal resistance of the evaporator walls due to insulation, it can be expressed by the following relationship:

$$\frac{1}{U.A_{evap}} = \frac{1}{h_{chil\,w}.A_{i,evap}} + \frac{1}{h_{evap}.A_{o,evap}} \tag{9}$$

The parameters $A_{i,evap}$ and $A_{o,evap}$ indicated in relation (9) correspond respectively to the areas of the internal and external surfaces of the evaporator. The energy balance for the condenser coupled to the adsorptive reactor can be evaluated through the following relationship:

$$\begin{aligned}\left[M_{w,cond}.C_{p_{w\,cond}}(T_{cond}) + M_{hx,cond}.C_{p_{hx,cond}}\right]\frac{dT_{cond}}{dt} = -h_f(T_{cond})\frac{dM_{wd}}{dt} + \\ n.h_{fg}(T_{cond})\frac{dC_{des}}{dt}.M_{sg} + \dot{m}_{w,cond}.C_{p_{w\,cond}}(T_{cond}).\left(T_{w,cond\,in} - T_{w,cond\,out}\right)\end{aligned} \tag{10}$$

Where $M_{w,cond}$ is the mass of steam condensed in the condenser, $M_{wd}$ the mass of distilled water, extracted in the condenser, $h_{fg\,(T_{cond})}$ denotes the enthalpy of steam saturation evaluated at the condenser temperature $T_{cond}$ , $\dot{m}_{w,cond}$ is the mass flow rate of the cooling water flow in the condenser with the inlet temperature$T_{w,cond\,in}$ and the outlet temperature $T_{w,cond\,out}$. The value for the leaving condenser cooling water temperature is estimated using the logarithmic mean temperature difference (LMTD) method given by:

$$T_{w,cond\,out} = T_{cond} + \left(T_{w,cond\,in} - T_{cond}\right)exp\left\{\frac{-U.A_{cond}}{\dot{m}_{w,cond}.C_{p_{w,cond}}}\right\} \tag{11}$$

$$\frac{1}{U.A_{cond}} = \frac{1}{h_{w\,cond}.A_{i,cond}} + \frac{1}{h_{cond}.A_{o,cond}} \tag{12}$$

Where $A_{i,cond}$ and $A_{0,cond}$ , represent the inner and outer area of the condenser tube and $U.A_{cond}$ is the global heat transfer coefficient of the condenser, $h_{w,cond}$ and $h_{cond}$ represent the coefficients of heat transfer by internal (tube) and external (shell) convection respectively. The energy balance equation for the adsorptive bed reactor that contains the silica gel mass and the finned heat exchanger, and which is also coupled to the evaporator and condenser, is given by the expression:

$$\left[M_{sg}.C_{p\,sg} + M_{hx,bed}.C_{p_{hx,bed}} + M_{sg}.C_{p_v}.C^*\right]\frac{dT_{ads/des}}{dt} = \pm n.\Delta h_{isos,ads/des}(T_{ads/des},P_{ads/des}).M_{sg}\frac{dC_{ads/des}}{dt} \pm \dot{m}_{h/c\,w}.C_{p\,h/c\,w}(T_{h/c\,w}).(T_{h/c\,w,in} - T_{h/c\,w,out}) \tag{13}$$

The terms presented on the left side of the equality above represent the sensible heat of the heat exchanger set of the adsorptive bed where the specific heat of the silica gel, the mass of the metallic components and the mass of the adsorbent modelled as liquid phase are taken into account. The first term on the right side of the equality represents the enthalpy variation during the adsorption and desorption processes that occur inside the adsorptive bed. The parameter $\Delta h_{isos,ads/des}(T_{ads/des},P_{ads/des})$ is called isosteric heat and quantifies the heat supplied or rejected in the adsorptive bed during the adsorption and desorption processes, which is given by (Ruthven 2008):

$$\Delta h_{isos,ads/des} = h_{fg} + E.\left[ln\left(\frac{C}{C^*}\right)\right]^{\frac{1}{n}} + \frac{ET\alpha}{n}\left[ln\left(\frac{C}{C^*}\right)\right]^{\frac{1-n}{n}} \tag{14}$$

The terms $T_{h/cw,in}$ ,$T_{h/cw,out}$ respectively represent the inlet and outlet temperatures of the water used in the heating and cooling steps of the adsorptive reactor heat exchanger during the adsorption and desorption. $T_{h/cwout}$ can be estimated using, similarly to the other heat exchangers in the model, the logarithmic mean temperature method (LMTD) as:

$$T_{h/c\,w,out} = T_{hex} + (T_{h/c\,w,in} - T_{hex})exp\left\{\frac{-U.A_{hex}}{\dot{m}_{h/c\;w}.C_{p_{h/c\;w}}}\right\} \tag{15}$$

In order to evaluate the performance of the adsorption cycle with the use of the refrigeration effect, the performance indices are defined below: The SWP (specific water production) and to evaluate the cooling effect, two other parameters are used to evaluate the performance of the cycle: SCP (specific cooling power) and COP (coefficient of performance). These parameters are calculated using the equations:

$$SWP = \int_0^{t_{cycle}} \frac{\dot{m}_{w\,cond}.C_{p_{w\,cond}}(T_{cond}).(T_{w\,cond,out} - T_{w\,cond\,,in})}{h_{fg}(T_{cond}).M_{sg}}\,dt \tag{16}$$

$$SCP = \int_0^{t_{cycle}} \frac{\dot{m}_{chil\,w}.C_{p_{chil\,w}}(T_{chil}).(T_{chil,in} - T_{chil,out})}{M_{sg}}\,dt \tag{17}$$

$$COP = \int_0^{t_{cycle}} \frac{\dot{m}_{chil\,w}.C_{p_{chil\,w}}(T_{chil}).(T_{chil,in} - T_{chil,out})}{\dot{m}_{h\,w}.C_{p\,h\,w}(T_{h\,w}).(T_{h\,w,in} - T_{h\,w,out})}\,dt \tag{18}$$

### 2.1.2 Numerical simulation results

The SWP, SCP and COP indicators proposed for the model estimate the performance of an adsorption desalination system (AD/ADC), single or double bed, operating in different configurations: desalination or desalination using the refrigeration effect. Cycle steps are evaluated by changing parameters n, θ and γ. The numerical model is solved using the MATLAB 2017a program coupled to the REFPROP thermophysical properties platform. The system of variables was computed by numerical integration, from the differential equations of the model, with the implementation of the fourth-order Runge-Kutta-Felberg method with a relative error tolerance of $1.10^{-6}$. Table 1 presents the material properties, constants, the dimensional and operational parameters used as the initial value in the numerical simulation.

Table 1: Parameters used in numerical simulation

| Symbol | Description | Value | Unit |
|---|---|---|---|
| $\dot{m}_{h/cw}$ | water mass flow in adsorptive reactor | 0,25 | Kg/s |
| $\dot{m}_{chil\,w}$ | mass flow of cooling water | 0,25 | Kg/s |
| $\dot{m}_{w,cond}$ | mass flow of condenser cooling water | 1,0 | Kg/s |
| $C_{0,i}$ | initial mass of adsorbed vapor | 0,16 | Kg/kg |
| $C_m$ | maximum adsorption capacity | 0,45 | kg/kg |
| $C_{p\,sg}$ | specific heat silica gel | $0,924.10^3$ | J/kg.k |
| $C_{p,hx\,evap}$ | specific heat evaporator material / copper (Cu) | $0,386.10^3$ | J/kg.K |
| $C_{phx,cond}$ | specific heat condenser material/copper (Cu) | $0,386.10^3$ | J/kg.K |
| $C_{phx.bed}$ | specific heat exchanger material (AI 304) | 477 | J/kg.K |
| $C_{pv}$ | specific heat water vapor phase | $1,89.10^3$ | J/kg.K |
| $C_{pw}$ | specific heat water liquid phase | $4,18.10^3$ | J/kg.K |
| $D_{so}$ | adsorption kinetic constant | $2,9.10^{-4}$ | $m^2/s$ |
| $E_a$ | activation energy | $2,3.10^3$ | kJ/kg |
| $K_0$ | pre-exponential constant | $7,3.10^{-10}$ | 1/kPa |
| $M_{hx\,bed}$ | mass of adsorptive reactor material | 15 | kg |
| $M_{hx,evap}$ | heat exchanger material mass | 1,3 | kg |
| $M_{s,evap}$ | initial mass of saline water | 3 | kg |
| $M_{sg}$ | total silica gel mass in the reactor | 7,0 | kg |
| $R_p$ | average radius of the adsorbent particle (silica gel) | $0,8.10^{-3}$ | m |
| $T_{hw,in}$ | maximum temperature of the thermal source | 85 | °C |
| $T_{chil,in}$ | cooling water temperature | 25 | °C |
| $T_{cw,in}$ | cooling water temperature | 25 | °C |
| $T_{wcond\,in}$ | cooling water temperature | 25 | °C |
| $UA_{hex}$ | global heat transfer coefficient | 600 | W/K |
| $UA_{evap}$ | global evaporator heat transfer coefficient | 350 | W/K |
| $\chi_{sw,evap}$ | pre-determined concentration of brine for tailings | 100000 | ppm |
| $\chi_{sw,i}$ | initial concentration of saline water | 35000 | ppm |
| $\Delta h_{isos}$ | isosteric enthalpy variation | 2693 | kJ/kg |
| $R$ | universal gas constant | 0,461 | kJ/kg.K |
| $x$ | tòth heterogeneity constant | 12 | |

For the numerical simulation, the thermophysical properties of the used adsorptive medium were obtained from the characteristics of Fuji Davison type RD 2560 silica gel, which is an adsorbent commonly used by commercial chiller manufacturers. In (Chua et al. 2002) and (Thu et al. 2013) results of experimental studies of the adsorptive characteristics between silica gel and water used in this simulation are presented.

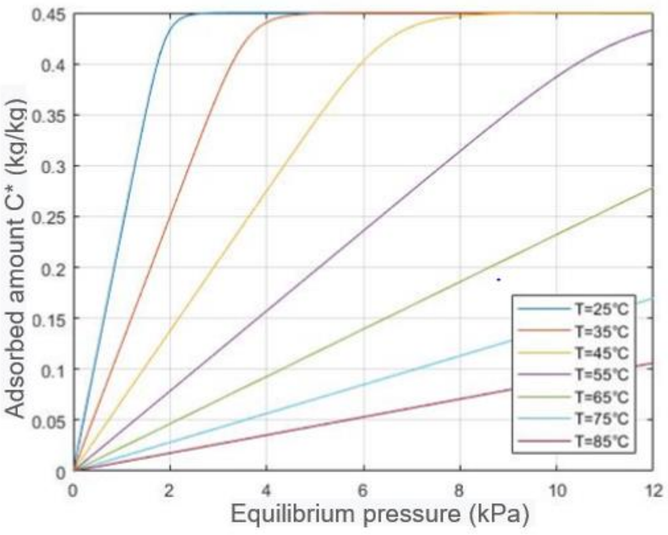

Figure 3: Adsorption isotherms for a pair of Fuji Davison type RD 2560 silica gel and water.

The isotherms and the behaviour of the adsorption process kinetics of the silica gel-water pair were simulated for different temperature ranges between 25°C and 85°C using the Tòth model presented in equation 1. In Figure 3, the isotherms of the adsorption process demonstrate that the adsorption capacity, under equilibrium conditions, of silica gel (C*) is a function of the partial vapour pressure (P) of the adsorbate (water) in the gas phase and the temperature of the medium adsorbent (silica gel) (T). For the adsorptive pair of silica gel type RD 2560 and water, for the same equilibrium pressure (P) the value of $C_m$ (0.45 kg/kg), which indicates the maximum adsorptive capacity of the medium, is reached faster when this medium is at lower temperatures. Otherwise, at a previously defined concentration for the adsorptive medium, as the temperature of the adsorbent medium increases, there is an increase in the vapour pressure of the adsorbate in the equilibrium condition.

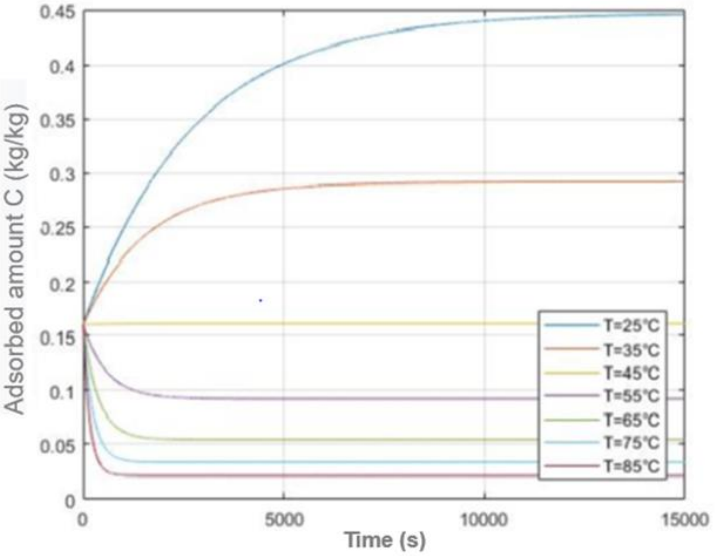

Figure 4: Transient of the amount of steam in the sorption/desorption in relation to the variation in bed temperatures

Figure 4 presents the values obtained for the numerical simulation of the transient of the amount of adsorbed vapour, evaluated from the LDF (Linear Drive Force) model with equations (2),(3) and (4) , with the parameters of the Table 1 and for adsorptive reactor temperatures ranging from 25°C to 85°C. Starting from an initial amount of adsorbed vapour of $C_{0,1}$ =0.16 kg/kg of silica gel, and a partial pressure of the adsorbate vapour in the pre-fixed equilibrium condition of 2.339 kPa ($T_{sat}$ = 20°C) it is verified that for the temperature of the adsorptive bed at 45°C the amount of steam is in equilibrium. The adsorption process takes place from temperatures below 45°C and desorption to bed temperatures above 45°C. For the adsorption process, considering the lowest temperatures of the adsorptive bed ($T_{cw,in}$) at T = 25°C and T = 35°C, they present 0.4 and 0.28 kg/kg of amount of adsorbed steam respectively up to the first 5000 s, and for the next periods, from 5,000 s to 10,000 s and 10,000 and 15,000 s these gains are no longer significant in relation to the adsorption time and this is due to the exponential nature of the adsorption kinetics. In the desorption processes, for the highest bed regeneration temperatures ($T_{hw,in}$) T = 85°C and T = 75°C were the ones that obtained the highest amounts of desorbed steam. The maximum amplitude obtained between the temperatures $T_{cw,in}$ and $T_{hw,in}$ , in the equilibrium condition indicates the maximum amount of steam in the sorption/desorption processes and, for a simulation time of 15,000 s , the maximum value obtained under these conditions was 0.41kg/kg. The bed(s) sorption and desorption times are part of the composition of the total cycle time of the system.

In Figures 5 and 6 are summarized as variations of the SCP, SWP and COP performance indices as a function of the simulation time. Values were captured from $T_{hw,in}$ = 85 °C, $T_{cw,in}$ = 25 °C for adsorptive reactor and 25 °C for evaporator and condenser cooling water. It can be seen from Figure 5 that the SCP and COP trends are similar. The number of refrigerant mass over the complete cycle, indicated by equation (5) of the mathematical model, implies that the average mass of the saline water that vaporizes in the evaporator is equal to the amount of condensate generated. Therefore, an average cooling capacity and a desalinated water production rate are proportional to each other and similar trends with variation in operating conditions. It is observed that for the one simulation time between 132 and 321 s these three indexes present their maximum values, therefore, when the system operational parameters are optimized, the cycle time will be between these two values. For extremely short cycle times, the adsorption and desorption processes are inefficient, as in this step a fraction of heat is transferred to or from the thermal mass of the adsorbent bed, leading to a reduction in the COP index, as shown in Figures 5 and 6. It also requires that for extremely long cycle times, an exponential nature of the absorption kinetics and the heat transfer process, decrease the rate of absorption or desorption leading to the observed reduction in performance indices. During this condition, although the heat transfer to the bed decreases, a large fraction of this heat is transferred to the adsorption or desorption process, thus increasing the efficiency of the system. Therefore, in an adsorptive system, it is not possible to optimize the COP and SWP performance indexes simultaneously from the manipulation of the cycle time variable.

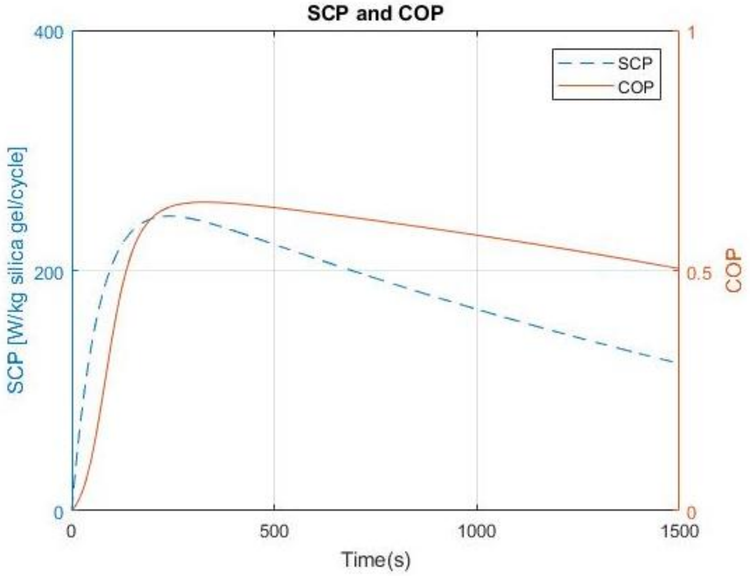

Figure 5: Variation SCP and COP

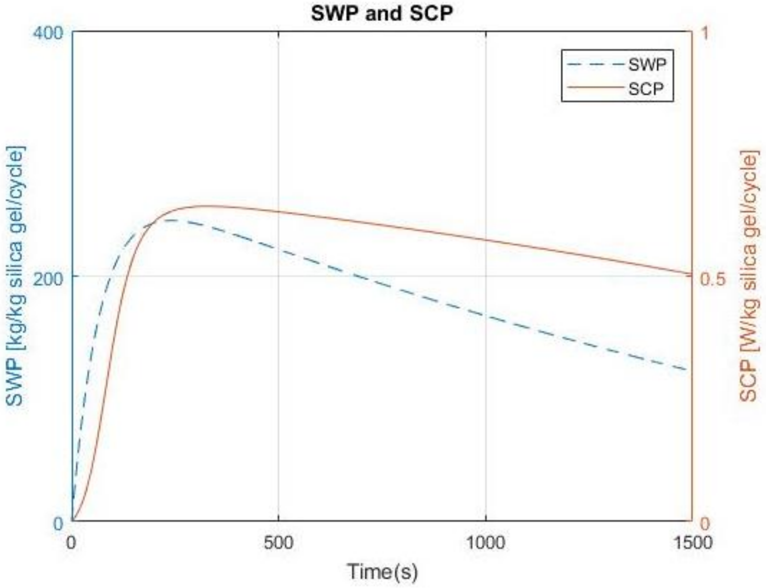

Figure 6: Variation SWP and SCP

## 3. CONCLUSIONS

The characteristics of the adsorptive kinetics of FUJI RD 2560 silica gel were evaluated in different temperature ranges. The maximum capacity of 0.45 kg/kg was reached for the simulation at various temperatures. In the adsorption process for the temperature evaluated at T=25°C, this value was only reached for simulation times above 15000 s. For medium temperature at T=35°C, the maximum value obtained and stabilized at 0.29 kg/kg was obtained in 10000 s of simulation time, indicating the saturation of the medium under the pressure conditions used in the simulation. For the medium temperature range between 55°C and 85°C used in this simulation, the best performances in the desorption process were obtained for T=85°C, with residual steam in stabilization of 0.025 kg/kg. For the temperature range between 25°C for adsorption and 85°C for desorption, the maximum yield obtained was 0.41 kg/kg in 15000 s of simulation. For smaller temperature ranges and shorter simulation times, the model indicates a reduction in efficiency, signalling a strong correlation between the simulation time (cycle time) and the temperatures of the thermal sources and cooling adopted in the system. Based on the numerical simulation results, the SWP achieved 4.1 kg per kilogram of adsorvent (silica gel) per day at $T_{cw,in}$=25°C and $T_{hw,in}$ =85°C . Applying the same initial conditions, the maximum values obtained for the SCP and COP indices were 245.3 W/kg (t = 236 s), and 0.6422 (t= 321 s) respectively.

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## 5. RESPONSIBILITY NOTICE

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