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Xio Lin Wang

*National University of Singapore*

Hui Tong Chua

*National University of Singapore*

Kim Choon Ng

*National University of Singapore*

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# SIMULATION OF SILICA GEL-WATER ADSORPTION CHILLERS

Xiaolin Wang <sup>1\*</sup>, Hui Tong Chua <sup>2</sup>, Kim Choon Ng <sup>3</sup>

<sup>1)</sup> Department of Mechanical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260, Singapore  
Tel No.: (65)68747877, Fax No.: (65)67791459, E-mail id: [mpewx@nus.edu.sg](mailto:mpewx@nus.edu.sg)

<sup>2)</sup> Department of Mechanical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260, Singapore  
Tel No.: (65)68746627, Fax No.: (65)67773525, E-mail id: [mpecht@nus.edu.sg](mailto:mpecht@nus.edu.sg)

<sup>3)</sup> Department of Mechanical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260, Singapore  
Tel No.: (65)68742214, Fax No.: (65)67791459, E-mail id: [mpengkc@nus.edu.sg](mailto:mpengkc@nus.edu.sg)

## ABSTRACT

A mathematical model describing the behaviors of current commercialized silica gel-water adsorption chillers is presented in this study. Comparing with the previous study, this model comprises (i) a realistic representation of the thermal mass of the associated piping materials and fins; (ii) a distributed modeling of the reactor bed for the sorption processes. The model is demonstrated on a two-bed adsorption chiller with circular fin sorption heat exchanger. A comparison of simulated results and experimental data shows that good agreement can be achieved when a realistic time constant for temperature sensors has been considered. Thereafter, the chiller performance is analyzed and discussed for a two-bed adsorption chiller. A detailed study on the 4-bed adsorption chiller with rectangular fin heat exchanger is currently being carried out.

## 1. INTRODUCTION

Adsorption chillers have been commercialized for many years and silica gel-water has been proven as an excellent adsorbent-adsorbate working pair for such chillers. In order to predict the system performance and provide the design guidance for manufacturers, researchers have put a lot of efforts on simulation of adsorption chillers. Karagiorgas et al. (1987), Passos et al.(1989), and Cho et al.(1992) presented the uniform temperature and pressure models in which equilibrium conditions of pressure and temperature are assumed for the adsorbent layer, as well as the solid and gas phases, and neglected the heat-and-mass transfer resistance in the adsorbent layer. Such equilibrium models are unable to predict the accurate vapor uptake due to uncertain temperature and pressure distributions within the sorption beds. Subsequently, Amar et al. (1996) considered both the heat-and-mass transfer resistance within the sorption beds in their simulation for an adsorption heat pump with temperature wave heat generation. The influence of the operating parameters, such as cycle time, permeability and heating temperature, on the COP was discussed. It was found that for the packed bed design, and the mass transfer resistance can influence the performance of heat pump substantially. Based on this framework, Zhang (2000) studied an intermittent adsorption cooling system using a 3-D non-equilibrium model, where both internal and external mass transfer resistances within the adsorbent bed have been accounted for. However, the assumptions of ideal gaseous adsorbate and ideal condenser and evaporator render the model unrealistic. Recently, Chua et al. (2004) presented a distributed-parameter model for a two-bed adsorption chiller that correctly incorporated the evaporator & condenser thermal dynamics.

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\* Corresponding author

In this paper, a detailed mathematical model that handles all the major components of an adsorption chiller is presented. The simulation work focused on the performance of the adsorption chillers with current market-available bed structures as shown in figure 1. It considers the thermodynamic representation of the heat-and-mass transfer processes of adsorbed phase and heat-and-mass transfer in the condenser and evaporator. It is one-step close to the real process of the adsorption chiller and provides a useful tool for the engineers to optimize the system design and performance estimation.

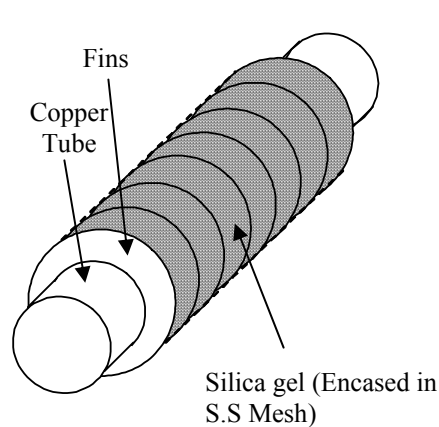


Fig. 1a A circular fin heat exchanger made by Nishiyodo

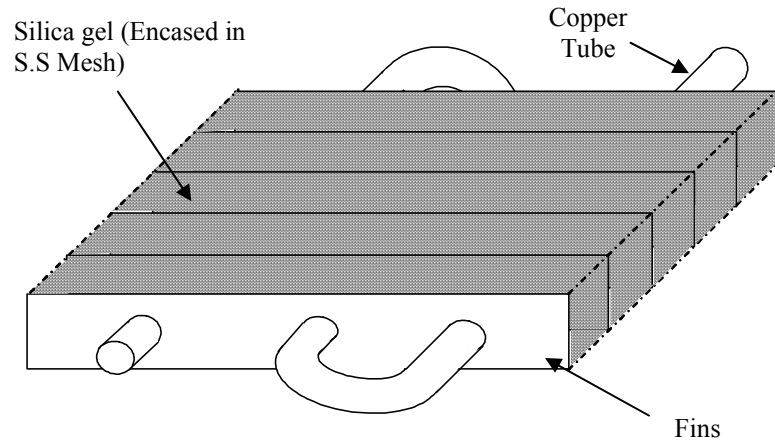


Fig. 1b A rectangular fin heat exchanger made by Mycom

## 2. SIMULATION MODEL

Our model focused on the two types of current commercialized chiller bed structures as shown in the figure 1. Figure 1a is a circular fins heat exchanger design which is used in the Nishiyodo adsorption chiller and figure 1b is a rectangular fin heat exchanger design which is commonly used in the Mycom adsorption chiller. We employed linear driving force equation (Sakoda et al. 1984) to determine the sorption rate. All the thermodynamic properties of water are calculated by the formulation of Wagner and Kruse (1997).

### 2.1 Adsorption bed

Based on the abovementioned bed structures, schematics of the control volume selections are shown in figure 2a and 2b. Cylindrical coordinate is adopted for the circular fin heat exchanger so as to exploits its axisymmetry. Rectangular coordinate is chosen for rectangular fin heat exchanger since we consider only the changes along the  $x$ - and  $z$ - direction due to relatively small dimension along the  $y$ - direction.

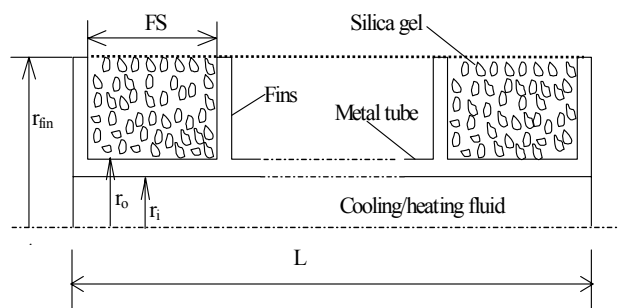


Fig. 2a Schematic of the control volume selections for a circular fin heat exchanger

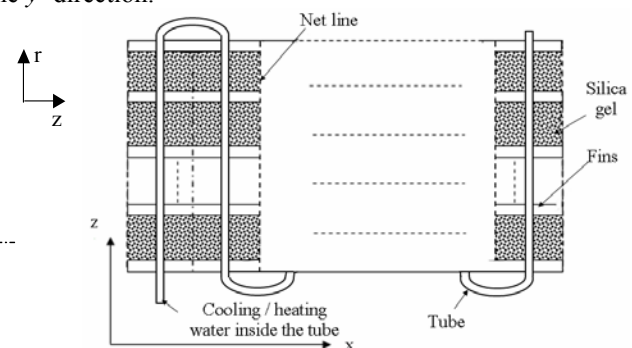


Fig. 2b Schematic of the control volume selections for a rectangular fin heat exchanger

### 2.1.1 Adsorbent and adsorbate system

The overall mass conservation in the porous bed is described as

$$\int_V \left[ \varepsilon_t \frac{\partial \rho_v}{\partial t} + (1 - \varepsilon_t) \rho_s \frac{\partial q}{\partial t} \right] dV = \dot{m}_{c/e}, \quad (1)$$

The energy balance on the control volume (adsorbent + adsorbate + inter-particle vapor) can be written as

$$\frac{(1 - \varepsilon_t) \rho_s c_{ps} \partial T_s + \varepsilon_t \partial(\rho_v u_v)}{\partial t} = k_s \frac{\partial \left( \frac{\partial T_s}{\partial X} \right) \hbar}{\hbar \partial X} + \frac{h_{fins}}{FS} (T_{finl} - T_s) - \frac{h_{fins}}{FS} (T_s - T_{fin}) + \frac{h_{ms}}{MS} (T_m - T_s) \quad (2)$$

where

$\varepsilon_t = \varepsilon_b + (1 - \varepsilon_b) \varepsilon_p$ . For the rectangular coordinate,  $\hbar = 1$ ,  $X = x$  and for the cylindrical coordinate,  $\hbar = r$ ,  $X = r$ .

This definition is applicable to all the following formulae.

Temperature boundary conditions

$$-k_s \frac{\partial T_s}{\partial X} \Big|_{X=X_0} = 0, \quad \frac{\partial T_s}{\partial X} \Big|_{X=X_l} = h_v (T_s - T_v) \quad (3)$$

Pressure boundary conditions

$P_s \Big| = P_c$  when connecting to the condenser

$P_s \Big| = P_e$  when connecting to the evaporator

$P_s \Big| = P_{cham}$  during switching time

$P_{cham}$  can be determined by

Mass balance equation:

$$\frac{d(\rho_{cham})}{dt} = -\frac{1}{V_{cham} V_h} \int_V \left[ \varepsilon_t \frac{\partial \rho_v}{\partial t} + (1 - \varepsilon_t) \rho_s \frac{\partial q}{\partial t} \right] dV, \quad (4)$$

Energy balance equation:

$$\frac{d(\rho_{cham} u_{cham})}{dt} = -\frac{1}{V_{cham} V_h} \int_V \left[ \varepsilon_t \frac{\partial(\rho_v u_v)}{\partial t} + (1 - \varepsilon_t) \rho_s \frac{\partial q}{\partial t} \right] dV, \quad (5)$$

### 2.1.2 Fins

The fin thickness is very small and the heat transfer in the fin is assumed to be one dimensional. The energy balance equation of the control volume in the fins is

$$\delta \rho_{fin} c_{pfin} \frac{\partial T_{fin}}{\partial t} = k_{fin} \delta \frac{\partial \left( \frac{\partial T_{fin}}{\partial X} \right) \hbar}{\partial X} + h_{fins} (T_{sl} - T_{fin}) - h_{fins} (T_{fin} - T_s), \quad (6)$$

The boundary conditions are

For cylindrical coordinate:  $T_{fin} \Big|_{r=r_o} = T_m$ ,  $\frac{\partial T_{fin}}{\partial r} \Big|_{r=r_{fin}} = 0$

For rectangular coordinate:  $T_{fin} \Big|_{X=x_0=x_L} = T_{cham}$

### 2.1.3 Metal tube

Two kinds of situations should be considered (with and without fin)

Without fin:

$$\rho_m c_{pm} \frac{\partial T_{bm}}{\partial t} (r_o^2 - r_i^2) = k_m \frac{\partial^2 T_{bm}}{\partial z^2} (r_o^2 - r_i^2) + 2r_i h_{fm} (T_f - T_{bm}) - 2r_o h_{ms} (T_{bm} - T_s), \quad (7)$$

With fin:

$$\rho_m c_{pm} \frac{\partial T_{bm}}{\partial t} (r_o^2 - r_i^2) = k_m \frac{\partial^2 T_{bm}}{\partial z^2} (r_o^2 - r_i^2) + 2r_i h_{fm} (T_f - T_{bm}) + 2r_o k_{fin} \frac{\partial T_{fin}}{\partial r}, \quad (8)$$

The boundary conditions are

$$\frac{\partial T_{bm}}{\partial z} \Big|_{z=0} = \frac{\partial T_{bm}}{\partial z} \Big|_{z=L} = 0$$

### 2.1.4 Cooling water/hot water

Since  $r_i/L \ll 1$ , the heat transfer in the fluid is assumed to be one dimensional. Energy balance on the cooling water control volume can be written as

$$\rho_f c_{pf} \frac{\partial T_f}{\partial t} = -u_f c_{pf} \rho_f \frac{\partial T_f}{\partial z} - \frac{2h_{fm}}{r_{bi}} (T_f - T_{bm}), \quad (9)$$

where  $h_{fm}$  is calculated with the aid of the Dittus-Boelter correlation for smooth tube.

The boundary conditions are

$$T_f \Big|_{z=0} = T_{cooling} \text{ when cooling, } T_f \Big|_{z=0} = T_{hot} \text{ when heating, } \frac{\partial T_f}{\partial z} \Big|_{z=L} = 0 \text{ at the system outlet.}$$

## 2.2 Condenser and evaporator

### 2.2.1 Metal tube

The energy balance equation of the control volume in condenser or evaporator tube can be expressed as:

$$\rho_m c_{pm} \frac{\partial T_m}{\partial t} \frac{d_o^2 - d_i^2}{4} = k_m \frac{\partial^2 T_m}{\partial z^2} \frac{(d_o^2 - d_i^2)}{4} - d_i h_i (T_m - T_{cooling}) + d_o h_o (T_{c/e} - T_m), \quad (10)$$

The boundary conditions are

$$\frac{\partial T_m}{\partial z} \Big|_{z=0} = 0; \quad \frac{\partial T_m}{\partial z} \Big|_{z=L_{c/e}} = 0$$

where  $h_{ci}$  is calculated with the aid of the Dittus-Boelter correlation for smooth tube:

### 2.2.2 Water inside the condenser or evaporator tube

Considering energy balance, the equation for the water control volume in the condenser or evaporator

$$\frac{\partial(\rho_f c_{pf} T_{water})}{\partial t} = -u_{water} c_{pf} \frac{\partial(\rho_f T_{water})}{\partial z} + \frac{\partial}{\partial z} \left( \lambda_f \frac{\partial T_{water}}{\partial z} \right) - \frac{4h_i}{d_i} (T_{water} - T_m), \quad (11)$$

The boundary conditions are

$$T_{water} \Big|_{z=0} = T_{water-in}; \quad \frac{\partial T_{water}}{\partial z} \Big|_{z=L_{c/e}} = 0$$

### 2.2.3 Refrigerant in the condenser and evaporator space

#### a. In the condenser

Here we assume that the water vapor coming from the adsorption bed can be condensed on the condenser tubes. Therefore the condensing temperature can be determined using an iterative procedure.

Mass balance equation

$$\frac{d(\rho_{vc})}{dt} V_c = -\dot{m}_c, \quad (12)$$

Energy balance equation

$$\frac{d(\rho_{vc} u_{vc})}{dt} V_c = -\dot{m}_c h_{vc}, \quad (13)$$

where  $V_c$  is the volume of space in the condenser.

### b. In the evaporator

We assume that the refrigerant inside the evaporator is in saturated state.

Mass balance equation on the refrigerant outside the evaporator tube.

$$\frac{d(m_e)}{dt} = \dot{m}_c - \sum \Delta m_s \frac{dq}{dt}, \quad (14)$$

Energy balance equation on the refrigerant outside the evaporator tube.

$$\frac{\partial(m_e u_e)}{\partial t} = \dot{m}_c h_c - \sum \Delta m_s \frac{dq}{dt} h_v + \int_0^{L_e} h_{eo} \pi d_{eo} (T_{em} - T_e) dz, \quad (15)$$

The set of partial differential equations developed above can be numerically solved using a finite difference method. The whole computational domain was discretized into a number of equal step discrete elements. Since the fin thickness and space are very small. In the computer code, a group of neighboring fins and silica gel are separately grouped as two interacting control volume which in turn forms a grand control volume. The diffusion terms in the equations were approximated by a central difference scheme and the convection terms were replaced by an upstream difference scheme. Finally, a set of coupled ordinary differential equations was obtained and solved using the fifth-order Gear's Backward Differentiation Formulae method. Double precision was used and the tolerance set to  $1 \times 10^{-6}$ . Mesh independence was ensured, with no obvious difference after further refining the mesh size.

The cooling capacity  $Q_{evap}$  and COP are respectively defined as:

$$Q_{evap} = \frac{dM_{cooling}}{dt} [c_{pf} (T_{chilled}^{in})] \int_0^{t_{cycle}} (T_{chilled}^{in} - T_{chilled}^{out}) dt, \quad (16)$$

$$COP = \frac{Q_{evap}}{\frac{dM_{heating}}{dt} [c_{pf} (T_{heating}^{in})] \int_0^{t_{cycle}} (T_{heating}^{in} - T_{heating}^{out}) dt}. \quad (17)$$

## 3. RESULTS AND DISCUSSIONS

We demonstrate this simulation on a two-bed adsorption chiller with circular finned sorption beds. The operating conditions of this chiller are listed in the table 1. The typical half-cycle and switching time for this two-bed adsorption chiller is 442s and 30s respectively. Figure 3 shows the chiller response in terms of the temporal history of outlet water temperatures. It was found that regardless of the initial adsorbed mass distribution in the sorption beds, cyclic-steady-state can be achieved within three cycles which reflects the robustness of the code.

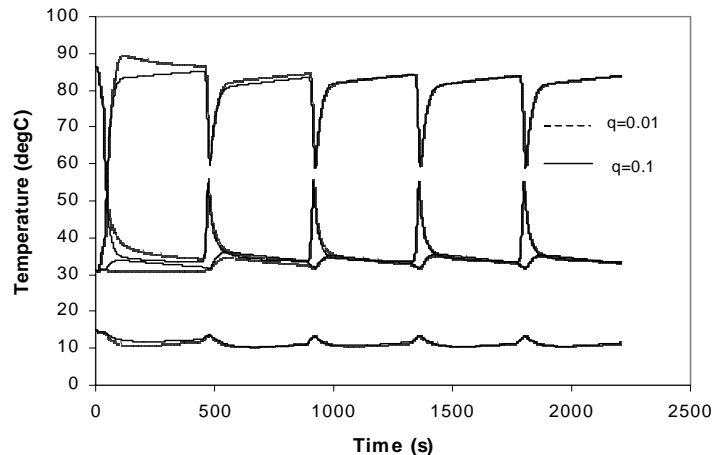


Fig.3 Temporal histories of outlet temperatures of heat source, cooling and chilled water circuits under different initial refrigerant mass distribution.

To study the reliability of this simulation method, we compared the simulation results with the experimental data of Boelman et al. (1995) for the two-bed adsorption chiller. Figure 4 shows the temperatures of the cooling and hot

waters at the outlet of the bed system, condenser and evaporator. Good agreement between simulated and experimental results has been observed. The predicted cooling capacity and COP are 10.7kW and 0.38 respectively which is very similar to the experimentally measured values to within a few percent (less than 5%).

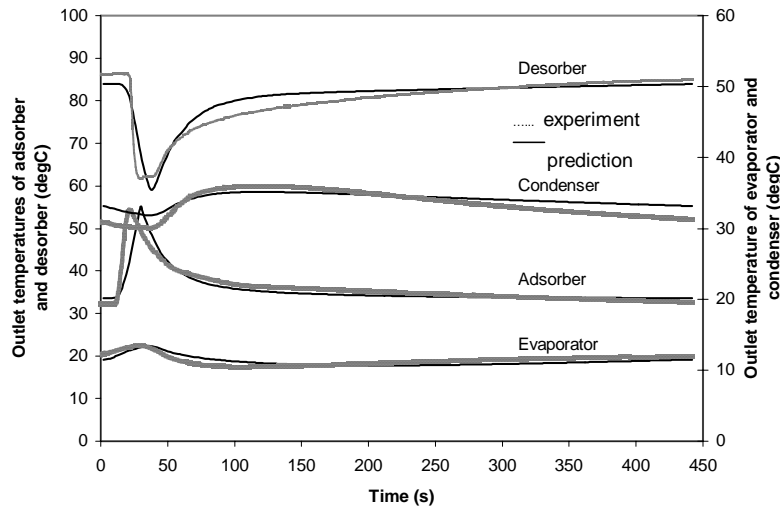


Fig.4 Comparison between the simulated and measured temperatures at the outlet of the bed system, condenser and evaporator.

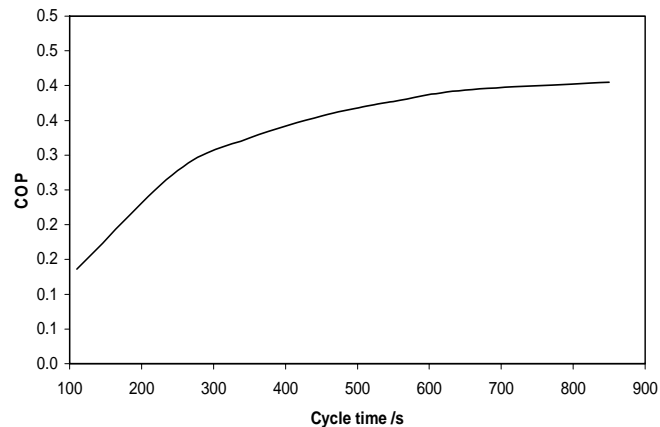


Fig.5 Effect of cycle time on COP of a two-bed adsorption chiller.

Figure 5 presents the effect of cycle time on the COP of the two-bed adsorption chiller. It is clearly seen that the COP increases monotonically with the cycle time. The reason can be explained as follows. With a longer cycle time, the relative time frame occupied by bed switching which involves significant sensible heat exchange is reduced vis-à-vis that of a shorter cycle time. This leads to a favorable effect on the COP.

The effect of cycle time on the cycle average cooling capacity is presented in the figure 6. The variation of cooling capacity is not monotonic. There is an optimum cooling capacity. If the cycle time is short, it reduces the extent of adsorption and desorption due to insufficient cooling and heating of the sorption beds. However, if the cycle time is long, it also reduces the extent of adsorption and desorption due to the near saturated condition in the beds. We have also compared our present prediction with the previous lumped-parameter model [Chua et al. 1999]. For the lumped-parameter method we employed before, the overall heat transfer coefficients of the beds are identical to those of our present model at the standard operating condition and their values do not change in other operating conditions. The effective overall  $U$  values of adsorber and desorber are  $1297.3 \text{ W/m}^2\text{K}$  and  $1327.6 \text{ W/m}^2\text{K}$ , respectively. It was

observed that the lump-parameter model can predict the system performance at the nominal operating condition and it results in an underestimation of the chiller performance at long cycle times.

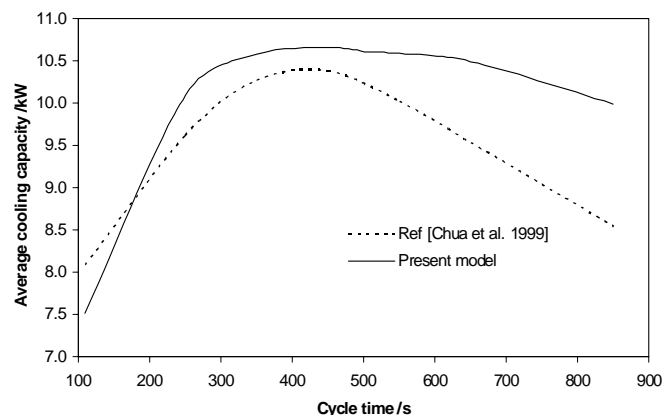


Fig.6 Effect of cycle time on cycle average cooling capacity.

#### 4. CONCLUSIONS

A distributed-parameter approach has been developed to capture the behaviors of a batch-operated adsorption chiller where dissipative losses in the major components of the chiller have been accounted for in the simulation code. It was successfully demonstrated on a standard two-bed adsorption chiller. It was found that this model tended to be more accurate than the lump-parameter model in its prediction of the cooling capacity at off-rated conditions due to its correctly handling the cycle-time dependent heat transfer coefficients in the beds. The application of this approach to a four-bed adsorption chiller is currently on going.

Table 1 Chiller operating conditions

$T_{chilled}^{in}$	14.8 °C	$dM_{chilled} / dt$	0.71 kg/s
$T_{heating}^{in}$	86.3 °C	$dM_{cond} / dt$	1.37 kg/s
$T_{cooling}^{in}$	31.1 °C	$t_{cycle}$	442s
$dM_{cooling} / dt$	1.52 kg/s	$t_{switching}$	30s
$dM_{hot} / dt$	1.28 kg/s	$\tau$	15s

#### NOMENCLATURE

$c_p$	specific heat capacity	J/kg.K		<b>Superscripts/Subscripts</b>
$d$	diameter	m	l	liquid water, left
$D_s$	surface diffusivity	$m^2/s$	v	water vapor
$D_{so}$	pre-exponent constant	$m^2/s$	p	Particle
$E_a$	activation energy of surface diffusion	kJ/kg	f	fluid(water)
FS	fin space		m	metal tube
$h$	heat transfer coefficient	$W/m^2.K$	fin	Fin
$h$	enthalpy	J/kg	s	silica gel
$h_{fg}$	latent heat of condensation or vaporization	J/kg	b	Bed
$k_D$	permeability of porous media	$m^2$	c	Condenser
$k$	thermal conductivity	$W/m.K$	e	Evaporator
$L$	length	m	i	Inner



m	mass	kg	o	Outer
$\dot{m}$	mass flow rate	kg/s	chilled	chilled water
P	pressure	Pa	cooling	cooling water
q	fraction of refrigerant adsorbed by the adsorbent	kg/kg dry adsorbent	heating	hot water
q*	fraction of refrigerant which can be adsorbed by the adsorbent under saturation condition	kg/kg dry adsorbent	cond	condenser cooling water
r	radius	m	t	total
t	time	s	cham	chamber in the adsorption bed
T	temperature	°C	r	radial direction, right
u	specific internal energy	J/kg	z	axial direction
u	velocity	m/s	in	Inlet
V	volume	m <sup>3</sup>	sorp	adsorption/desorption related to corresponding stage
$\Delta H_{ads}$	isosteric heat of adsorption	J/kg	water	cooling water in condenser or chilled water in evaporator
$\delta$	fin thickness	m		
$\rho$	density	kg/m <sup>3</sup>		
$\mu$	viscosity	N·s/m <sup>2</sup>		
$\varepsilon$	porosity			
$\tau$	time constant	s		
COP	coefficient of performance			

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