



Effects of porosity on heat and mass transfer in a granular adsorbent bed[☆]

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ABSTRACT

In the present study, the mechanism of heat and mass transfer in an annulus adsorbent is handled. The heat and mass transfer equations for the adsorbent bed and the mass balance equation for the adsorbent granules are numerically solved to obtain the distributions of temperature, pressure, adsorptive density and adsorbate concentration in the adsorbent bed. The study is performed for the silica gel–water pair and for three different values of porosity as 0.1, 0.2 and 0.3. The distributions of temperature and adsorbate concentration are considerably influenced from the bed porosity. The adsorption period increases with the increase of the porosity value. The porosity affects the pressure and adsorptive density distributions at the beginning of the process and after a relatively short time, the averages of these dependent variables approach to the final equilibrium state.

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1. Introduction

Adsorption heat pump (AHP) is a kind of thermal heat pumps which can operate with thermal sources such as solar energy, geothermal energy and waste heat of industrial processes. It has significant advantages over the conventional systems which are absorption and mechanical heat pumps [1]. A simple adsorption heat pump consists of an adsorbent bed, an evaporator, a condenser and an expansion valve, and can operate without any mechanical or electrical power input. The working principle and the recent developments of the adsorption heat pump are discussed in literature [2].

The main drawback of the solid adsorbents, used in the adsorption heat pump, is their poor thermal conductivity. Additionally, voids between the granules lead a discontinuity in the adsorbent bed and as a result the thermal conductivity of the adsorbent bed considerably decreases. The decrease of granule size enhances the contact area between the granules and consequently heat transfer rate through the bed; however it causes the increase of mass transfer resistance. In order to improve the heat and mass transfer in a granular adsorbent bed, the mechanism of heat and mass transport in the bed should be well known [3]. The solution of heat and mass transfer equations for an adsorbent bed provides valuable information and helps researchers in designing of an adsorbent bed.

Numerical studies on the adsorption heat pump cycle can be found in literature. Liu and Leong [4] numerically investigated the influence of the operation temperatures on the performance of an adsorption heat pump operating with zeolite 13X–water pair. They found that the

operation temperatures significantly affect the performance, and they optimized the operating conditions for the considered system. Di et al. [5] performed numerical and experimental studies to investigate the effect of heat source temperature on the coefficient of performance of an adsorption heat pump. Chahbani et al. [6] employed numerical simulation to study the influence of heat and mass transfer limitations on the adsorption heat pump efficiency. They declared that the low heat and mass transfer rates through the adsorbent bed significantly reduce the coefficient of performance and the specific cooling power values. Yong and Sumathy [7] compared the heat and mass transfer models for simulation an adsorbent bed according to conductance dominant and negligible mass transfer resistance states. A numerical study is also performed on the effects of coupled heat and mass transfers on the performance of a waste heat adsorption cooling unit by Zhang and Wang [8]. Ruivo et al. [9] performed an investigation for simplifying assumptions for the numerical modeling of the heat and mass transfer in a porous desiccant medium. Sphaier and Worek [10] proposed a novel solution scheme for the periodic heat and mass transfer in adsorption problems since the optimization of computational solution codes play a significant role on the implementation of numerical methods. Hajji and Lavan [11] performed a numerical study to carry out a parametric study on the effect of various design parameters and operating conditions on the system performance, including the evaporator and condenser temperatures and inert material thermal capacitance.

In the performed studies, the attentions have been focused on the influences of COP and SCP of an AHP from the different parameters such as porosity, operation temperature and pressure. However; in the present study, the attentions are focused on the mechanism of heat and mass transfer in the adsorbent bed of AHP. The influences of porosity on the variations of temperature, pressure, adsorbate concentration

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Nomenclature

C_p	specific heat of adsorbent, $\text{J kg}^{-1} \text{K}^{-1}$
D_{eff}	effective mass transfer diffusivity, $\text{m}^2 \text{s}^{-1}$
D_K	Knudsen diffusivity, $\text{m}^2 \text{s}^{-1}$
D_m	molecular diffusivity, $\text{m}^2 \text{s}^{-1}$
D_{bed}	effective diffusivity of adsorptive in adsorbent bed, $\text{m}^2 \text{s}^{-1}$
D_0	reference diffusivity, $\text{m}^2 \text{s}^{-1}$
E	diffusional activation energy, J mol^{-1}
K	inherent permeability of adsorbent bed, m^2
K_{app}	apparent permeability of adsorbent bed, m^2
M	molecular weight of adsorptive, kg mol^{-1}
P	pressure, Pa
r_p	radius of adsorbent granule, m
R	radius of bed, m; ideal gas constant, $\text{J mol}^{-1} \text{K}^{-1}$
T	temperature, K
u	adsorptive velocity, m s^{-1}
W	average adsorbate concentration, $\text{kg}_w \text{ kg}_s^{-1}$
W_∞	adsorbate concentration in equilibrium, $\text{kg}_w \text{ kg}_s^{-1}$
W_0	limiting adsorbate capacity of adsorbent, $\text{kg}_w \text{ kg}_s^{-1}$

Greek symbols

ρ	density, kg m^{-3}
ΔH_{st}	heat of adsorption, J kg^{-1}
ε	porosity
φ	a dependent variable
λ_{eff}	effective thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
μ	adsorptive viscosity, Ns m^{-2}
σ	collision diameter for Lennard–Jones potential, Å
Ω	collision integral
τ	tortuosity

Subscriptions

ads	adsorption
eff	effective
ev	evaporation
init	initial
o	outer
i	inner
s	adsorbent
sat	saturation
w	adsorbate
∞	equilibrium

and adsorptive density profiles in a thick granular silica gel bed are studied. The governing equations which are the heat and mass transfer equations for the bed and mass balance equation for the granule are presented and the solution method is described. The results are discussed via graphics which depict the variations of temperature, pressure, adsorbate concentration and adsorptive density in the radial direction of the bed during an adsorption process.

2. The annulus adsorbent bed

Fig. 1 shows the schematic view of the analyzed annulus adsorbent bed filled with the adsorbent granules. In this study, the adsorbent granules are silica gel grains and the adsorptive is water vapor. The adsorbent bed has a cylindrical annulus shape. The adsorptive can flow easily in the center of the annulus and enter with a uniform velocity to the portion filled with granules. The adsorptive flows from the inner surface, $R = R_i$, toward the outer surface, $R = R_o$. The upper and bottom

surfaces of the adsorbent bed are insulated and the transfer of heat and mass is assumed only in radial direction. The thermal resistance of the metal casing is neglected. The inner and outer radii of the annulus are $R_i = 0.06 \text{ m}$ and $R_o = 0.19 \text{ m}$. The equivalent radius of the adsorbent granule is $r_c = 0.0016 \text{ m}$. The study is performed for the adsorption process and three values of bed porosity as 0.1, 0.2 and 0.3.

3. Formulation of the problem

Two types of mass transfer occur in a granular adsorbent bed; mass transfer within the adsorbent granules and mass transfer through the voids between the granules (i.e. intra-particle and inter-particle mass transfers). The mechanism of heat and mass transfer in a granular adsorbent bed is complicated; hence some assumptions have to be made to pose the governing equations. The main employed assumptions in this study are; 1) the adsorbent bed consists of uniform size adsorbent granules, thus the bed porosity is assumed constant; 2) the adsorptive and adsorbent granules are in thermodynamic equilibrium; 3) the adsorptive behaves as an ideal gas; 4) thermal resistance within the adsorbent granule is neglected; 5) the temperature of an adsorbent granule equals to its surrounded adsorptive; 6) thermal properties of the adsorbent and adsorptive are constant; 7) heat transfer rate at $R = R_i$ is negligible.

3.1. Governing equations

Under the above assumptions, the governing equations for the problem can be written as:

$$\left((\rho C_p)_{\text{eff}} + \rho_s C_{pw} W \right) \frac{\partial T}{\partial t} = \lambda_{\text{eq}} \frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T}{\partial R} \right) - \frac{1}{R} \frac{\partial}{\partial R} (\rho_w C_{pw} R u T) + \rho_s \Delta H_{\text{st}} \frac{\partial W}{\partial t} \quad (1)$$

$$\frac{\partial \rho_w}{\partial t} + \left(\frac{1}{\varepsilon} \right) \rho_s \frac{\partial W}{\partial t} + \frac{1}{\varepsilon R} \frac{\partial}{\partial R} (R \rho_w u) = 0 \quad (2)$$

$$\frac{\partial W}{\partial t} = \frac{15 D_{\text{eff}}}{r_p^2} (W_\infty - W) \quad (3)$$

where W is the average adsorbate concentration. The Eqs. (1) and (2) are the heat and mass transfer equations for the adsorbent bed. As is seen, the heat and mass are transferred in the radial direction of the

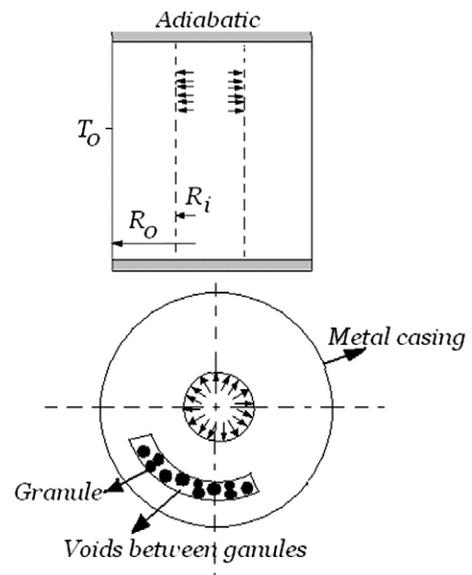


Fig. 1. A schematic view of the adsorbent bed.

bed and the effect of adsorption rate within the granule is contributed by $\partial W/\partial t$. The Eq. (3) represents the mass balance equation for the adsorbent granule. The distribution of adsorptive pressure in the bed can be found from the distribution of adsorptive density by using the ideal gas relation. By the application of ideal gas relation to the Darcy law, the following equation can be used to determine the velocity field.

$$u = -K_{app} \frac{R}{M\mu} \frac{\partial(\rho_w T_w)}{\partial r} \quad (4)$$

where R is the ideal gas constant and M represents molecular weight of adsorptive. The apparent permeability of the adsorbent bed, K_{app} , can be calculated by the following relation [12].

$$K_{app} = K + \frac{\varepsilon\mu}{\tau P} D_{bed} \quad (5)$$

where K is the inherent permeability of the adsorbent bed and it can be obtained by using Blake–Kozeny relation which is valid for void fractions less than $\varepsilon = 0.5$ [13].

$$K = \frac{r_p^2 \varepsilon^3}{37.5(1-\varepsilon)^2} \quad (6)$$

The symbol D_{bed} represents the diffusion flow due to the two diffusion mechanisms of the adsorptive in the adsorbent bed which are Knudsen and molecular diffusions. It can be predicted by the following relations [14].

$$\frac{1}{D_{bed}} = \frac{1}{D_m} + \frac{1}{D_K} \quad (7)$$

$$D_K = 97r_p \sqrt{T/M} \quad (8)$$

$$D_m = 0.02628 \frac{\sqrt{T^3/M}}{PO^2\Omega} \quad (9)$$

All physical and thermal properties of the silica gel and water are given in Table 1 [14–17]. The symbol W_∞ in Eq. (3) shows the equilibrium concentration of the adsorbate and it can be determined by the following model;

$$W_\infty = W_0 \left(\frac{P_{sat}}{P} \right)^{1/n} \quad (10)$$

where n represents linear driving for relationship constant and its value is given in Table 1. The effective mass diffusivity of the adsorbent

Table 1
Thermophysical properties of silica gel granule and water

Parameter	Symbol	Value
Molecular weight of water, kg mol ⁻¹	M	18
Density of adsorbent, kg m ⁻³	ρ_s	670
Specific heats of adsorbent, kJ kg ⁻¹ K ⁻¹	C_{p_s}	0.88
Specific heats of adsorptive 30 °C, kJ kg ⁻¹ K ⁻¹	C_{p_w}	4.1784
Thermal conductivity of adsorbent, kW m ⁻¹ K ⁻¹ [15]	λ_s	0.198×10^{-3}
Thermal conductivity of adsorptive, kW m ⁻¹ K ⁻¹ [16]	λ_w	1.96×10^{-5}
Heat of adsorption for water on silica gel, kJ kg ⁻¹ [15]	ΔH_{st}	2560
Limiting adsorption capacity of adsorbent kg _w kg _s ⁻¹	W_0	0.552
Linear driving force relationship constant	n	1.6
Reference diffusivity, m ² s ⁻¹ [15]	D_0	2.54×10^{-4}
Diffusion activation energy, J mol ⁻¹ [15]	E	4.2×10^4
Collision diameter for Lennard–Jones potential, Å [17]	σ	2.641
Collision integral [17]	Ω	2.236
Boltzmann's constant (J K ⁻¹ molecule ⁻¹) [16]	k	1.38×10^{-23}
Tortuosity [14]	τ	3
Viscosity of water vapor, kNs m ⁻² at 300K [16]	μ	9.09×10^{-9}

Table 2
Initial and boundary conditions for the problem

Dependent parameter	Boundary conditions at $R=R_i$	Boundary conditions at $R=R_o$	Initial condition at $t=0$
Temperature (K)	$\partial T/\partial R=0$	$T=300$	$T=300$
Adsorptive pressure (kPa)	$P=P_{ev}=1.917$	$\partial P/\partial R=0$	$P=f(t, \rho)$
Adsorptive density (kg/m ³)	$\rho_w=f(P, T)$	$\rho_w=f(P, T)$	$\rho_w \approx 0$
Amount of adsorbate (kg _w /kg _s)	$W=f(P, T)$	$W=f(P, T)$	$W=0$
Adsorptive velocity (m/s)	$U=f(\rho_w, K_{app})$	$\partial U/\partial R=0$	$U=0$

varies with the granule temperature and it can be calculated by using Arrhenius equation [15]:

$$D_{eff} = D_0 e^{-E/RT} \quad (11)$$

The effective thermal conductivity and effective thermal capacitance of the bed (ρC_p)_{eff} are determined as follows [18]:

$$\lambda_{eff} = \lambda_s^{(1-\varepsilon)} \lambda_w^\varepsilon \quad (12)$$

$$(\rho C_p)_{eff} = \varepsilon (\rho C_p)_w + (\rho C_p)_s \quad (13)$$

3.2. Initial and boundary conditions

The initial and boundary conditions for the unknown dependent variables which are temperature, adsorptive density, adsorbate concentration, adsorptive pressure and velocity during an adsorption process are presented in Table 2.

4. Solution procedure

The set of the governing equations are highly nonlinear and coupled. Furthermore, the mass diffusivity within the granule and the value of the adsorbent bed apparent permeability are function of the dependent variables. The governing equations are discretized in time and in radial direction of the bed, and solved by finite difference solution method. The finite difference forms of the convection and diffusion terms are written based on the central difference scheme and implicit method is applied. Firstly, the average adsorbate concentration within adsorbent granule is calculated by using granule mass balance equation (Eq. (3)). The energy equation (Eq. (1)) is solved to find the temperature in the adsorbent bed. Based on the obtained adsorbate concentration and temperature fields, the mass transfer equation for the adsorbent bed (Eq. (2)) is solved to determine the distribution of the adsorptive density. The pressure field and velocity distribution in the bed are determined by using the new values of the adsorptive density. An inner iteration is performed before increasing a time step. The inner iteration is continued until the following defined convergence criterion is satisfied;

$$\left| \frac{(\varphi^{n+1} - \varphi^n)}{\varphi^n \cdot \Delta t} \right|_{\max} < 10^{-4} \quad (14)$$

where n is a step of inner iteration and φ represents values of the temperature and adsorptive density. The criterion for the outer iteration which provides the termination of program is $W < 0.34$. The grid distribution is uniform and number of grids are 14. The computer code is written by FORTRAN language. The following equation is used

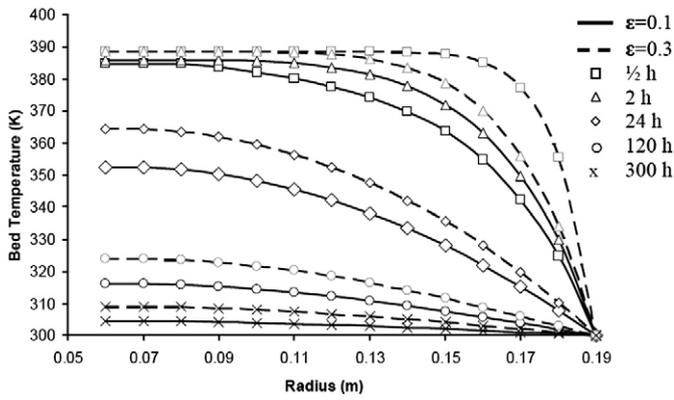


Fig. 2. The variations of bed temperature in the radial direction with time for two adsorbent beds.

to determine the average value of a dependent variable (T, P, ρ_w, W) in the bed.

$$\bar{\varphi}(t) = \frac{\int_{R_i}^{R_o} 2R\varphi(R, t)dR}{(R_o^2 - R_i^2)} \quad (15)$$

5. Results and discussions

The distributions of the bed temperature, adsorbate concentration, adsorptive density and pressure for 0.1 and 0.3 porosities during the adsorption process according to the initial and boundary conditions presented in Table 2 are illustrated in Figs. 2–5. The temperature distribution in the bed can be seen from Fig. 2. The temperature of the bed initially is at 300 K. The temperature of both adsorbent beds increases with time due to the adsorption of adsorptive. The differences between the thermal behaviors of 0.1 and 0.3 porosity cases can be observed. After half an hour, the temperature at the inner shell of annulus with $\varepsilon=0.1$ rapidly rises such that it becomes as $T=384$ K at $R=R_i$. The low thermal conductivity of the bed reduces the transfer of generated heat to the outer surface of the bed maintained at $T=300$ K and therefore the temperature of the inner region increases. For $\varepsilon=0.3$, the temperature at the inner shell of annulus increases more compared to the increase of bed temperature with $\varepsilon=0.1$ due to its lower thermal conductivity. The adsorbent temperature at inner shell of annulus reaches 388 K after 30 min for the 0.3 porosity. Due to the decreasing of the adsorption rate, the temperature of the bed decreases with time and the temperature of the bed with $\varepsilon=0.1$ at $R=R_i$ falls to $T=350$ K after 24 h. This value for the bed with

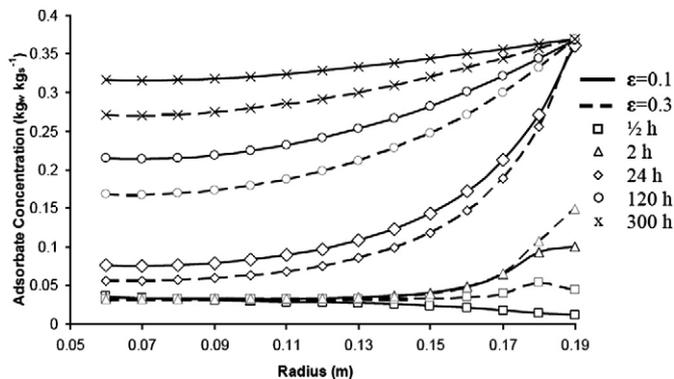


Fig. 3. The changes of adsorbate concentration in the radial direction with time for two adsorbent beds.

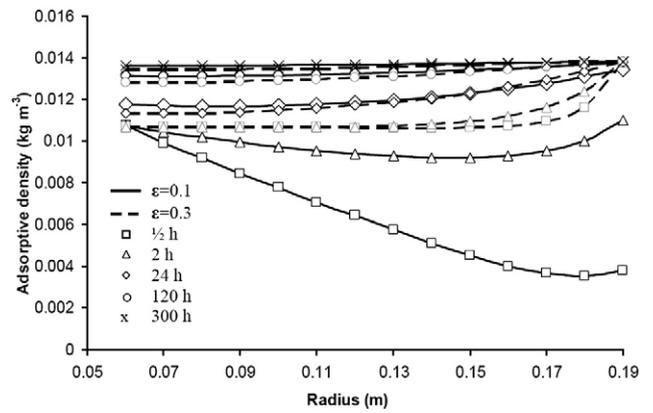


Fig. 4. The variations of adsorptive density in the radial direction with time for two adsorbent beds.

$\varepsilon=0.3$ is $T=360$ K. The adsorption rate and consequently the generation of heat in the bed decrease with time and finally the bed temperature reaches to the outer surface temperature which is 300 K.

The adsorbate concentration profiles in the bed during the adsorption process are shown in Fig. 3. The initial value of the adsorbate concentration is zero and it reaches to $0.34 \text{ kg}_w \text{ kg}_s^{-1}$ (or 34%) when the computer program is terminated. As is seen, the adsorbate concentration in the bed increases with time. For the bed with $\varepsilon=0.1$ at 1/2 h, the adsorbate concentration at the inner shell of the annulus, where the adsorptive enters, is slightly higher than the adsorbate concentration at the outer shell. However; the same behavior is not observed for the bed with $\varepsilon=0.3$. For the adsorbent bed with $\varepsilon=0.3$ at 1/2 h, the adsorbate concentration in the outer region is higher than the concentration at the inner shell of the annulus bed. The increase of porosity reduces the mass transfer resistance; hence the adsorptive reaches to the outer region of the bed faster. The temperature at the outer shell of annulus (at $R=R_o$) is lower than the inner shell of annulus temperature and therefore the adsorption rate at the outer shell of annulus is higher. After 24 h, the adsorbate concentration at the outer surface reaches to its maximum value while a small change of the concentration is seen in the inner region of the annulus. This behavior of the adsorptive transfer clearly shows that the thermal resistance of the bed controls the heat and mass transfer through the bed. The temperature at the inner shell of annulus decreases by time and as a result the adsorbate concentration increases. Although the adsorbate concentration in the bed with $\varepsilon=0.3$ is higher than the adsorbate concentration of the bed with $\varepsilon=0.1$ at the beginning periods of the adsorption process, it becomes below the concentration of $\varepsilon=0.1$ due to the high rate of heat transfer in the bed with smaller porosity.

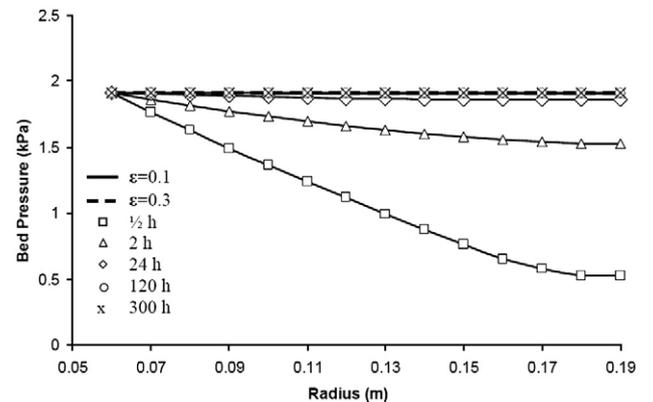


Fig. 5. The changes of bed pressure in the radial direction with time for two adsorbent beds.

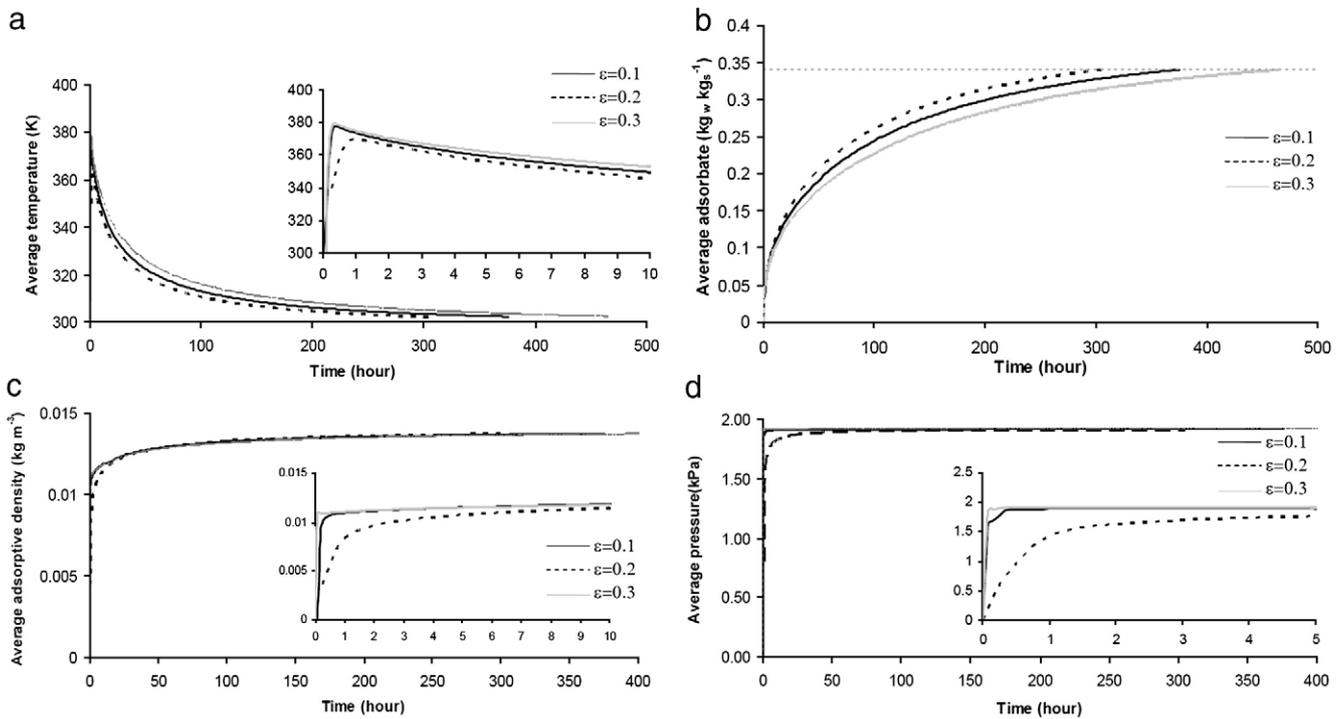


Fig. 6. The averages of temperature, adsorbate concentration, adsorptive density and pressure during the adsorption process for three different adsorbent beds, a) average temperature, b) average adsorbate concentration, c) average adsorptive density, d) average pressure.

The variation of the adsorptive density through the bed during the adsorption process is shown in Fig. 4. Initially, there is no adsorptive in the bed. For $\epsilon=0.1$, a steep density gradient is seen after the first 30 min since slow adsorptive transfer between the granules exists. For the case of $\epsilon=0.3$, the distribution of the adsorptive density in radial direction is completely different. There is small adsorptive density gradient in the most regions of the bed except in the region close to the outer shell because of temperature. The adsorptive density in the outer region of the bed is higher due to the lower temperature of this region. The adsorptive density profiles of two cases approach to each other because of slow rate of adsorption in the bed with $\epsilon=0.3$.

The variations of adsorptive pressure for both cases are shown in Fig. 5. The low porosity of the bed with $\epsilon=0.1$ causes a steep pressure gradient in the radial direction at the beginning of the process as seen from the pressure profile for $t=1/2$ h. The gradient of pressure in the radial direction decreases with the increasing of time. The pressure distribution of the bed with $\epsilon=0.3$ is different. The gradient of pressure for $t=1/2$ h and $t=2$ h is considerably smaller than the gradients of the bed with $\epsilon=0.1$ due to the larger voids between the granules. It should be mentioned that the pressure distribution in the radial direction for $\epsilon=0.3$ in Fig. 5 may seem uniform due to the scale of the Y axis chosen to plot the pressure distributions for the both beds in a graphic. There is no doubt that, a pressure gradient and consequently an adsorptive flow in the radial direction must exist until the final equilibrium condition.

The averages of the bed temperature, adsorbate concentration, adsorptive density and pressure during the adsorption process are shown in Fig. 6. The averages of these dependent variables are calculated by using Eq. (15). The change of average temperature during the adsorption process is presented in Fig. 6(a). For the starting period, the variation of average temperature is also shown as a small graph in Fig. 6(a) due to the rapid increase of average temperature at the beginning of the adsorption process. After starting of the adsorption process, the temperature of the bed rapidly increases due to the generated heat in the bed. For $\epsilon=0.1$, the average bed temperature rapidly increases from 300 K to 370 K. The increase of the porosity from 0.1 to 0.2 causes the rise of the maximum average

temperature and the maximum temperature becomes as 378 K. The average temperature increases with the increase of porosity since the generated heat cannot be transferred to the outer shell of annulus due to the poor thermal conductivity. The increase of porosity from 0.2 to 0.3 has a smaller effect on the maximum average temperature. Further increase of porosity reduces the amount of adsorbent granules in the bed and the amount of the generated heat in the bed. After the maximum temperature, the average temperature slowly decays with time and reaches to the outer surface temperature for the three adsorbent beds.

The variations of the average adsorbate concentration with time for the three beds are shown in Fig. 6(b). The increase of porosity extends the period of adsorption process. As it was mentioned before, mass transfer rate within a granule decreases with increase of temperature. The increase of porosity reduces the thermal conductivity of bed and extends the required time for transferring the generated heat from the bed to the environment. The periods of adsorption process in order to reach to the limiting adsorbate concentration which is $0.34 \text{ kg}_w \text{ kg}_s^{-1}$ for the beds with porosities as 0.1, 0.2 and 0.3 are 304, 376 and 465 h, respectively.

The variations of the average adsorptive density and pressure are shown in Fig. 6(c) and (d), respectively. After starting of adsorption process, the averages of both dependent variables rapidly approach to the steady state. These graphics again reveal that the thermal resistance of the bed controls heat and mass transfer through the bed for the studied granular adsorbent since both the adsorptive density and pressure values rapidly attain to the final equilibrium condition.

6. Summary remarks

The heat and mass transfer in a cylindrical annulus adsorbent bed filled with silica gel granules during adsorption of the water vapor are numerically analyzed. The governing equations are solved by finite difference method for three different porosity values as 0.1, 0.2 and 0.3. After starting of the adsorption process, the temperature of the adsorbent bed rapidly increases due to the generated heat by

adsorption. The bed temperature at $R=R_i$ reaches to 370, 378 and 380 K for 0.1, 0.2 and 0.3 porosity values. The increase of porosity reduces the thermal conductivity of the bed, heat transfer rate in the bed and the period of the adsorption process. A steep pressure gradient in the radial direction of the bed having low porosity occurs at the beginning of the adsorption process, but the gradient disappears after a short period.

For the studied adsorbent bed and porosity values, the averages of both pressure and adsorptive density rapidly increase and approach to the steady condition; however the changes of the temperature and adsorbate concentration parameters are slow. Thermal resistance controls heat and mass transfer through the studied bed and the increase of thermal conductivity of the bed without decreasing mass diffusivity improves heat and mass transfer rates in the bed.

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