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ANALYSIS OF HEAT AND MASS TRANSFER IN THE ADSORBENT BED OF A THERMAL WAVE ADSORPTION COOLING CYCLE

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ABSTRACT

A coupled heat and mass transfer analysis of the adsorbent bed of a thermal wave adsorption cooling cycle is performed. The adsorbent bed is modeled two dimensionally. Governing equations for energy, mass and momentum transfers are solved by Comsol Multiphysics simultaneously. Variations of temperature, pressure, adsorption capacity, equilibrium adsorption capacity and mass transfer coefficient for a finless tube adsorbent bed are presented with multicolored plots. Desorption process is simulated in the model. Results show that the adsorbent bed reaches the maximum cycle temperature uniformly after 5000s. Uniform pressure assumption can be used in the bed due to small pressure gradient during the process. Adsorption capacity decreases from 26.1% to 8.89% in 5000s. Temperature front progresses along the bed creating a thermal wave. The thermal wave length is needed to be short to enhance the bed effectiveness regenerating more heat between the beds of the thermal wave cycle. It can be concluded that a parametric study is recommended for a future work in order to investigate the effects of design and operational parameters on the dependent variables and thermal wave length.

INTRODUCTION

Energy consumption all around the world increases uncontrollably. Using electricity for heating and cooling demands causes a significant increase in the consumption of fossil based fuels that cause the global warming. Sustainable energy solutions must be found to meet the growing energy demand. Adsorption cooling technology is a sustainable solution to the energy problem as it can use waste or solar energy instead of electricity. Many researches on adsorption cooling cycles are performed [1-4]. Basic adsorption cooling cycles are intermittent and nonregenerative since they have a single adsorbent bed. On the other hand, thermal wave cycles are both continuous and regenerative since they have at least two beds. Heat and mass recovery can be made between the beds to increase specific cooling power (SCP) and coefficient of performance (COP).

NOMENCLATURE

A_i	[m^2]	HTF tube inner surface area
A_o	[m^2]	HTF tube outer surface area
b	[m]	HTF tube thickness
c	[J/kgK]	Specific heat
D_o	[m^2/s]	Reference diffusivity
E_a	[J/mol]	Activation energy of surface diffusion
h_i	[W/m^2K]	Convective heat transfer coefficient between tube and fluid
h_o	[W/m^2K]	Wall heat transfer coefficient between tube and adsorbent
k	[W/mK]	Thermal conductivity
P	[Pa]	Pressure
R	[J/molK]	Universal gas constant
R_v	[J/kgK]	Ideal gas constant for water vapor
r	[m]	Radius
T	[K]	Temperature
t	[s]	Time
$\mathbf{u}$	[m/s]	Vapor velocity vector
X	[kg_w/kg_s]	Amount of water vapor adsorbed by adsorbent per unit mass of adsorbent
v_{ave}	[m/s]	HTF mean velocity
v_f	[m/s]	HTF velocity
V	[m^3]	Volume

Special characters

ε	[-]	Total porosity
κ	[m^2]	Permeability
μ	[kg/ms]	Dynamic viscosity
ρ	[kg/m^3]	Density

Subscripts

f	Fluid
p	Particle
s	Adsorbent
sat	Saturation
t	Tube
v	Vapor

Several studies were made on thermal wave cycles. COP limits were predicted by Baker [5] for an ideal cycle with thermal regeneration using energy and exergy models. Critoph first proposed a forced convection adsorption cycle that achieves heat transfer enhancement by storing heat in a packed bed of inert material [6]. Tierney [7] investigated the effects of heat capacity and thermal conductivity of both refrigerant and adsorbent bed on SCP and COP for a convective thermal wave cycle. Entropy production concept was used for comparing COP of a thermal wave cycle with Carnot COP and thermal coupling between the adsorbers and heat reservoirs was seen to cause low COPs [8]. Local equilibrium assumption was used and the effects of resistances on heat and mass transfer were neglected to provide the asymptotic maximum performance obtainable from a thermal wave cycle [9]. Qu et al. [10] investigated the influence of mass and heat recovery on SCP and COP and results showed that a thermal wave cycle with mass and heat recovery had the highest COP amoung the cycles examined. Taylan et al. [11] modeled thermal wave cycles without mass recovery, with adiabatic mass recovery and with isothermal mass recovery.

The adsorbent bed of adsorption cooling cycle is especially focused on by several researchers since heat and mass transfer inside the bed have significant influence on the system performance. COP can be improved significantly as the mass and especially heat transfer inside the bed are enhanced. Poor heat and mass transfer problem was handled by several models that investigates system parameters affecting the performance. Pons et al. [12] investigated the thermal regeneration process for a straight tube adsorber defining two dimensionless parameters, number of transfer units and dimensionless outlet fluid temperature. Using these dimensionless parameters, Pons also investigated the axial temperature profile [13] and entropic mean temperature profile [14] in the adsorber. A one dimensional, coupled heat and mass transfer model was used for investigating temperature and pressure profiles and it was concluded that for low operating pressures, uniform-pressure assumption was not acceptable due to poor mass transfer [15].

In this paper, a two dimensional model that analyses transient coupled heat and mass transfer in the adsorbent bed is presented. The shape of thermal wave formed in a finless tube adsorbent bed is investigated during the desorption process of the cycle. In the literature, analyses were generally made by one-dimensional models. There is a gap in a two-dimensional solution and representation of heat and mass transfer in the adsorbent bed. The variations of temperature, pressure, adsorption capacity, equilibrium adsorption capacity and mass transfer coefficient are represented two dimensionally by multicolored plots. In the model, temperatures of adsorbent (solid), adsorbate (liquid) and adsorptive (vapor) are taken equal to each other using local temperature equilibrium assumption.

MODEL DESCRIPTION

There are three subdomains in the model and they have a cylindrical geometry. The three subdomains are heat transfer fluid (HTF) flowing inside a tube, the tube itself, an adsorbent bed. The adsorbent bed is also called porous media since it is filled with a porous material like zeolite, silica gel or activated carbon. Porous materials have very large surface area and can adsorb refrigerant vapor into their pores. 3-D and 2-D geometry of the model is represented in Figure 1.

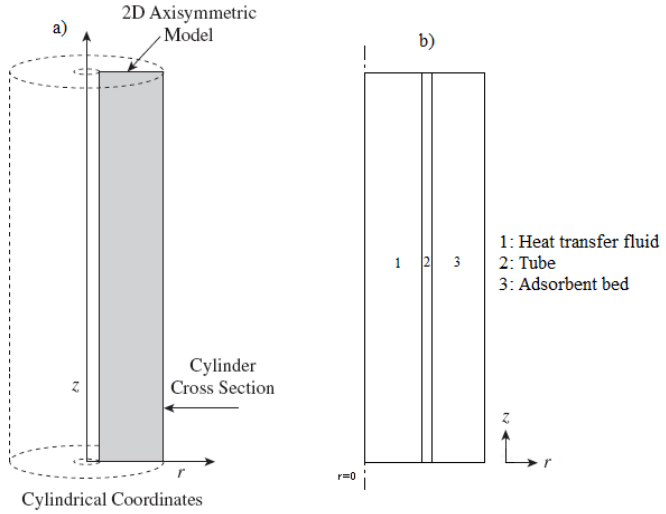

Figure 1 a) 3-D, b) 2-D model geometry

The three subdomains, the HTF, tube and adsorbent bed, are placed in a vacuum chamber. Refrigerant vapor flows inside or outside the vacuum chamber during the processes of cycle and the adsorbent bed adsorb or desorb the vapor in this vacuum chamber. 3-D model can be reduced to 2-D axisymmetric model by using the symmetry in tangential direction of the cylinder in Figure 1 (a). The 2-D model can be simulated faster and more accurately avoiding from the complexity of 3-D model whereas the 3-D model can result in less accurate results because of its limitations on the number of mesh elements. Only one side of the axis line is taken in Fig. 1 (b) since there is also an axial symmetry. It should be noted that 3-D simulation is necessary if the model has not symmetry in tangential direction and cannot be reduced to 2-D like in the case of using a rectangular adsorbent bed instead of the cylindrical geometry.

MATHEMATICAL MODEL

Energy equation for the HTF and tube, and energy, mass and momentum equations for the adsorbent bed are solved. Energy equation for the HTF including conduction and convection heat transfers can be written as [16]:

$$k_f \nabla^2 T_f = \rho_f c_f \frac{\partial T_f}{\partial t} + \rho_f c_f v_f \nabla T_f + \frac{2}{r_t} h_i (T_f - T_t) \qquad (1)$$

Velocity of HTF can be expressed as following for a fully developed laminar flow:

$$v_f = 2 v_{ave} \left(1 - \frac{r^2}{r_t^2} \right) \qquad (2)$$

Energy equation for the HTF tube including the heat conduction in the tube can be written as [16]:

$$k_t \nabla^2 T_t + \frac{h_i A_i}{V_t} (T_f - T_t) = \rho_t c_t \frac{\partial T_t}{\partial t} + \frac{h_o A_o}{V_t} (T_t - T_s) \qquad (3)$$

Energy balance in a porous media has a complex form due to three different phases; solid, gas and adsorbate phases. The energy equation in the adsorbent bed can be written as follows [17]:

$$0=(1-\varepsilon)\rho_s c_s\frac{\partial T_s}{\partial t}+\varepsilon\rho_v c_v\frac{\partial T_s}{\partial t}+(1-\varepsilon)\rho_s X c_l\frac{\partial T_s}{\partial t} -(1-\varepsilon)\rho_s\left|\Delta H\right|\frac{\partial X}{\partial t}-\varepsilon\frac{\partial P}{\partial t}-k_s\nabla^2 T_s+\rho_v c_{p,v}\mathbf{u}\nabla T_s +\frac{h_o A_o}{V_s}(T_s-T_t) \quad (4)$$

In equation (4), temperatures of adsorbent material, refrigerant vapor and adsorbate are taken equal to each other using local thermal equilibrium assumption. ΔH represents heat of adsorption and is taken as constant. The adsorbate that is refrigerant adsorbed by the adsorbent is assumed to be in liquid phase. c_v and c_l represent specific heats of refrigerant in vapor and liquid phases, respectively, and they are taken as constant. The working pair examined in the present study is zeolite-water pair which is operated under vacuum conditions. Water vapor behaves as an ideal gas in low pressure conditions and its density can be calculated by ideal gas relation:

$$P=\rho_v R_v T_s \quad (5)$$

The momentum equation for the adsorbent bed can be expressed by Darcy flow that gives a relation between refrigerant gas velocity and pressure:

$$\mathbf{u}=-\frac{\kappa}{\mu}\nabla P \quad (6)$$

Conservation of refrigerant mass in the adsorbent bed can be written as follows [17], neglecting diffusive mass transfer:

$$\varepsilon\frac{\partial\rho_v}{\partial t}+(1-\varepsilon)\rho_s\frac{\partial X}{\partial t}+\nabla(\mathbf{u}\rho_v)=0 \quad (7)$$

Adsorption capacity, X, can be found by Linear Driving Force (LDF) model that estimates the desorption rate assuming a parabolic concentration profile within the adsorbent particle [18]:

$$\frac{\partial X}{\partial t}=k_m(X_e-X) \quad (8)$$

The internal mass transfer coefficient, k_m, can be calculated by the following expression [18]:

$$k_m=\frac{15}{r_p^{\,2}}D_o\exp\left(-\frac{E_a}{RT_s}\right) \quad (9)$$

Dubinin–Astakhov equation is used for the equilibrium adsorption capacity, X_e, [19]:

$$X_e=X_o\exp\left[-B\left(\frac{T_s}{T_{sat}}-1\right)^n\right]$$

Coefficients X_o, B and n can be taken as 0.261, 5.36 and 1.73 respectively for zeolite-water pair [3].

Initial and boundary conditions

Temperature distributions for HTF, tube and adsorbent bed are initially uniform at cycle cooling temperature:

$$T_f(t=0,r,z)=T_t(t=0,r,z)=T_s(t=0,r,z)=T_i \quad (10)$$

Pressure and adsorption capacity in the bed are also initially uniform at condenser pressure (P_c) and maximum adsorption capacity (X_o) respectively:

$$P(t=0,r,z)=P_c,\quad X(t=0,r,z)=X_o \quad (11)$$

The HTF tube is insulated at the inlet and outlet of the adsorbent bed and this yields no temperature gradient at $z=0$ and $z=L$. Furthermore, there is no temperature gradient in HTF in the axial direction at the tube outlet due to the insulation. The adsorbent bed is also insulated on both sides. The presence of adjacent bed elements undergoing the same cycle yields a reflective condition on the lateral surface of the bed, $r=r_{bed}$. These conditions are all represented as follows:

$$\frac{\partial T_t}{\partial z}(t,r,z=0)=\frac{\partial T_t}{\partial z}(t,r,z=L)=\frac{\partial T_f}{\partial z}(t,r,z=L)=0,\qquad \frac{\partial T_s}{\partial z}(t,r,z=0)=\frac{\partial T_s}{\partial z}(t,r,z=L)=\frac{\partial T_s}{\partial r}(t,r=r_{bed},z)=0 \quad (12)$$

Heat conduction into the adsorbent bed is equal to heat transfer from the tube wall, $r=r_t$, yielding:

$$-k_s\frac{\partial T_s}{\partial r}(t,r=r_t,z)=h_o(T_t-T_s) \quad (13)$$

HTF enters the tube from the bottom side ($z=0$) at constant heating temperature yielding the following boundary condition:

$$T_f(t,r,z=0)=T_{hot} \quad (14)$$

On the other hand, at the other boundaries $z=0$, $z=L$ and $r=r_{bed}$, the adsorbent bed is open to the vacuum chamber that enables the refrigerant vapor to flow out at condenser pressure during desorption process. These boundary conditions can be given as follows:

$$P(t,r,z=0)=P(t,r,z=L)=P(t,r=r_{bed},z)=P_c \quad (15)$$

The flow of refrigerant vapor is restricted at the boundary $r=r_t$ since the surface at this boundary is enclosed by the tube wall. Therefore the pressure gradient at this boundary in the adsorbent bed is zero:

$$\frac{\partial P}{\partial r}(t,r=r_t,z)=0 \quad (16)$$

Model parameters used in simulations are given in Table 1.

Table 1
Model parameters [3,17]

Parameter	Value	Unit
c_f	1930	J/kgK
$c_{p,l}$	4180	J/kgK
$c_{p,v}$	1880	J/kgK
c_s	837	J/kgK
c_t	385	J/kgK
D_o	5.8e-9	m^2/s
E_a	1e4	J/mol
h_o	100	W/m^2K
k_f	0.115	W/mK
k_t	400	W/mK
P_c	4.247	kPa
R	8314	J/molK
R_v	461.5	J/kgK
r_p	1e-3	M

T_{hot}	473	K
T_i	313	K
X_o	0.261	kg_w/kg_s
ΔH	3300	kj/kg
ε	0.635	
κ	5e-12	m^2
μ	1e-5	kg/ms
ρ_f	914	kg/m^3
ρ_s	1000	kg/m^3
ρ_t	8700	kg/m^3
b	0.001	m
L	0.25	m
r_t	0.01	m

RESULTS AND DISCUSSION

Fully coupled model that includes heat, mass and momentum transfers is simultaneously solved by Comsol Multiphysics software package. In this model, temperature distributions for the HTF, tube and adsorbent bed, and variations of pressure, adsorption capacity, equilibrium adsorption capacity and mass transfer coefficient in the adsorbent bed are investigated for desorption process. Solutions are presented by domain plots that show the results in multi-colored 2D domain.

The model geometry is meshed by using extremely fine mesh having 15656 triangular elements. To test the mesh goodness, the model also simulated with the increasing number of mesh elements. Meshing the model with 44560 elements changed the results only ±0.2% at most. Solver parameter has a relative tolerance of 0.01 and an absolute tolerance 0.001 enabling high accuracy and convergence. The model is solved with a time step of one second, but results are presented for only the times t=0s, t=100s, t=1000s and t=5000s for brevity.

Temperature distributions in the HTF, tube and adsorbent bed are presented in Figure 1. The adsorbent bed reaches a uniform temperature after about 5000s. A poor heat transfer is seen in radial direction inside the adsorbent bed. A thermal wave or temperature front is formed in the adsorbent bed by heat transfer from HTF. However, the thermal wave length is long due to poor heat transfer in the bed. Thermal wave length is a key factor for a thermal wave adsorption cooling cycle to obtain high heat regeneration between the beds of the cycles [20,21]. High heat regeneration between the beds provides high performance. For this reason, thermal wave length should be shortened by enhancing heat transfer in radial direction inside the bed. Researches have focused on this problem and have performed several experimental studies [1]. In the present study, a finless tube adsorbent bed with an equivalent thermal conductivity of 0.5 W/mK is examined. Modifying the geometry with a finned tube and increasing the thermal conductivity of the bed, one can enhance the heat transfer in the bed.

Operating conditions also influence the heat transfer in the adsorbent bed. HTF enters the tube and reaches the cycle maximum temperature (423 K) in a short time as seen in Figure 2. This is due to high HTF velocity. Average HTF velocity is taken as 0.005 m/s in this study. HTF transfer its energy not in radial direction but axial direction. If lower velocities are used HTF can transfer more heat in radial direction yielding a straighter thermal wave. Thus, heat regeneration and cycle performance can be enhanced. It can be concluded that a parametric study is needed for investigating the effect of design and operating parameters on the heat transfer inside the bed.

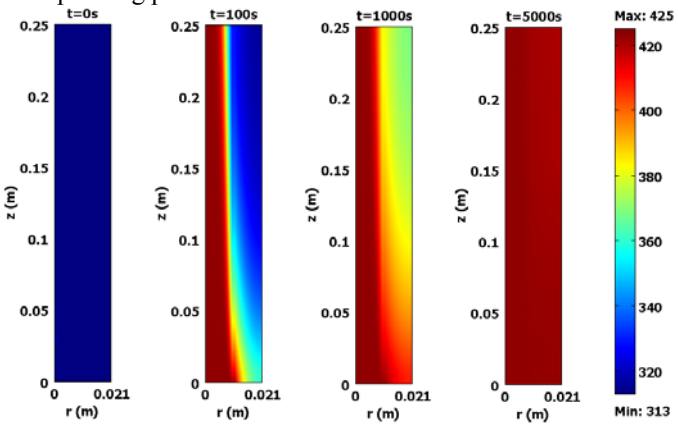

Figure 2 Temperature distributions in the HTF, tube and adsorbent bed with time (K)

Pressure distribution in the adsorbent bed is shown in Figure 3. Depending on the boundary conditions, pressure starts to increase at the region where temperature increases. The pressure wave expands to upward as temperature increases. The increase in pressure is due to mass transfer resistances as refrigerant vapor is desorbed and removed from the adsorbent material. The permeability of the adsorbent bed has significant effect on the vapor flow through the adsorbent particles. For larger permeability values, the resistance to mass transfer decreases and hence the vapor passes easier through the adsorbent particles yielding smaller pressure gradients in the bed. In Figure 3, pressure inside the adsorbent bed returns to its initial value after 5000s since desorption process is completed and the vapor flow is ended. Pressure varies between 4247-4545 Pa during the process. Consequently, the pressure gradient in the bed is not so significant and the pressure may be assumed uniform over the bed.

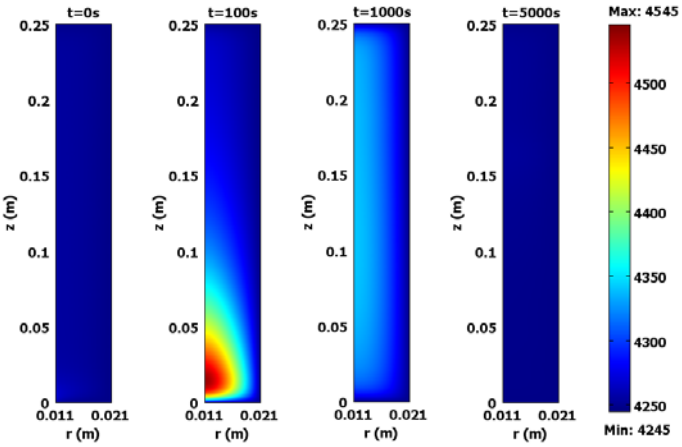

Figure 3 Pressure distribution in the adsorbent bed with time (Pa)

Figure 4 and Figure 5 represent the variations of adsorption capacity and equilibrium adsorption capacity, respectively. As the bed is heated, the adsorption capacity and equilibrium adsorption capacity decrease as expected from desorption process. At the beginning of the desorption process, the adsorption capacity decreases slowly due to the mass transfer resistances as expressed in the discussion of pressure variation. However, equilibrium adsorption capacity shows a similar profile with the temperature. The equilibrium adsorption capacity is theoretical maximum capacity which the adsorbent bed can desorb at given conditions. In practice, it takes a long time to reach the equilibrium state and LDF model can estimate the practical desorption rate taking the adsorption kinetics into account. Adsorption capacity varies between 0.261-0.0889 (26.1%-8.89%) kg water per kg adsorbent material.

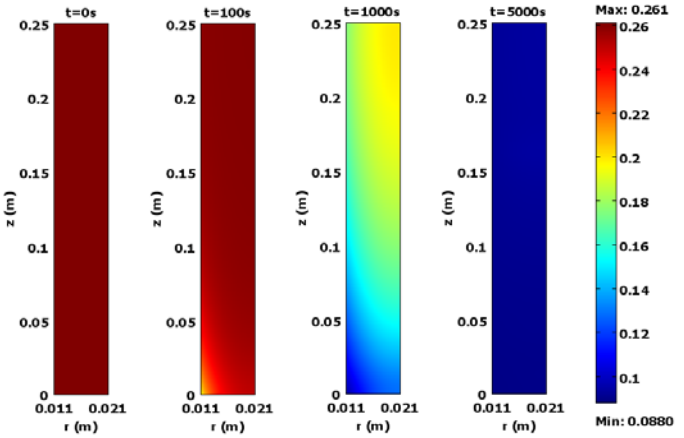

Figure 4 Variation of adsorption capacity in the adsorbent bed with time (kg_w/kg_s)

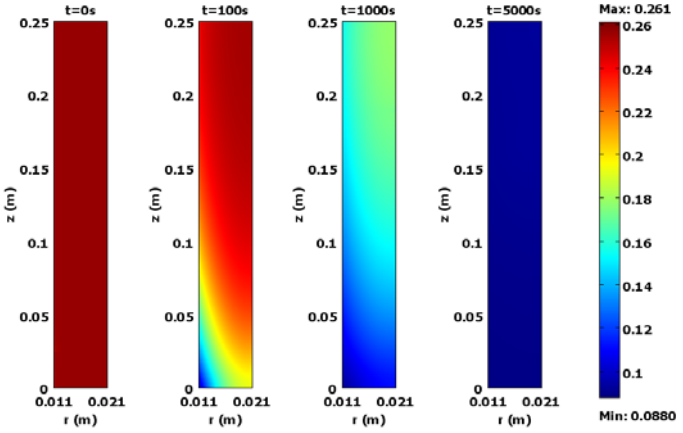

Figure 5 Variation of equilibrium adsorption capacity in the adsorbent bed with time (kg_w/kg_s)

Variation of the mass transfer coefficient in the bed is represented in Figure 6. The mass transfer coefficient varies between 0.00186-0.0052 1/s during the process. It increases with time and shows a behavior similar to temperature since it depends only on the adsorbent temperature for a fixed particle size and fixed adsorbent/refrigerant pair as understood from equation (9). The increase in the mass transfer coefficient implies the increase in desorption rate or decrease in adsorption capacity. On the other hand, the mass transfer coefficient changes for different particle sizes and different pairs. When particle size is increased, for example, a uniform mass transfer coefficient with high value may be expected since mass transfer resistances will decrease. A further study may be performed for investigating the effects of design parameters on the mass transfer coefficient.

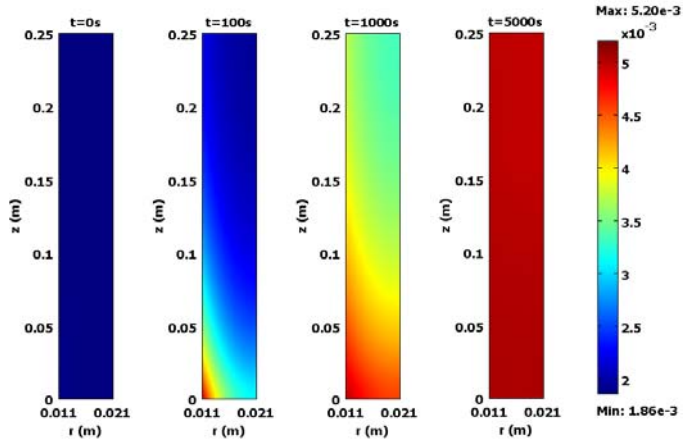

Figure 6 Variation of mass transfer coefficient in the adsorbent bed with time (1/s)

CONCLUSION

A finless tube type adsorbent bed has been analyzed two dimensionally for the coupled heat and mass transfer based on a thermal wave adsorption cooling cycle. Zeolite-water pair is used for simulations. Temperature and pressure distributions and variations of adsorption capacity, equilibrium adsorption capacity and mass transfer coefficient are investigated. Pressure inside the bed varies between 4245-4545 Pa and may be assumed to be uniform throughout the process. Adsorption capacity varies between 0.261-0.0889 kg water per kg zeolite. The mass transfer coefficient varies between 0.00186-0.0052 1/s and has a similar wave with temperature due to its temperature dependence.

The results presented are valid for model parameters used in this study. A parametric study that investigates the effects of design and operation parameters on the distributions is recommended. In this way, solutions for enhancing the heat transfer in the adsorbent bed and the performance of a thermal wave cycle may be developed. This type of parametric study is planned for the future work.

ACKNOWLEDGEMENTS

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