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Comparison between heat transfer and heat mass transfer models for transportation process in an adsorbent bed

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Abstract

The heat and mass transfer (HMT) model for transportation process in adsorbent bed is studied in relation to heat transfer (HT) model, which is dependent on assumptions such as the conduction dominance and negligible mass transfer resistance. Two general criteria are generated by performing an order of magnitude analysis to determine when the HT model can be applied in practical situation as a good approximation in the evaluation of the temperature field as well as dimensionless uptake and the criteria are validated with the numerical results. It is seen that the criterion for conduction dominance (CR1) is usually satisfied for all practical situations, but the criterion towards negligible mass transfer resistance (CR2) turns out to be more important for the selection of an appropriate model.

Keywords: Adsorption; Criterion; Model; Numerical analysis

1. Introduction

Accurate, time-dependent, spatially resolved predictions of heat transfer and desorption/adsorption rate in the adsorbent bed will be of great assistance in the design of the recently introduced adsorption cooling and heat pump. Various analytical and numerical studies on performance of adsorbent bed can generally be classified under two groups: (i) heat transfer model (HT) and (ii) heat and mass transfer model (HMT) [1].

Several researchers have used the heat transfer model to obtain temperature distributions in a porous medium with uniform pressure distribution, owing to its simplicity [2–5]. Guilleminot et al. [2] introduced the uniform pressure model to analyze the heat transfer in a fixed bed of solid adsorbent in a finned reactor of rectangular cross-section. Later, Hajji et al. [4,5] have presented a numerical and experimental analysis of the adsorption process and reported that the assumption of uniform pressure is valid only when the rate of heat transfer to or from the adsorbent is sufficiently slow.

The above listed models based on uniform pressure distribution have invariably neglected the mass transfer phenomenon and have failed to justify their approach. An analysis on the influence of mass transfer phenomena in the adsorbent bed can be avoided under following situations only: (i) convection heat transfer is small, i.e. when conduction is the dominant heat transfer mode; (ii) there exists negligible resistance to the desorbed/adsorbed vapor flow, and the desorption/adsorption occurs at uniform pressure. The heat transfer model (HT) is sufficient enough to analyze heat transfer in an adsorbent bed provided the above two mentioned aspects/assumptions, such as: (i) conduction dominance; (ii) negligible mass transfer resistance are valid in the adsorbent side. Though a wide range of engineering applications can be limited to the above said assumptions, there do occur certain situations, that one has to reckon to heat and mass transfer analysis. That is, when the mass transfer is far from zero, the Heat Transfer model need to be replaced with the Heat and Mass

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Nomenclature

c	constant in Dn_2
c_p	specific heat at a constant pressure (kJ/kg K)
d_p	diameter of adsorbent particles (m)
Diff_T	percentage difference for temperature calculated
Diff_w	percentage difference for uptake of adsorbate calculated
Dn_1	potential number
Dn_2	dimensionless heat transfer rate
h	heat transfer coefficient (W/m^2 K)
ΔH	heat of adsorption (J/kg)
k	thermal conductivity (W/m K); constant parameter of adsorption equilibrium equation (21)
k_D	permeability of porous media (m^2)
L	adsorbent thickness (m)
m	mass (kg)
$\dot{m}$	mass flow rate (kg/m^2 s)
n	constant parameter of adsorption equilibrium equation (21)
p	pressure (Pa)
q	local heat transfer rate (W/m^2)
Q	heat transfer rate (W/m^2)
r	radial coordinate in the adsorbent bed
R	gas constant, (J/mol K); radius of the cylindrical adsorbent bed (m)
R_k	thermal conductivity ratio
R_p	dimensionless pressure difference
R_ρ	density ratio
s	dependent variable
S	cross section area of adsorbent (m^2)
t	time (s)
T	temperature (K)
u	velocity (m/s)
V	volume of adsorbent (m^3)
w	mass adsorption capacity (kg/kg adsorbent)
w_0	maximum mass adsorption capacity (kg/kg adsorbent)
x, y, z	axial coordinate

Greek symbols

α	thermal diffusivity (m^2/s)
ε_t	total porosity of adsorbent bed
μ	viscosity (N s/m^2)
ρ	density (kg/m^3)
σ	convergence tolerance
ω	dimensionless uptake

Subscripts

a	adsorbate
b	bed
c	condenser
cd	conduction
cv	convection
e	evaporator
eff	effective
h	high temperature heat source
in	initial
m	metal
p	constant pressure
r	refrigerant
sat	saturation
t	total
ti	inner metal tube
to	outer metal tube
v	vapour
z	adsorbent

Transfer model, so that the conduction and the fluid flow or mass diffusion can be treated for a perfect analysis simultaneously. Similarly, when the mass transfer resistance is significant, the desorption/adsorption processes are controlled by the mass transfer, and hence, the mass transfer equation should also be included. However, an analysis of transport process in a porous medium based on the heat and mass transfer is more complex because it requires more detail information on the properties of adsorbent and the numerical calculation is time consuming, especially when dealing with two-dimensional or three-dimensional models. Due to the said difficulties, investigators have mostly used the heat transfer model with certain limitations to obtain temperature distributions in a porous adsorbent medium without examining the validity of the above-mentioned two assumptions.

In recent years, more attention is given to the models that include both heat and mass transfer so as to obtain accurate results. Sun et al. [6] have developed a model to study the performance of a long cylindrical adsorbent bed. Besides considering the one dimensional heat balance equations, the mass balance of refrigerant in the adsorbent bed has also been taken into account. A more complex, three-dimensional heat and mass transfer numerical analysis had been proposed by Zhang et al. [7]. The most recent model in this category has been established by Marletta et al. [8] to simulate of innovative consolidated-type adsorbent beds which is treated as a two-dimensional case. The governing equations take into account of the transport phenomena and are solved using advanced numerical methods both in the time and space domain. It has been reported that permeability plays an important role in adsorption phase. However, they have not reported the reason for using heat and mass transfer model and also have failed to list/identify other major parameters that influence the mass transfer resistance.

Selection of an appropriate mathematical and computational model is quite often the most important step in obtaining valid computer simulations of physical events [9]. Hence, the purpose of the present study is to analyze the influence of mass transfer on the temperature field as well as on sorption kinetics in adsorbent bed and present general criteria for selection of mathematic model in terms of parameters of engineering importance. Also, an effort is made to identify the factors that influence the mass transfer process through order of magnitude analysis, which could suggest a proper adsorber design, avoiding the mass transfer resistance in the desorption/adsorption process. In order to check the validity of the proposed criteria for conduction dominance and negligible mass transfer resistance, a cylindrical adsorbent bed being heated or cooled externally, is studied using numerical method.

2. Criterion for conduction dominance

The assumption of conduction dominance is valid when the heat transferred due to convection of desorbed vapor in a representative elementary volume (REV) is much less than that due to conduction:

$$Q_{\mathrm{cd}} \gg Q_{\mathrm{cv}}. \tag{1}$$

In order to estimate Q_{cd} and Q_{cv} in an adsorbent bed, an order of magnitude analysis has been used. The system under consideration is illustrated in Fig. 1, showing different modes of heat transfer. It is assumed that the heat transfer is effected mainly through conduction and convection, since the temperature difference across the bed thickness is not significant enough and hence the radiation mode is neglected. The local heat transfer rate by conduction through solid phase and fluid phase in the REV can be expressed as:

$$q_{\mathrm{cd}} = -k_{\mathrm{eff}}\frac{\mathrm{d}T}{\mathrm{d}x}, \tag{2}$$

where, the effective thermal conductivity can be estimated using [10]:

$$k_{\mathrm{eff}} = k_{\mathrm{z}}^{(1-\varepsilon_{\mathrm{t}})}k_{\mathrm{v}}^{\varepsilon_{\mathrm{t}}}. \tag{3}$$

Hence, the heat transfer rate by conduction mode in the overall system is:

$$Q_{\mathrm{cd}} \sim k_{\mathrm{eff}}\frac{T_L}{L}, \tag{4}$$

where ΔT_L is the temperature difference across the adsorbent bed thickness, L is the characteristic length of the adsorbent, representing the thickness of the adsorbent layer.

The amount of heat, which is transferred by convection to or from the fluid flowing through adsorbent bed, can be evaluated by:

$$Q_{\mathrm{cv}} \sim \dot{m}c_{p\mathrm{v}}\Delta T_L = \rho_{\mathrm{v}}c_{p\mathrm{v}}u_{\mathrm{v}}\Delta T_L. \tag{5}$$

By substituting Eqs. (4) and (5) into Eq. (1), the criterion for conduction dominance is expressed by the following equation:

$$\frac{(\rho_{\mathrm{v}}c_{p\mathrm{v}}u_{\mathrm{v}})L}{k_{\mathrm{eff}}} \ll 1. \tag{6}$$

In the above equation, the superficial velocity of the gaseous phase in the adsorbent bed can be estimated by using the Darcy equation:

$$u_{\mathrm{v}} = -\frac{k_{\mathrm{D}}}{\mu}\frac{\partial p}{\partial r} \sim -\frac{k_{\mathrm{D}}}{\mu}\frac{\Delta p}{L}, \tag{7}$$

where ΔP is the pressure difference across the adsorbent bed thickness. By substituting the expression for u_{v} (Eq. (7)) and k_{eff} (Eq. (3)) in Eq. (6), results in criterion for conduction dominance, CR1:

$$DaR_k^{1-\varepsilon_{\mathrm{t}}}Dn_1 \ll 1, \tag{8}$$

where the Darcy number (Da), the thermal conductivity ratio (R_k), and the new dimensionless number referred as potential number, Dn_1 are defined respectively as:

$$Da = \frac{k_{\mathrm{D}}}{L^2}, \quad R_k = \frac{k_{\mathrm{v}}}{k_{\mathrm{z}}}, \quad Dn_1 = -\frac{\Delta pL^2}{\alpha_{\mathrm{v}}\mu}.$$

3. Criterion for negligible mass transfer resistance

The assumption of negligible mass transfer resistance is valid only when the actual fluid velocity in a

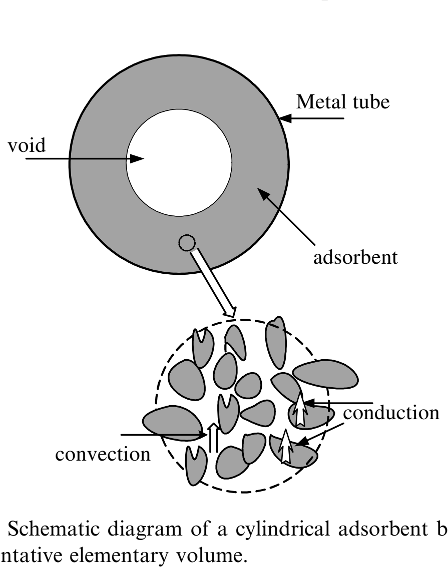

Fig. 1. Schematic diagram of a cylindrical adsorbent bed and representative elementary volume.

representative elementary volume (REV) is nearly same as the velocity produced under uniform pressure condition. That is to say, if the actual fluid velocity in a REV is much less than the velocity corresponding to the uniform pressure condition, the mass transfer resistance will be significant affecting the desorption process. Under such situations, heat and mass transfer model must be used, and the criterion for small mass transfer resistance can be expressed as:

$$\frac{u_\mathrm{v}}{u_p} \sim 1. \tag{9}$$

The average fluid (vapor) velocity, u_p, in uniform pressure in the system can be estimated as:

$$u_p = \frac{\rho_\mathrm{z}}{\rho_\mathrm{v}} \frac{\mathrm{d}w}{\mathrm{d}t} \frac{V}{S}. \tag{10}$$

Though the actual adsorption/desorption rate $\mathrm{d}w/\mathrm{d}t$ is difficult to estimate, it can be deduced in terms of heat transfer rate. This is acceptable for the fact that, the adsorption/desorption process is mainly governed by the heat output/input when subjected to uniform pressure conditions:

$$\frac{\mathrm{d}w}{\mathrm{d}t} = c\left(\frac{qS}{m\Delta H}\right), \tag{11}$$

where c is a positive constant whose value is obtained from comparing the numerical results predicted by HT and HMT model using regression method. It is found that when the c is 310.4, the CR2 turns out to be in the order of 10^{-1}, and error percentages being less than 1%. In this Eq. (11), ΔH reflects to the heat of adsorption, and q represents the heat transfer rate which is the most dominant parameter influencing the adsorption/desorption process. By substituting Darcy equation (7), Eqs. (10) and (11), the Eq. (9) becomes:

$$\frac{k_\mathrm{D}}{L^2} \frac{\rho_\mathrm{v}}{\rho_\mathrm{z}} \frac{-\Delta p}{\mu c(qS/\Delta H m)} \sim 1. \tag{12}$$

The above equation can be transformed to simple terms and be expressed as:

$$\frac{Da R_\rho R_p}{Dn_2} \sim 1, \tag{13}$$

where the Darcy number (Da), has been defined in the previous section. The density ratio (R_ρ), the dimensionless pressure difference (R_p) and the new dimensionless heat transfer rate (Dn_2) can be expressed respectively as:

$$R_\rho = \frac{\rho_\mathrm{v}}{\rho_\mathrm{z}}, \quad R_p = -\frac{\Delta p}{p_0}, \quad Dn_2 = \frac{\mu c q S}{p_0 \Delta H m}.$$

Since, the actual fluid velocity in the adsorbent bed is determined by the mass of refrigerant desorbed/adsorbed by the adsorbent, the quantity in the LHS of Eq. (13) is always lower than 1; the actual fluid velocity is always less than the average fluid velocity under uniform pressure condition ($u_\mathrm{v} < u_p$). From the criterion Eq. (13), the effect of mass transfer resistance become stronger as either any one of the Darcy number, density ratio, dimensionless pressure difference decreases, or the dimensionless heat transfer rate increases. Hence, the criterion CR2 can identify the major factors that influence the mass transfer resistance, and numerical method can be used to predict and analyze to what extent each of these factors affect the mass transfer resistance.

4. Numerical solution for the cylindrical adsorption bed

4.1. Problem description and modeling

In order to check the validity of the proposed criteria, Eq. (8), named CR1, for conduction dominance and Eq. (13), named CR2, for negligible mass transfer resistance quantitatively, a cylindrical adsorption bed with void in the center, being heated/cooled externally (Fig. 1) is studied. The reason for that the proposed criterion is benchmarked against the problem of cylindrical bed is because this kind of bed is a typical geometry which performances are widely studied [3,6–8]. The desorbed vapor transfers from the bed through the void and gets accumulated in the condenser/evaporator.

Two different adsorption pairs are selected as base case such as, monolith activated carbon/ammonia and activated carbon/methanol. Methanol and ammonia are the two refrigerants which are often used in adsorption systems of which methanol operates at very low pressure, whereas ammonia operates at very high pressures. By considering ammonia and methanol, this research provides insight into the behavior adsorption systems under different pressure conditions. The physical properties of activated carbon/ammonia pair and activated carbon/methanol are listed in Tables 1 [11] and 2 [12,13], respectively. The configuration and operational parameters are listed in Table 3.

The model of the adsorber consists of dynamic heat balance of the metal tube, the adsorbent bed and the mass transfer kinetic equations. The heat balance for the metal tube is given by:

$$\frac{1}{2}\rho_\mathrm{m} c_{p\mathrm{m}} (r_\mathrm{to}^2 - r_\mathrm{ti}^2) \frac{\partial T_\mathrm{m}}{\partial t} + h_\mathrm{mz} r_\mathrm{ti}(T_\mathrm{m} - T_\mathrm{z}) - h_\mathrm{fm} r_\mathrm{to}(T_\mathrm{f} - T_\mathrm{m}) = 0, \tag{14}$$

where h_fm and h_mz are the heat transfer coefficient corresponding to the fluid–metal and metal–adsorbent, respectively [8].

In analyzing the problem, the temperature of heat transfer fluid and all physical properties are assumed to be constant. To analyze the adsorbent bed, the govern-

Table 1
The physical properties of monolith activated carbon/ammonia pair

Parameters	Value
Heat capacity of the adsorbent (monolith carbon)	1125 J/kg K
Density of the adsorbent (monolith carbon)	750 kg/m^3
Thermal conductivity (monolith carbon)	0.44 W/m K
k	3.6571
n	0.94
w_0	0.3629
Heat of adsorption	1,380,808.7 J/kg

Table 2
The physical properties of activated carbon/methanol pair

Parameters	Value
Heat capacity of the adsorbent (activated carbon)	900 J/kg K
Density of the adsorbent	450 kg/m^3
Thermal conductivity of the adsorbent	0.35 W/m K
k	9.3
n	0.86
w_0	0.365
Heat of adsorption (q_{st})	1,100,000 J/kg

Table 3
The geometry parameters and operational parameters

	Value
Geometry parameters	
Diameter of the metal tube × thickness	40 mm × 2 mm
Thickness of the adsorbent	10 mm
Diameter of the inner void channel (r_0)	20 mm
Operating conditions	
Condensation temperature (T_c)	313.15 K
Evaporation temperature (T_e)	278.15 K
Ambient temperature (T_a)	308.15 K
The heating temperature (T_h)	453.15 K

ing equations are established by applying the volume-averaging technique [6–8]. The general criteria CR1 and CR2 are verified by results obtained both from HT model and HMT model and are compared in terms of the temperature profile and the variation in uptake of adsorbate. The criteria are further validated by numerical method considering the geometry to be one-dimensional, which is sufficient enough to provide insight of the physical process involved in the adsorbent bed.

4.2. Heat transfer model

A very simple tool to analyze the adsorbent bed, is the heat transfer model, hence, the governing equation is obtained based only on the heat transfer from solid phase and fluid phase in the adsorbent bed by conduction mode alone, therefore, neglecting convection and radiation terms, the heat balance equation can be expressed as:

$$\frac{\partial(\rho c_p T_z)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(k_{\mathrm{eff}} r \frac{\partial T_z}{\partial r}\right) + \rho_z \Delta H \frac{\partial w}{\partial t}, \tag{15}$$

where ρc_p is the total heat capacity in the control volume of the bed, which includes adsorbent, refrigerant vapor as well as adsorbate can be estimated as:

$$\rho c_p = \rho_z (c_{pz} + w c_{pa})(1 - \varepsilon_t) + \varepsilon_t (\rho c_p)_v. \tag{16}$$

4.3. Heat and mass transfer model

Heat and mass transfer model is featured in which temperature or mass content of adsorbate varies not only with time but also with space and the governing equations are always partial differential equations. The heat and mass transfer analysis involves four main governing equations such as: energy balance equation, mass conservation equation, momentum equation and state equation of the adsorbent–adsorbate system. These equations are usually nonlinear due to the adsorption isotherms and physical properties and become even more complex to solve if the adsorption process is considered as a cyclic process with varying boundary and initial conditions.

The heat balance equation taking into account of conduction as well as convection for vapor and solid adsorbent can be given as:

$$\frac{\partial(\rho c_p T_z)}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}\left(r \rho_v c_{pv} u_r T_z\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(k_{\mathrm{eff}} r \frac{\partial T_z}{\partial r}\right) + \rho_z \Delta H w \frac{\partial w}{\partial t}. \tag{17}$$

The overall mass conservation in the porous bed is described as:

$$\varepsilon_t \frac{\partial \rho_v}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r \rho_v u_r) = -\rho_z \frac{\partial w}{\partial t}. \tag{18}$$

In the above equation, the vapor superficial velocity in the adsorbent bed is determined using the Darcy equation. This is done because of the complexity of fluid flow in the porous media, and hence a simplest momentum equation is deduced from Darcy's law:

$$u_r = -\frac{k_D}{\mu}\frac{\partial p}{\partial r}. \tag{19}$$

The vapor density ρ_v is related to pressure and temperature by using the ideal gas state equation:

$$\rho_v = \frac{p_v}{R T_z}. \tag{20}$$

The variation in uptake of adsorbate is estimated using modified Dubinin–Radushkevich equation:

$$w = w_0 \exp\left[-k\left(\frac{T}{T_{\text{sat}}} - 1\right)^n \right], \tag{21}$$

where T is the sample temperature (K); w_0 is the uptake under saturation conditions corresponding to the maximum uptake; T_{sat} is the saturation temperature (K) corresponding to gas pressure and n is an exponent constant.

The above given governing equations Eqs. (17) and (18) are solved using the initial and boundary conditions. The initial temperature and pressure distribution is supposed to be uniform. Hence,

$$T_{\text{m}} = T_{\text{z}} = T_{\text{in}} \quad \text{at } t = 0, \tag{22}$$

$$P_{\text{b}} = P_{\text{c/e}}$$

for bed connected to the condenser/evaporator at $t = 0$.

(23)

For the adsorbent bed, the two temperature boundary conditions are:

$$h_{\text{mz}}(T_{\text{m}} - T|_{r=r_{\text{m}}}) = -k\frac{\partial T_{\text{z}}}{\partial r}\bigg|_{r=r_{\text{m}}} \tag{24}$$

and

$$T|_{r=r_0} = T_{\text{c/e}}$$

for bed connected to the condenser/evaporator.

(25)

Similarly, the two boundary conditions for pressure are:

$$\frac{\partial P}{\partial r}\bigg|_{r=r_{\text{m}}} = 0 \tag{26}$$

and

$$P|_{r=r_0} = P_{\text{c/e}}$$

for bed connected to the condenser/evaporator,

(27)

where $P_{\text{c/e}}$ is the pressure of the condenser or evaporator, which can be predicted as a function of the corresponding temperatures of condensation or evaporation, $T_{\text{c/e}}$.

4.4. Numerical method

The complexity and nonlinearity of such coupled heat and mass transfer models in general exclude the possibility of having an analytical solution. Therefore, numerical methods are the only feasible alternative to meet the requirements for simulation of adsorbent bed dynamics. In this study, the numerical method used is the finite volume method. To avoid numerical instabilities, an implicit scheme is adopted. For spatial derivatives, the convection terms in the equations are approximated by the quadratic upstream differencing scheme (QUDS) [14] and the diffusion terms are replaced by the central difference analogs. The nonlinearity of the equations is solved by iterative techniques. The iteration procedure is continued until a convergence tolerance is satisfied:

$$\frac{\sum_i |s_i^{m+1} - s_i^m|}{\sum_i |s_i^m|} \leqslant \sigma, \tag{28}$$

where s_i is the dependent variable which is being numerically calculated (velocity, temperature, uptake). The subscripts i implies spatial position in the computational mesh, and m refers to the iteration number. In this work, the value assigned to σ is 10^{-6}. A grid-dependence check has been carried out; the time step and spatial grid size used in the calculation are fine enough to obtain accurate computations.

The progress of the desorption/adsorption process can be measured by dimensionless uptake which is the ratio of average uptake of adsorbate, to the maximum uptake under saturated condition, and be expressed as:

$$\omega(t) = \frac{w(t)}{w_0}. \tag{29}$$

To quantify the outcome based on qualitative ratings for the assumptions on conduction dominance and negligible mass transfer, the percentage difference is defined as:

$$\text{Diff\_T } (\%) = \frac{\max(T_{\text{HMT}} - T_{\text{HT}})}{T_{\text{c}} - T_{\text{e}}} \times 100, \tag{30}$$

$$\text{Diff\_w } (\%) = \frac{\max(w_{\text{HMT}} - w_{\text{HT}})}{w_0} \times 100. \tag{31}$$

5. Results and discussion on the criterion

5.1. Conduction dominance

Simulations of the thermal behavior in the adsorbent bed are initially performed to check the validity of criterion for conduction dominance, CR1. As mentioned before, the criterion CR1, comprises of three parameters such as Darcy number, thermal conductivity ratio and the potential number (listed in Section 2). In this study, methanol and ammonia are chosen as two different refrigerants to provide insight into the behavior of adsorption systems under different pressure conditions. It should be pointed out that the validity of CR1 has not been carried out for the activated carbon/methanol pair since methanol operate under low pressure and hence will not oblige to the condition of "negligible mass resistance".

To begin with, the first parameter such as the Darcy number of CR1 is checked for its influence on the desorption process for AC/ammonia pair based on two models are plotted in Fig. 2. Fig. 2(a) shows the variation in temperature across the bed thickness for Darcy number in a higher range. It should be pointed out that, though the simulation was carried out for a longer time scale, only two typical results are presented here, corresponding to 400 and 800 s, respectively. It is seen that, the temperatures profiles are similar for the chosen times, but the absolute temperature values are comparatively higher when using the HMT model. This is because, desorption is not restrained as well as heat transfer through convection is also included, along with conduction mode.

The variation in the dimensionless uptake of the adsorbent is compared for the said two models in Fig. 2(b). It is seen that, the dimensionless uptake estimated by HT and HMT model is nearly the same, which proves that the actual desorption occurs at uniform pressure conditions.

In order to further check the validity of CR1, in term of second parameters such as the thermal conductivity ratio, the influence of k_v on thermal performance of the adsorbent bed has been compared (Fig. 3). It is clearly seen that, there exists not much of difference between the results attained by the HT and HMT models.

The third parameter of CR1, such as the potential number Dn_1 is expected to have no significant impact in validity the criterion, because of the fact that, the pressure difference would be negligible for the situation when there exists no mass transfer resistance.

Based on the above results, it is seen that the criterion CR1 in terms of the Darcy number in high range as well as thermal conductivity ratio, are nearly the same (percentage difference < 1%) obtained by HT and HMT models. This can be attributed to two reasons: (i) the mass rate of vapor desorbed/adsorbed during the

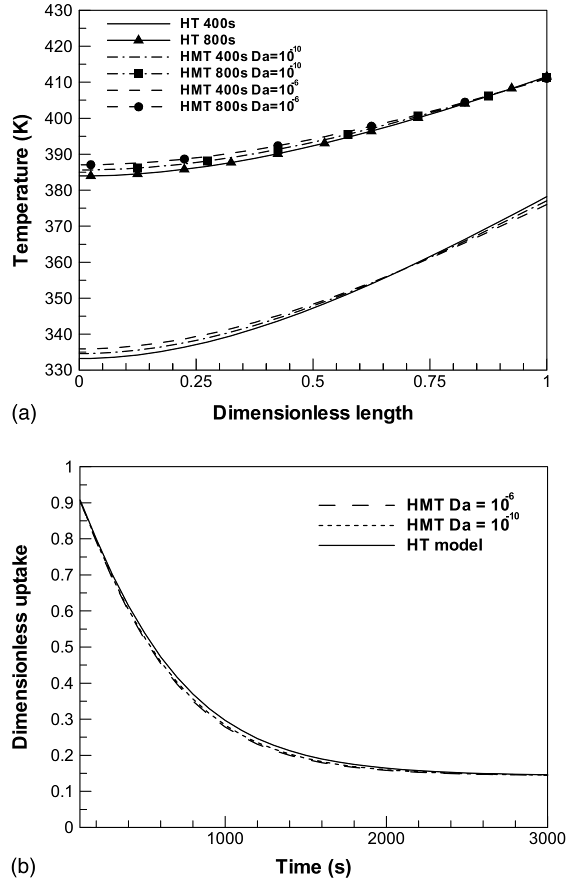

Fig. 2. (a) Variation of the temperature field, and (b) dimensionless uptake in adsorbent bed for high Darcy number using AC/ammonia pair.

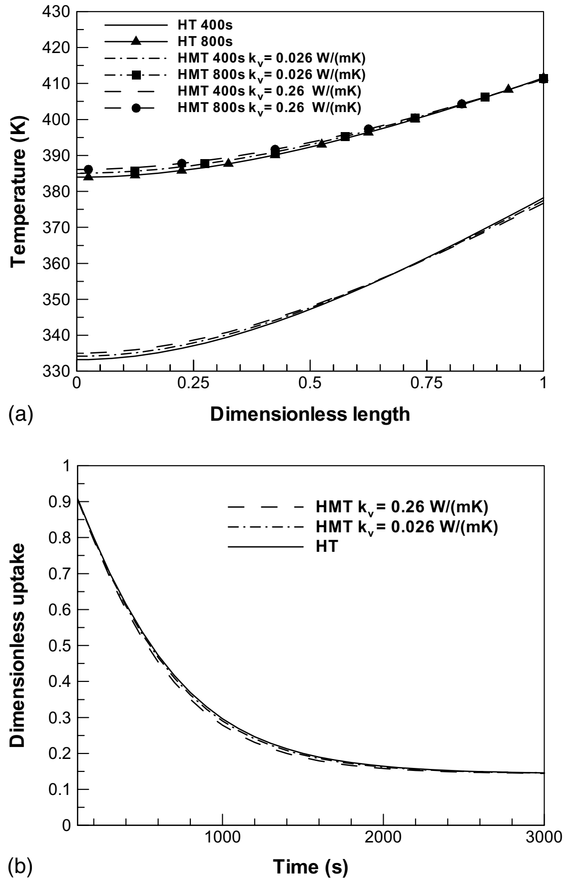

Fig. 3. (a) Influence of effective thermal conductivity ratio on temperature field, and (b) dimensionless uptake in adsorbent bed using AC/ammonia pair.

desorption/adsorption process is small; and (ii) the permeability is less in almost all adsorbent material. This confirms the validity of criterion on conduction dominance ($CR1 < 10^{-3}$). In practical situations, the absolute value of CR1 is too low in the order of 10^{-3}, reflecting that, conduction dominance is valid for adsorption systems under consideration.

5.2. Negligible mass transfer resistance

As stated in the earlier discussion, though the conduction dominance is easy to be satisfied, the HT model cannot yield accurate results, if the second criterion CR2 is not satisfied. Hence to check the negligible mass transfer resistance criterion CR2, the four parameters such as the dimensionless pressure difference R_p, Darcy number (Da), Density ratio (R_ρ) and the new dimensionless heat transfer rate (Dn_2) has to be verified. Among these parameters, R_p is a complex parameter, which is dependent on the other three parameters, and also, it is related to the adsorption pair properties such as adsorption equilibrium relation, pressure and density of refrigerant vapor under saturation condition. Here, R_p, is defined as a ratio of ($\Delta p/p_0$) maximum pressure difference across the bed during the desorption/adsorption process to the pressure corresponding to condensation/evaporation.

The study on the effect of Darcy number in low range on the dimensionless pressure difference is carried out for both the AC/ammonia pair and AC/methanol pair. The low range Darcy number can be obtained by reducing the permeability of the adsorbent material or by increasing the adsorbent thickness, for the given heat transfer rate and vapor density. Fig. 4(a) shows the variation in maximum pressure difference for AC/ammonia pair. It can be seen that, as the Da decreases, the R_p increases implying that maximum pressure difference increase steadily. However, it should be noted that, when the Darcy number is further reduced beyond the order of 10^{-12}, there exists no appreciable increase in the maximum pressure difference. Fig. 4(a) also shows the influence of low range Da on the criterion for neg-

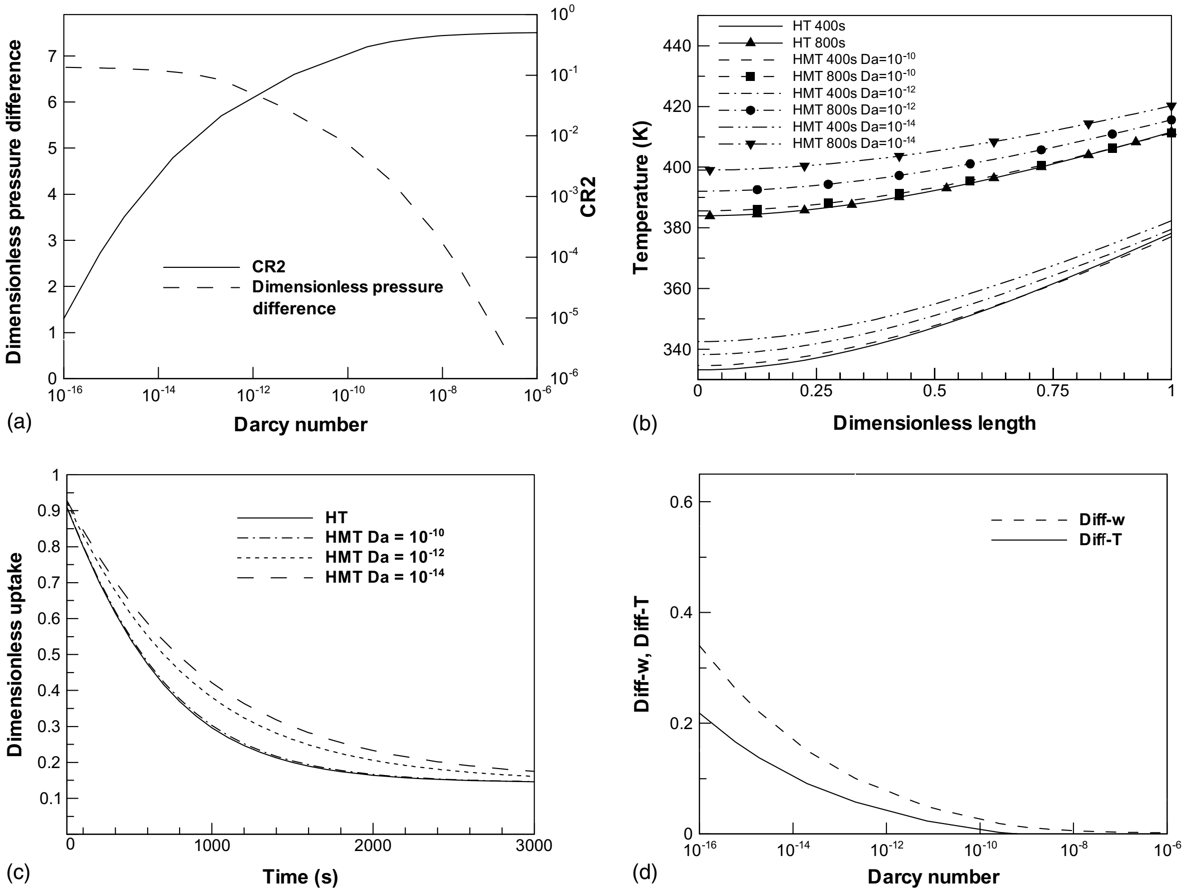

Fig. 4. Effect of low Darcy number on: (a) CR2 and maximum dimensionless pressure difference, (b) temperature field, (c) dimensionless uptake, and (d) percentage difference for AC/ammonia pair.

ligible mass transfer resistance, CR2. To begin with, the CR2 decreases until the *Da* is of the order 10^{-12} and sharply decreases thereafter. The reason for this trend can be explained with the help of adsorption equilibrium equation (21) and Darcy equation (19). For instance, the rate of desorption is effected by the permeability of the material, velocity of the vapor and the pressure difference across the bed. If the rate of desorption be maintained at a constant rate, for the given velocity of the vapor, the pressure difference has to increase for low permeability values (reflecting the reduction in *Da*). This increase in pressure difference is induced by desorption of vapor due to increase in the adsorbent bed temperature. The pressure difference cannot be unduly increased and would be limited by the pressure corresponding to the temperature difference between the bed temperature and the condensation temperature. Expressing the limitation in the terms of pressure, it yields,

$$\Delta p < p_{\mathrm{sat\,max}} - p_{\mathrm{sat}}, \tag{32}$$

where, $p_{\mathrm{sat\,max}}$ and p_{sat} represents the saturation pressure corresponding to the maximum adsorbent bed temperature, and condensation temperature, respectively. Using the above given equation and recalling Eq. (21), it can be discerned that when adsorbent temperature (T) is higher than the local saturation temperature (T_{sat}), the desorption will occur. On the other hand, when adsorbent temperature is less than the local saturation temperature, the desorption would cease. This indirectly explains the reason for the slow increase in the variation of pressure difference for very low *Da*.

The variation of temperature field and uptake in an AC/ammonia system is shown in Fig. 4(b) and (c). It can be seen that, when *Da* is in the order of around 10^{-10}, the results obtained by the two models such as HT and HMT model are similar. However, the results deviate from each other for low *Da* values below 10^{-12}. This is so because, as explained before, at low *Da*, the increase in the pressure difference becomes negligible when the desorption of vapor is restrained. This is reflected indirectly by the deviation in uptake at low *Da* values (Fig. 4(c)), which in turn raises the bed temperature (Fig. 4(b)). The percentage difference estimated using two models are presented in Fig. 4(d). It can be clearly seen that the percentage difference for both temperature and uptake increases when *Da* reduces. It becomes more prominent when *Da* is further less than 10^{-14}. Hence when porous media of low permeability are used for analysis, numerical results indicate that the HT model overestimates the desorption rate and underestimate the temperature field.

In addition to the AC/ammonia pair, numerical analysis has been carried out for AC/methanol pair to obtain the effects of low *Da* on the pressure difference and criterion CR2, temperature field and uptake. The results show a similar trend to that obtained for AC/ammonia pair (Fig. 4(a)), except for the shift in the order of magnitude, due to the fact that there exists a large difference in the properties (Tables 1 and 2).

The third parameter of CR2, such as the density ratio is studied by comparing the results obtained by the HT and HMT models. To have the variation in density ratio, the vapor density (ρ_{v}) is changed for the given density value of the adsorbent (ρ_{z}). Practically, such situations could be achieved in several ways: (i) using different adsorbates such as ammonia, methanol or water; (ii) varying the condensation temperature or evaporation temperature; (iii) shifting the cycle either to adsorption or desorption phase. In this numerical study the change in density of the adsorbate is accomplished by varying the condensation temperature, such that the density ratio varies in the range of 1–10^{-4}. Though such large variation will not occur in actual systems, the analysis is carried out for the specified range, in order to check if at all the change in density ratio will influence the pressure difference, similar to that of the *Da*.

The effect of the density ratio on variation in maximum pressure difference and CR2 is shown in Fig. 5(a). It can be clearly seen that its influence is very much similar to that of *Da* in Fig. 4(a). It is noticed that there is a sharp increase in the pressure difference when R_{ρ} is higher than 10^{-2}. This is because, velocity of vapor has to rise with reduction in vapor density, in order to maintain constant mass flow rate. Vapor velocity reflects the increase in pressure difference which results in a large resistance to mass transfer for the given permeability of the adsorbent. On the other hand, if the R_{ρ} is reduced beyond 10^{-2}, increase in the pressure difference becomes negligible. This is experienced because of the limitation on the pressure difference as listed in Eq. (32). This leads to a significant variation of the uptake values estimated using HT model and HMT model, especially for very low-density ratios. The variation in values is expressed in the form of percentage difference as shown in Fig. 5(b). As said, it could be seen from the figure that the percentage difference is about 30% for very low R_{ρ} of the order 10^{-4}, while the error is just 5%, when R_{ρ} is around 10^{-2}.

As known both the density as well as working pressure condition for methanol is lower compared to the ammonia. Hence, the above discussion on influence of low R_{ρ}, can be well realized in terms of the desorption/adsorption process of AC/methanol system. Fig. 5(c) and (d) shows the variation in uptake during desorption and adsorption process predicted using the HT and HMT models. It is seen that, the uptake values predicted by HT model overestimates the amount of desorption compared to HMT model. This deflection is higher compared to the results obtained for AC/ammonia as shown in Fig. 4(c). Also, it should be pointed out that, compared to the desorption process, the deviation

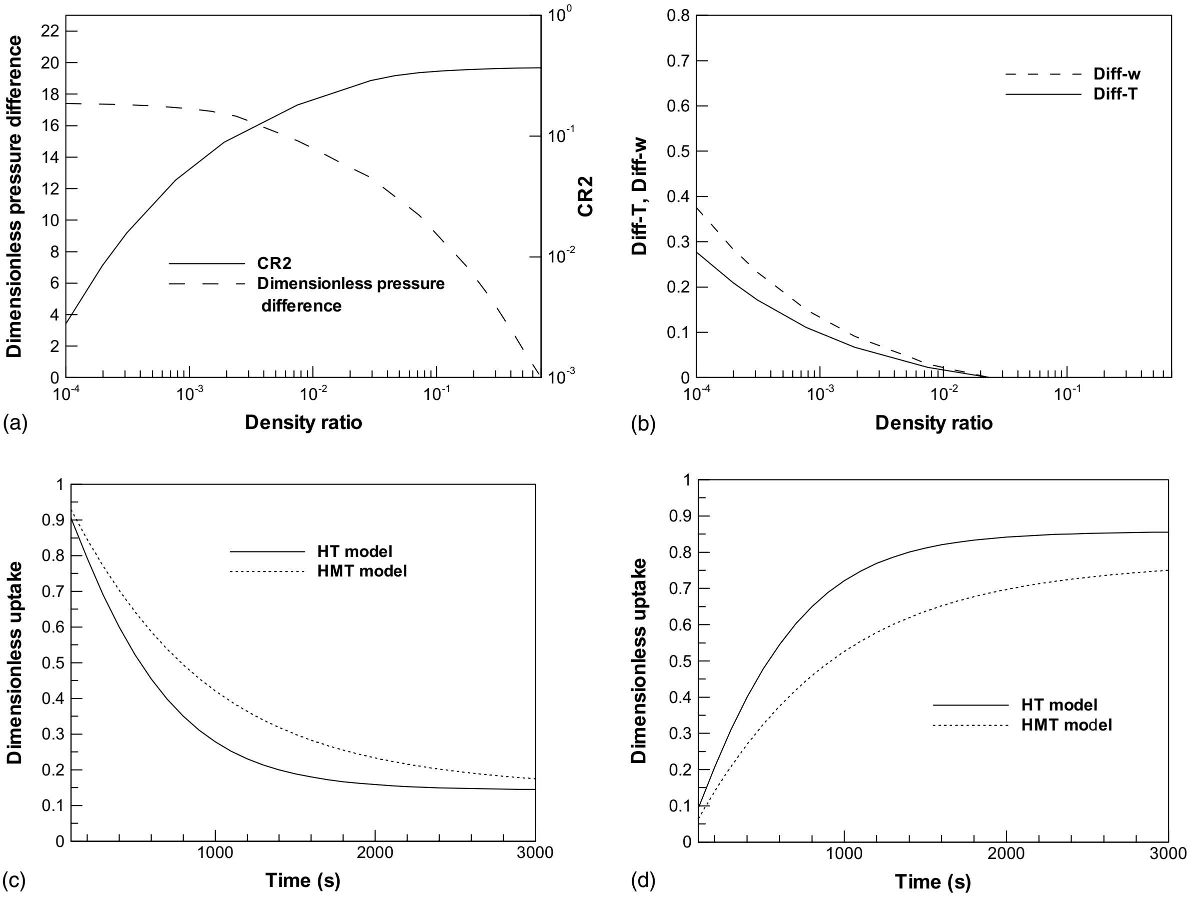

Fig. 5. Effect of density ratio on: (a) CR2 and maximum dimensionless pressure difference, (b) percentage difference, (c) dimensionless uptake-desorption phase, and (d) dimensionless uptake-adsorption phase for AC/methanol pair.

between HT and HMT becomes much more higher (Fig. 5(d)) when considering adsorption process. This is obviously because of the low prevailing density values during adsorption process. The same phenomenon was experienced by Marletta et al. [8].

The dimensionless heat transfer rate Dn_2 is yet another complex parameter in the CR2. As stated in Section 3, "q" is the most important parameter that influences the desorption/adsorption process and hence, its effect is studied to reflect the influence of Dn_2. It can be seen from the Fig. 6(a) that increase in the pressure difference is negligible, when the heat transfer rate (q) is low about 100 W/m^2. This is due to the fact when q is low, the amount of ammonia desorbed will be less as shown in Fig. 6(d). Hence, the results estimated both by HT and HMT model are same as seen in Fig. 6(c) and (d), for low heat transfer rates. On the contrary, when q is high, say about 5000 W/m^2 (applicable to high temperature source), the desorption rate increases in turn leading to a gradual increase in the maximum pressure difference. This situation results in the deflection of results obtained by HT and HMT model (Fig. 6(c) and (d)) and thereby a significant increase in the percentage difference is realized (Fig. 6(b)).

It should be noticed from Fig. 6(d), that a further increase in heat transfer rate will not effect more desorption of vapor, because of the limitation on increase in pressure difference, as listed in Eq. (32). The above results, more specially, Fig. 6(b) proves that it is sufficient to use HT model in analyzing any low heat transfer rate application such as solar powered adsorption system.

In summary, the parameters such as the Darcy number (Fig. 4(a)), the refrigerant vapor density (Fig. 5(a)), and the heat transfer rate (Fig. 6(a)) are the three main factors that influence the mass transfer resistance. That is, either $Da \to 0$, or $R_\rho \to 0$, or $Dn_2 \to \infty$, the mass resistance will significantly increase thereby restraining the desorption/adsorption leading to an increase in the local pressure. These effects can be combinely expressed by the criterion CR2 (Eq. (13)). The numerical results shows that when the CR2 > 10^{-2}, both

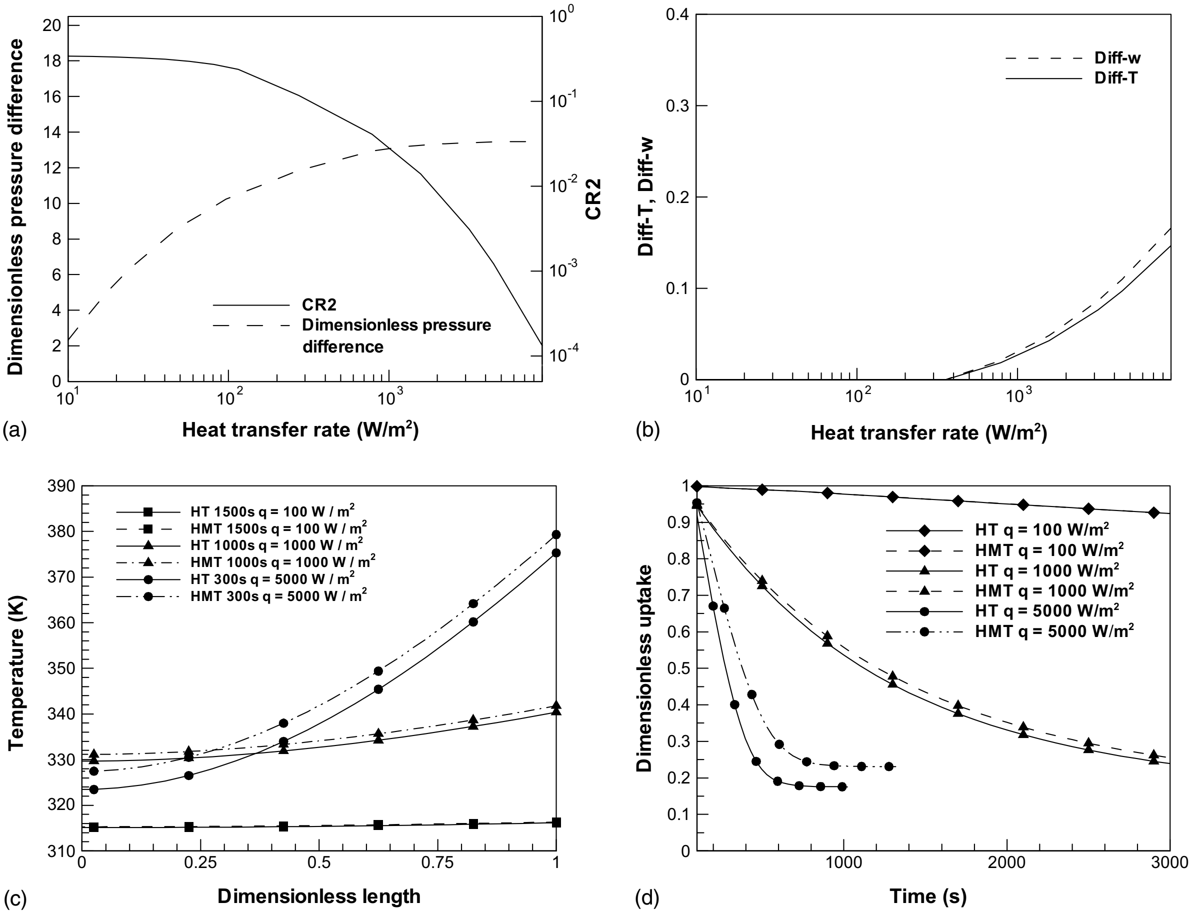

Fig. 6. Effect of heat transfer rate on: (a) CR2 and maximum dimensionless pressure difference, (b) temperature field, (c) dimensionless uptake, and (d) percentage difference for AC/methanol pair.

HT and HMT model yield similar results with percentage difference being less than 3%. And hence it is sufficient to use the HT model to analyze the systems that oblige the above criterion. On the other hand, if CR2 is less than 10^{-2}, the HT model is not valid, and hence the transportation process in the adsorbent bed must be analyzed using the HMT model.

6. Conclusion

In this work, the validity of Heat Transfer model is studied using two general criteria for conduction dominance and negligible mass transfer resistance. For this, an order of magnitude analysis is performed and the criteria are expressed in terms of parameters of engineering importance which include the Darcy number (*Da*), thermal conductivity ratio, density ratio, dimensionless pressure difference, potential number Dn_1 and the dimensionless heat transfer rate Dn_2.

In order to validate the proposed criterion, the numerical results obtained by Heat Transfer model and Heat Mass Transfer model are compared in terms of the temperature distribution and dimensionless uptake. It is found that the criterion of conduction dominance (CR1) is always valid for all adsorption system owing to the low mass flow rates involved during the adsorption/desorption process. However, the criterion for negligible mass transfer resistance is more complex and requires a careful scrutiny to check for its validity. The mass transfer resistance can be influenced either by the properties of the adsorbent and adsorbate, bed geometry as well as the operational condition. As long as the value of CR2 is less than 10^{-2}, the HT model is not valid and the use of the HMT model is mandatory.

In addition, the results show that, there is a possibility to design a fast adsorption cycle with low mass transfer resistance, by either increasing the permeability of the adsorbent or reducing the thickness of the adsorbent bed. The general criteria developed in this study can be useful in selecting an appropriate model and to identify the factors that influence the mass transfer resistance which would be helpful in proper design of adsorbent bed and choosing appropriate working pair.

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