A non-uniform pressure and transient boundary condition based dynamic modeling of the adsorption process of an adsorption refrigeration tube

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ABSTRACT
The adsorption refrigeration tube (ART) has drawn increasing attention because of its advantages of no moving parts, compact structure and use of low grade heat as the heat source. A new design of ART was developed, in which activated carbon–methanol was selected as the working pair for either refrigeration or air-conditioning purposes. Based on the typical configuration of the generator of the ART, a dynamic mathematical model was developed under the non-uniform pressure assumption and the introduction of a transient boundary condition of diffusion equation. Moreover, experiments were conducted for validating the model. The experimental data and numerical results were compared in terms of temperature development inside the carbon bed, with the transient and two popular simplified boundary conditions of vapor density respectively. The comparison shows that the transient boundary condition improves accuracy of the model and more importantly it is capable of reflecting the dynamic shift of dominant driving forces of the adsorption process inside the generator, i.e. shifting to temperature driving gradually from diffusion driving.

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1. Introduction
Adsorption refrigeration has been studied extensively since the nineteen eighties for its low-grade energy requirement and environmentally-friendly refrigerant [1–6]. The coefficient of performance (COP) and specific cooling performance (SCP) of adsorption refrigeration systems have been improved in recent years due to system optimization with advanced thermal cycles [4,5,7,8]. However, the optimization increases the complexity of the system, which in turn leads to a decrease in performance reliability of the adsorption refrigeration systems.

Over the last ten years, some researchers studied ART that only consists of integrated adsorber, condenser and evaporator, which was aimed at improving system reliability through multi-ART integration to achieve continuous and large scale refrigeration capacity. Tamaninot-Telto and Critoph [9], in 1993, initially proposed a cooling tube with monolithic carbon–ammonia as working pair, in which the monolithic carbon was made in situ within the generator in order to reduce contact heat transfer resistance between the generator wall and the adsorbent. Zhao et al. [10] proposed a solar powered ART, in which vacuum glass tube was employed to contain the adsorbent bed and adsorb solar energy efficiently. Wang and Zhang [11] developed a fin-type adsorption cooling tube that finned tube was adopted to improve heat transfer within the adsorbent bed.

On the other hand, various mathematical models describing the adsorption process were proposed. Some mathematical models used lumped parameter method based on the uniform pressure assumption to study the thermal performance [11–13]. However, this kind of model may not represent the accurate system performance, especially when the thickness of the adsorbent bed exceeds a certain value which results in the uneven temperature profile becoming significant. Moreover, the assumption of uniform pressure may be not accurate as the pressure gradient within the adsorbent bed would act as the principal driving force of adsorption at the very beginning of an adsorption process. For the side of non-uniform pressure based model, although these kinds of models have been proposed and studied, one important boundary condition of the diffusion equation (or mass transfer equation), i.e. gas density from the evaporator, all applied simplified constant values [14,15]. This simplification is not accurate to some extent since the dynamic shift of adsorption driving forces cannot be presented under the circumstances. In fact, the shift of driving forces at the very beginning of the adsorption process, i.e. from diffusion driving (gradient of gas density) to temperature driving, plays an important role in following adsorbent temperature development and adsorption performance.

The aim of this study is to establish a non-uniform pressure and transient vapor density based model to investigate the adsorption process of a real adsorption refrigeration cycle. Experiments were
conducted for validating the model. Moreover, numerical studies of the model under two constant vapor densities were conducted and compared with the experimental data.

2. Configuration description

The ART proposed is comprised of a generator, a condenser, an evaporator, insulation sectors, a circulation pipe, a water jacket and a control valve, as shown in Fig. 1. Activated carbon (Calgon activated carbon WS-480) and methanol are selected as the working pair for either refrigeration or air-conditioning purposes. In the generator, a porous tube is placed centrally in the carbon as the mass transfer channel for the methanol vapor. This ART has two major advantages, compared to Critoph’s and other researchers’ models [16,17]. First, the condenser and evaporator are separated and located at two ends, which thoroughly helps to avoid heat losses and heat disturbances. Second, the valve on the external circulation pipe provides convenience to control the evaporating pressure, which could enhance the production of useful refrigeration capacity.

3. Working principle

A non-valve controlled adsorption refrigeration cycle normally includes two processes, which are heating-desorption process and cooling-adsorption process (purposes 1–2, 3–4, shown in Fig. 2). However, a valve is usually added to control the effective evaporating temperature by connecting the evaporator

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Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>x</td>
<td>concentration of adsorbed methanol, kg kg⁻¹</td>
</tr>
<tr>
<td>t</td>
<td>time, s</td>
</tr>
<tr>
<td>r</td>
<td>radial coordinate</td>
</tr>
<tr>
<td>T</td>
<td>temperature, K</td>
</tr>
<tr>
<td>p</td>
<td>pressure, Pa</td>
</tr>
<tr>
<td>M</td>
<td>mass, kg or molar mass, kg mol⁻¹</td>
</tr>
<tr>
<td>H</td>
<td>heat of adsorption, J kg⁻¹</td>
</tr>
<tr>
<td>R₀</td>
<td>specific gas constant, J mol⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Rᵢ</td>
<td>inside radius of carbon column, m</td>
</tr>
<tr>
<td>Rₒ</td>
<td>outside radius of carbon column, m</td>
</tr>
<tr>
<td>l</td>
<td>serial number of carbon layers</td>
</tr>
<tr>
<td>N</td>
<td>number of total layers divided</td>
</tr>
<tr>
<td>C</td>
<td>gas density, mol m⁻³</td>
</tr>
<tr>
<td>cₚ</td>
<td>specific heat, J kg⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Q</td>
<td>internal heat source, W m⁻³</td>
</tr>
<tr>
<td>Dₑd</td>
<td>effective diffusion coefficient of porous media, m² s⁻¹</td>
</tr>
<tr>
<td>Dₖ,m</td>
<td>diffusivity of Knudsen and molecular diffusion, m² s⁻¹</td>
</tr>
<tr>
<td>Dₖ</td>
<td>Knudsen diffusivity, m² s⁻¹</td>
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<tr>
<td>Dₘ</td>
<td>molecular diffusivity, m² s⁻¹</td>
</tr>
<tr>
<td>D</td>
<td>coefficient of D–A equation</td>
</tr>
<tr>
<td>n</td>
<td>coefficient of D–A equation</td>
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Greek symbols

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<thead>
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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>ρ</td>
<td>density, kg m⁻³</td>
</tr>
<tr>
<td>λ</td>
<td>thermal conductivity, W m⁻¹ K⁻¹</td>
</tr>
<tr>
<td>ε</td>
<td>total porosity</td>
</tr>
<tr>
<td>α</td>
<td>coefficient of the transient boundary condition</td>
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</table>

Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>s</td>
<td>solid adsorbent</td>
</tr>
<tr>
<td>l</td>
<td>liquid phase</td>
</tr>
<tr>
<td>g</td>
<td>gaseous phase</td>
</tr>
<tr>
<td>c</td>
<td>condensing</td>
</tr>
<tr>
<td>e</td>
<td>evaporating or gas from evaporator</td>
</tr>
<tr>
<td>t</td>
<td>transient</td>
</tr>
<tr>
<td>am</td>
<td>ambient</td>
</tr>
<tr>
<td>cb</td>
<td>activated carbon</td>
</tr>
<tr>
<td>eb</td>
<td>equivalent property of the adsorbent bed</td>
</tr>
<tr>
<td>sat</td>
<td>saturation status</td>
</tr>
<tr>
<td>ini</td>
<td>initial condition</td>
</tr>
<tr>
<td>max</td>
<td>maximum value in studied cycle</td>
</tr>
<tr>
<td>min</td>
<td>minimum value in studied cycle</td>
</tr>
<tr>
<td>1 2 3 4 2' 3' 4'</td>
<td>status of relevant processes</td>
</tr>
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</table>
to the generator until the pressure in the generator has dropped to the required pressure. In such valve controlled cycle, the entire cycle has four processes, which are isosteric heating, isobaric desorption, isosteric cooling and isobaric adsorption (i.e. processes 1–2, 2–3, 3–4, 4–1).

The overall working processes of the ART are next described. In the first half cycle (i.e. process 1–2–3), the generator is heated up by circulating heat transfer fluid in the water jacket of the ART. At this moment, the refrigerant (methanol) is desorbed from the carbon bed and the gaseous methanol via the porous tube rises to the condenser and then flows to the evaporator via the circulation pipe after condensing. When this process completes, heat transfer fluid is switched to cooling fluid to start the second half cycle (i.e. 3–4–1). When the pressure in the generator drops to the designed evaporating pressure, valve is turned on to connect the evaporator to the generator to generate the refrigeration process (4–1), which is a key process that refrigeration effect is generated.

4. Modeling

4.1. Model assumptions

In this study, the heat and mass transfer processes in the generator is considered to be one dimensional (radial). Fig. 3 shows the simplified one dimensional scheme, in which uniform grid (layer) is adopted. Besides the one dimensional assumption, the other modeling assumptions are made as follows:

(1) The temperature of heat transfer fluid is considered as constant.
(2) The particles of activated carbon are uniformly distributed and have identical adsorptive property.

4.2. Governing equations

4.2.1. Adsorption state equation

The Dubinin–Astakov equation (D–A) [16] is used as the state equation, which can be rewritten as:

\[
x = x_0 \exp \left( -D \left( \frac{T \ln \frac{P_{sa}}{T}}{T} \right)^n \right)
\]

(1)

where \(x_0\) is the maximum possible concentration of adsorbate; \(T\) is the local temperature of solid adsorbent; \(P_{sa}\) is the saturation pressure at local temperature \(T\); \(P\) is the local adsorption pressure; \(D\) and \(n\) are the constants determined experimentally by the adsorbate/adsorbent pair involved.

4.2.2. Energy governing equation

Adsorption process is considered as coupled heat transfer and gas diffusion processes within the adsorbent bed. The energy conservation equation in cylindrical coordinates is:

\[
\frac{(\rho \epsilon c_p)_{eb}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + Q
\]

(2)

where \((\rho \epsilon c_p)_{eb}\) denotes the total heat capacity of the control volume of the adsorbent bed; \(\lambda_{eb}\) refers equivalent thermal conductivity of the adsorbent bed and \(Q\) represents internal heat source. Total heat capacity \((\rho \epsilon c_p)_{eb}\) and internal heat source can be calculated as follows [18]:

\[
(\rho \epsilon c_p)_{eb} = \rho_r c_{pr} + \epsilon \rho_r c_{ps} + x \rho_s c_{ps}
\]

(3)

\[
Q = (1 - \epsilon) \cdot H \cdot \rho_r \frac{\partial \xi}{\partial r}
\]

(4)

4.2.3. Diffusion equation

During the adsorption process, adsorbates (i.e. methanol vapor) from the evaporator travel towards the inner positions of the carbon layers resulted from diffusion as well as adsorption effects. The driving forces of the methanol vapor transfer, including the inner mass transfer within micropores of carbon particles and external mass transfer within the void space of the bed, are the local pressure gradient and the local methanol density difference. When taking porosity of the carbon bed into account, the equation of methanol diffusion can be written as [19]:

\[
\frac{\epsilon \partial C}{\partial t} + (1 - \epsilon) \cdot \rho_r \frac{\partial (\xi x/M)}{\partial t} = D_{ed} \cdot \epsilon \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right)
\]

(5)

where \(C\) is the local density of gaseous methanol; \(x\) is the concentration of adsorbed methanol (in micropores of the carbon); \(M\) is the molar mass of methanol; \(\epsilon\) is the total porosity of the carbon bed and \(D_{ed}\) is the effective diffusion coefficient.

The local density of gaseous methanol is evaluated with the ideal gas law, Eq. (6), in which \(R_0\) is the gas constant. The temperature of gaseous methanol in Eq. (6) is approximately evaluated with the correlation of methanol saturation vapor pressure and corresponding temperature, Eq. (7) [12].

\[
C = \frac{P}{R_0 T}
\]

(6)

\[
\ln P = 18.587 - 3626.55/(T - 34.29)
\]

(7)

For porous media with random twisted and interconnected pores, \(D_{ed}\) can be calculated approximately using Eq. (8), in which \(\epsilon_i\) is the total porosity of the bed and \(D_{ed,m}\) is the diffusion coefficient.
that depends on double effects resulted from Knudsen diffusion \((D_k)\) and molecular diffusion \((D_m)\). Expressions for calculating the diffusion coefficient \(D_{k-m}\) and corresponding mass diffusion and molecular diffusion are given in Eqs. (9)–(11) respectively [20].

\[
\begin{align*}
D_{ed} & = \rho^2 D_{k-m} \\
\frac{1}{D_{k-m}} & = \frac{1}{D_k} + \frac{1}{D_m} \\
D_k & = 4850 d_{pore} \left( \frac{T}{M} \right)^{1/2} \\
D_m & = \frac{2}{3} \pi \frac{r_s^3}{\kappa^2 N_a} \left( \frac{T}{M} \right)^{1/2}
\end{align*}
\]

In above two equations, i.e. Eqs. (10) and (11), \(d_{pore}\) is the pore diameter of activated carbon; \(T\) is the temperature of gas methanol; \(M\) is the molar mass of methanol; \(\sigma\) is the Lennard-Jones diameter of the spherical molecules of gas methanol; \(P\) is the local adsorption pressure; \(\kappa\) is the Boltzmann constant; \(N_a\) is the Avogadro’s number [20].

4.3. Initial and boundary conditions

4.3.1. Initial conditions

The adsorption process numerically studied is assumed starting from point 4 (see Fig. 2), which could be practically achieved by holding system at the point 4 status long enough, with circulating cooling water of temperature \(T_a\). The temperature of the activated carbon and concentration of methanol at point 4 are evenly profiled cross the generator, whose values can be calculated using Eq. (1) associated with \(P_e\) and \(x_{min}\). Therefore, the initial conditions of the above governing equations (Eqs. (2) and (5)) are:

\[
\begin{align*}
T &= 0, \quad T_{in} = T_4 \\
C &= 0, \quad C_{in} = C_4
\end{align*}
\]

4.3.2. Boundary conditions

Dirichlet and Neumann boundary conditions [21] are used respectively for the heat transfer equation (Eq. (2)), which are:

\[
\begin{align*}
T_{r=R_0} & = T_c \\
\frac{\partial T}{\partial r}_{r=R_0} & = 0
\end{align*}
\]

For the diffusion equation, Eq. (5), boundary condition at \(R_0\) applies mass insulation while that at \(R_i\) equals to the vapor density from the evaporator. Therefore two boundary conditions can be written as:

\[
\begin{align*}
\frac{\partial C}{\partial r}_{r=R_0} & = 0 \\
C_{r=R_0} & = C_e
\end{align*}
\]

The value of \(C_e\) in Eq. (17) depends on the vapor pressure and its temperature as shown in Eqs. (6) and (7).

In previous models developed by other researchers [13–15], \(C_e\) (or system pressure \(P_e\)) was assumed to be a constant that equals to \(C_{e_0}\) (or \(P_0\)) in the process 4–1. However, the system pressure and the density of methanol vapor from the evaporator are not constants, especially when the evaporator is just connected to the generator (i.e. status at point 4 in Fig. 2). There is a (quick) process for the pressure and corresponding methanol vapor density to stabilize from \(P_e\) and \(C_e\) to \(P_0\) and \(C_{e_0}\), which results in a transient condition of vapor density for the diffusion effect. After this beginning stage, the pressure and the density of methanol vapor in the evaporator reach and remain at the stable values. To present this process, a concept of the transient system pressure \((P_t)\) is introduced to reflect the corresponding transient vapor density \((C_t)\). The transient pressure \((P_t)\) is defined as Eq. (18):

\[
P_t = P_e - P_e \frac{t}{1 + \alpha t} + P_e
\]

where \(P_e\) and \(P_e\) denote the pressure in the evaporator at status point 3’ and 4’ (see Fig. 2); \(t\) is time; \(\alpha\) is a coefficient that reflects the time taken by the pressure dropping to \(P_e\) from \(P_e\).

Since the pressure falling off process is relatively quick compared to the time needed for the whole adsorption process, \(\alpha\) is in the range \(0 < \alpha < 1\), which means that the bigger value \(\alpha\) is, the shorter time needs for the evaporating pressure dropping. When \(\alpha = 1\), the evaporating pressure falls off to the designed evaporating pressure and is dominated by the generator in dozens of seconds. The value of \(\alpha\) depends on the practical operating situation and system inner structure, which can be an empirical value and obtained experimentally. Substituting the defined transient pressure into Eq. (6), the transient density of methanol vapor \((C_t)\) is then:

\[
C_t = P_t / R_0 T_t
\]

4.4. Numerical solutions

The operating conditions, \(T_0 = 30^\circ C, T_4 = T_{in} = 10^\circ C, T_0 = T_{in} = 25^\circ C\) and \(T_4 = 65^\circ C\) were chosen for the numerical study. The data used in numerical calculations is given in Table 1. The thermal properties of methanol and physical property of carbon were obtained from literature [22,23]. The adsorptive properties of the carbon-methanol working pair were obtained experimentally in our lab.

The set of governing equations (i.e., Eqs. (1), (2), and (5)) associated with corresponding initial and boundary conditions were solved by finite-volume technique [24] in Matlab environment. For the spatial grids, as schematic diagram shown in Fig. 3, the adsorbent bed was divided into a number of elementary layers/ rings in radial direction and each elementary layer was small enough to be considered having the uniform temperature and pressure within each layer. In the grid scheme, \(R_i\) is the inside radius of the carbon column while \(R_0\) is the outside radius of the carbon column; \(\Delta r\) represents the uniform thickness of each layer in spatial discretization. Thus, each carbon layer has an even thickness of \((R_0 − R_i)/N\) \((N\) denotes the number of total layers).

The central difference and forward difference approaches were adopted to convert the differential equations into a set of linear equations. The linear equations were solved by Thomas algorithm and Gauss–Seidel iteration technique [24].

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho_0)</td>
<td>420</td>
<td>kg m (^{-3})</td>
<td>(R_0)</td>
<td>8314</td>
<td>J mol (^{-1}) K (^{-1})</td>
</tr>
<tr>
<td>(\rho_3)</td>
<td>0.8</td>
<td>kg m (^{-3})</td>
<td>(C_{gh})</td>
<td>930</td>
<td>J kg (^{-1}) K (^{-1})</td>
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<tr>
<td>(C_{gh})</td>
<td>6.6</td>
<td>mol m (^{-3})</td>
<td>(C_{ps})</td>
<td>2530</td>
<td>J kg (^{-1}) K (^{-1})</td>
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<tr>
<td>(C_{ps})</td>
<td>3</td>
<td>mol m (^{-3})</td>
<td>(C_{pg})</td>
<td>1370</td>
<td>J kg (^{-1}) K (^{-1})</td>
</tr>
<tr>
<td>(T_0)</td>
<td>298</td>
<td>K</td>
<td>(L)</td>
<td>1102000</td>
<td>J kg (^{-1})</td>
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<tr>
<td>(T_4)</td>
<td>338</td>
<td>K</td>
<td>(R_0)</td>
<td>0.105</td>
<td>m</td>
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<tr>
<td>(P_e)</td>
<td>16360</td>
<td>Pa</td>
<td>(\Delta_{st})</td>
<td>0.175</td>
<td>W m (^{-1}) K (^{-1})</td>
</tr>
<tr>
<td>(P_e)</td>
<td>7140</td>
<td>Pa</td>
<td>(\Delta_{st})</td>
<td>10</td>
<td>m</td>
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<tr>
<td>(x_{0})</td>
<td>0.269 (exper.)</td>
<td>kg kg (^{-1})</td>
<td>(\alpha)</td>
<td>0.005</td>
<td>(exper.)</td>
</tr>
<tr>
<td>(n)</td>
<td>1.781 (exper.)</td>
<td>N</td>
<td>(D)</td>
<td>500</td>
<td>(assumed)</td>
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<tr>
<td></td>
<td>9.08e-6</td>
<td>(exper.)</td>
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</table>
5. Experiments

The schematic diagram and photo of the test rig are shown in Fig. 4a and b. The configuration of the experimental prototype of the ART was modified for the testing purpose, which includes spindled evaporator, enlarged generator and non-compact connection. Water baths were used as the simulated heating source and cooling source. Temperature was measured by the directly-inserted thermocouple (T type). The thermocouples and the data logger were calibrated separately by Fluke calibrators. The volume of the evaporator was calibrated using a volume calibration syringe.

The main procedures of the experiments conducted include the following steps:

1. Heat and degas the carbon bed simultaneously for twelve hours, and then isolate the generator by closing valve V2.
2. Fill methanol into the evaporator and maintain evaporator at $T_3$. The amount filled in the evaporator is slightly higher than the amount $x_{\text{max}}/M_{\text{cb}}$ for compensating the vacuuming process caused evaporation.
3. Charge methanol into the carbon bed. The amount charged is $M_4 = x_{\text{min}}/C_2M_{\text{cb}}$.
4. Set the status of the generator to point 4 (see Fig. 2) via circulating water (at $T_4$) in water jacket until the carbon bed temperature reaches $T_4$ evenly.
5. Connect the generator and evaporator and in the meantime circulate cooling water (at $T_c$) in water jacket to start the adsorption process.
6. Record temperatures and pressures.

6. Results and discussion

Fig. 5 shows the comparison of pressure development among experimental data and results calculated using the transient pressure $P_t$ with $\alpha = 0.001$, $\alpha = 0.005$ and $\alpha = 0.009$ respectively.

The experimental data shows that evaporating pressure in the evaporator takes about 3000 s to reach the designed evaporating pressure. In other words, system pressure is dominated by the generator after 3000 s. Moreover, this experimental data also indicates that the principal driving force of adsorption is shifted to temperature driving over this period (about 3000 s). Because in the following process only the decrease of adsorbent temperature could lead to concentration variation (i.e. adsorption) once the pressure throughout the adsorbent bed is almost stabilized, according to D–A equation (Eq. (1)).

For three values of $\alpha$, $\alpha = 0.005$ gives the best agreement of calculated data and experimental data. Therefore, $\alpha = 0.005$ is selected for this particular experimental setting up, for further simulation.

Fig. 6 presents three typical methanol vapor density changing trends assumed in following simulation models. They are (1) transient $C_t$ with $\alpha = 0.005$ proposed in current model, (2) setting $C_e$ as a constant that equals to $C_3$, and 3) setting $C_e$ as a constant that equals to $C_4$ which was used in almost all previous models [14,15,23]. Fig. 6 indicates that with the transient vapor density assumption, after some time (about 3000 s), value of $C_t$ would be stable towards $C_e = C_4$.

Fig. 7 shows the experimental data and simulated results of temperature development under three $C_e$ assumptions i.e. (a) $C_e = C_3$, (b) $C_e = C_4$ and (c) $C_e = C_5$. It can be seen from the group figures of Fig. 7 that the calculated temperature values under the assumption $C_e = C_5$ (with $\alpha = 0.005$) has the best agreement with the experimental data. In other words, introduction of transient boundary condition of vapor density ($C_t$) makes the simulation of the process more accurate, especially at the beginning stage, compared to that simulated with $C_e = C_3$ and $C_e = C_4$.

In Fig. 7a, when $C_e = C_3$ was chosen as the boundary condition for diffusion equation, the simulated temperature of the relative inside positions (layers) jumps dramatically, up to 25 $^\circ$C, at the very beginning of the process, before starting to decrease. This result indicates there is a strong adsorption process happened in the
inner layers, i.e. a lot of adsorption heat generated. However, the simulated values are much higher than the experimental data, reaching about 10 °C difference in the inner positions. This deviation generated is due to the inappropriate boundary condition \( C_e = C_3 \) because this high vapor density cannot exist over the entire adsorption process, but reaching the low level in about 1500 s, shown in Fig. 6.

In Fig. 7b, when using the popular boundary condition \( C_e = C_4 \), the simulated temperature of inner layers rises slightly, about 4 °C, and then starts to decrease. But for the outer position (e.g. \( r = 98 \) mm), the temperature decreases directly without a quick temperature jump. Comparing with the case at \( C_e = C_3 \), using boundary condition \( C_e = C_4 \) may bring a better agreement with experimental data. However, the temperature of outer layer and the temperature jump of the inner layers are lower than the experimental values, which resulted from missing the strong diffusion force several hundred seconds before the vapor density reaching and keeping at the stable value. In other words, if the process of transient pressure was neglected, the phenomenon of the temperature jump could not be well predicted, such as the numerical study in literature [14].

Fig. 7c shows the experimental and simulated results of temperature development under the introduced transient boundary condition \( C_e = C_t \) with \( \alpha = 0.005 \). There is a very good agreement between the calculated data and the experimental data. Therefore the model developed is valid in terms of predicting the temperature development. From Fig. 7, it can also be seen that the simulated temperature increases before starting to decrease, which agrees with the experimental data well. It indicates that the transient boundary condition introduced is able to present the shift of the dominant factors of the adsorption driving force, which is shifting to temperature driving from vapor density gradient caused diffusion driving with the diminishing of the gradient of vapor density.

Fig. 8 shows the dynamic adsorption amount calculated with \( C_e = C_4 \) and \( C_e = C_t \). The adsorption amount calculated with \( C_e = C_4 \) is about 20% lower than that calculated with the transient boundary
Fig. 7. Comparison of experimental data and modeling results of temperature variation at three positions with static and transient boundary conditions $C_e$: (a) $C_e = C_y$, (b) $C_e = C_q$ and (c) $C_e = C_t$. (Markers represent experimental data and solid lines denote numerical results.)
condition \(C_e = C_t\) in the first 2000 s, which is resulted from the neglect of the strong diffusion effect at the very beginning moment. However, with time goes on, the gap tends to reduce because the value of \(C_t\) approaches the constant boundary condition \(C_3\) as well.

7. Conclusions

A dynamic model describing the adsorption process in the carbon/methanol refrigeration tube was established based on coupled diffusion driving and temperature driving adsorption mechanism. A concept of transient boundary i.e. transient pressure (and transient vapor density) was introduced for the first time into the model. The model was preliminary validated in terms of adsorbent temperature development after the determination of \(x\) value using experimental data.

The introduced transient boundary condition provides an effective way to describe the shift of dominant driving forces of the adsorption process, which is very helpful for improving the accuracy of the model.

References