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Modeling of isobaric stages of adsorption cooling cycle: Transient and quasi-stationary regimes

Boris N. Okunev [a,*], Yuriy I. Aristov [b]

[a] Moscow State University, Vorobievi Gori, Moscow 119992, Russia
[b] Boreskov Institute of Catalysis, Novosibirsk 630090, Russia

HIGHLIGHTS

- ► A Fickian diffusion model is used to study dynamics of adsorption chillers.
- ► The formation of transient and quasi-stationary modes has been numerically studied.
- ► Heat transfer between the plate and the grain commonly is a rate limiting process.
- ► Intraparticle water diffusion dominates only at unfeasible values of the diffusivity.

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ABSTRACT

Isobaric water ad-/desorption on/from a spherical adsorbent grain of 1.5 mm in diameter, which is in thermal contact with a metal plate, is studied by numerical simulation based on a Fickian diffusion model. The plate is subjected to a fast temperature drop/jump (60 °C ↔ 70 °C) that initiates changing the adsorbed water uptake/release. Several model adsorption isobars (linear, exponential and stepwise) are used to describe the adsorbent–water equilibrium.

We have investigated the formation of quasi-stationary ad-/desorption regimes which are established after a short transient period right after the temperature drop/jump. The instant rate of water ad-/desorption is found to be a linear function of the difference of the metal plate temperature and the current temperature of the grain. As a result, the water ad-/desorption is faster when this average temperature difference is larger. Under studied conditions, the vapor pore diffusivity affects the overall ad-/desorption dynamics, although the dynamics is more sensitive to variation of heat transfer parameters. For a monolayer configuration, the heat transfer from the plate to the grain is the main rate limiting process at most realistic situations. Intraparticle water diffusion is the main rate limiting factor at unfeasible values of the pore diffusivity (lower than 10^{-10}–10^{-11} m^2/s).

1. Introduction

Various adsorption chillers, AC, have been developed during the past few years, and many of them have now passed over from the prototype stage to small serial production [1]. Despite significant progress achieved, there is still a big room for improvement in this technology [2], first of all, for enhancing the specific cooling/heating power (SCHP) and, hence, reducing the AC size. The main challenge is a dynamic optimization of the integrated unit “Adsorbent – Heat Exchanger” (Ad-HEx) [3] to enhance heat and mass transfer processes. Several ways have been considered for reaching this goal, e.g. a proper HEx design [4], consolidation of the adsorbent with HEx [5], heat transfer intensification [6], sophisticated Ad-Hex structure [7], heat and mass recovery [8], process control strategy [9], harmonization of the adsorbent and the cycle [10], etc.

Mathematical modeling is an important tool for study and optimization of heat and mass transfer in AC. Depending on the complexity, the dynamic models may be classified as lumped parameters (LP) and heat and mass transfer (HMT) models. The LP models give a simplified representation of the adsorption process, neglecting any space gradients. As to our knowledge, the LP model was first applied for analysis of ACs by Sakoda and Suzuki [11] and afterwards was replicated in both original or modified forms in many papers (see e.g. [12]). The HMT models take into account

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* Corresponding author.
E-mail addresses: okunev@tech.chem.msu.ru, nadar@ngs.ru (B.N. Okunev), aristov@catalysis.ru (Y.I. Aristov).

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Nomenclature

AC	Adsorption Chiller
Ad	Adsorber
Bi	thermal Biot number, dimensionless
C	concentration, mol/m^3
c_p	effective heat capacity, J/(kg K)
D	effective water diffusivity (m^2/s)
F	free energy of adsorption, J/mol
H	heat of adsorption (J/mol)
HEx	Heat Exchanger
P	pressure, Pa
q	water uptake, kg H$_2$0/kg adsorbent
R_p	grain radius, m
R	universal gas constant, J/(mol K)
r	radius, m
SWS-1L	composite sorbent “CaCl$_2$ in the silica gel pores”
T	temperature, K
t	time, s

Greek symbols

α	heat transfer coefficient, W/(m^2 K)
χ	water uptake, dimensionless
ε	grain porosity, dimensionless
λ	coefficient of heat conductivity of the grain, W/(m K)
μ	molar mass, kg/mol
ρ	density, kg/m^3
τ	characteristic time, s

Subscript

av	average
dr	driving force
dif	diffusion
f	final
g	grain
in	initial
kn	Knudsen
max	maximal
p	at constant pressure
s	saturated
st	step (of the adsorption isobar)

variation of the adsorbent temperature T_a, pressure P and the adsorbate concentration q both in time and space [13,14]. The governing equations are partial differential, hence, sophisticated and time-consuming numerical methods are required for solving these equations and simulation of adsorbent bed dynamics. Because of this, the HMT models are less wide-spread.

In this paper, we have applied an HTM model developed in [15] for analyzing a coupled heat and mass transfer in a monolayer of adsorbent grains which are in thermal contact with a metal plate serving as a heat source/sink. This model differs from the majority of model presented in literature because a) the mass transport is described by a Fickian diffusion equation but not by a Linear Driving Force equation [11]; and b) the water adsorption is initiated by a fast temperature jump/drop but not a pressure jump. Thus, the model closely simulates water adsorption process under isobaric stages of an AC and has been used for analyzing the experimental results obtained by a Large Temperature Jump (LTJ) method [16]. Recently, we used this model to realize how a shape of the adsorption isobar affects the dynamics of the AC isobaric stages [17]. Several model adsorption isobars (stepwise, linear and exponential) were considered (Fig. 1).

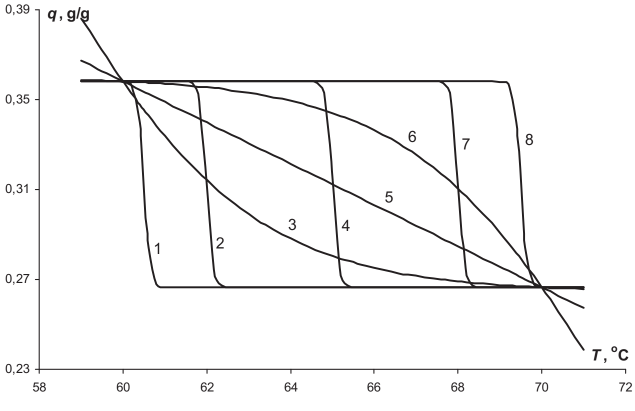

Fig. 1. a – Model isobars of water sorption at $P = 56.5$ mbar: 1 – step at 60.5 °C, 2 – step at 62 °C, 3 – exp (concave), 4 – step at 65 °C, 5 – linear, 6 – exp (convex), 7 – step at 68 °C, 8 – step at 69.5 °C.

In the course of that study, we found that the temporal evolution of the average grain temperature T_{av} and the average pressure P_{av} inside the grain can be divided into two parts, namely, fast transient and slow quasi-stationary modes [17]. The aim of this paper is to carefully investigate the process of coupling heat and mass transfer and the formation of the quasi-stationary regime. We have analyzed how long time does it take setting of the quasi-stationary regime and revealed the main features of this mode (energy balance, instant cooling power, etc).

Another principal question to be analyzed is “What are relative contributions of heat transfer and mass transfer to the overall dynamics of AC isobaric stages?” It is well known that these two processes are inevitably coupled and strongly affect each other. Indeed, a fast heating of an adsorbent grain readily causes water desorption and generates a pressure gradient inside the grain, thus, enhancing the mass transfer and water removal out of the grain. On the other hand, this fast water desorption prevents the rapid grain heating and, therefore, promotes the heat supply to the adsorbent grain. In this paper, we attempt to elucidate which contribution is more important by evaluating which parameter – the heat transfer coefficient or the vapor diffusivity – is the dynamics more sensitive to. This could be important for making practical recommendations on desirable strategy for improving the Ad-HEx dynamics.

2. Mathematical model

A mathematical model of coupled heat and mass transfer in a single adsorbent grain was described elsewhere [15] and here we just repeat its main features. Combined heat and mass transfer in a single adsorbent grain was described by the following system of differential equations:

a) The energy balance equation including the heat of adsorption ΔH:

$$\rho c_p(T,q)\frac{\partial T}{\partial t}-\frac{\rho\Delta H}{\mu_{H_2O}}\frac{\partial q}{\partial t}=\frac{\lambda}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) \qquad (1)$$

$$0<r<R_g$$

with the relevant initial and boundary conditions