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Insights from modeling dynamics of water sorption in spherical particles for adsorption heat pumps

A.I. Radu [a,b], T. Defraeye [a,b], P. Ruch [c], J. Carmeliet [a,b], D. Derome [b,*]

[a] Chair of Building Physics, Swiss Federal Institute of Technology Zürich (ETHZ), Stefano-Franscini-Platz 5, 8093 Zürich, Switzerland
[b] Laboratory of Multiscale Studies in Building Physics, Empa, Überlandstrasse 129, 8600 Dübendorf, Switzerland
[c] IBM Research – Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

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ABSTRACT

The coupled heat and mass transport in porous adsorbents, shaped as spherical particles is simulated in the context of finned heat exchangers for thermally-driven heat pumps. Water vapor sorption behavior triggered by a step change in fin temperature, representative for the isobaric stages of a thermodynamic cooling cycle, is modeled for two different particle diameters, both in mono- and multi-layer configurations. Numerical results confirm the experimental observations for adsorption and desorption, with faster dynamics for smaller particles in monolayer configurations. Simulations show that contact between particles influences heat transfer in the particle ensemble to a different extent, dependent on particle diameter. The characteristic time required to reach 80% of the equilibrium amount of moisture uptake is only slightly affected by the particle packing configuration for the studied cases. Parametric evaluations of heat and mass transport properties of the adsorbent are carried out for an operational scenario typical for air-conditioning using low grade heat. The aim is to identify the critical factors for improving the specific cooling power of the adsorbent. Sorption dynamics and the corresponding specific cooling power are mostly affected by the heat transfer parameters of the adsorbent-heat exchanger system. Results indicate that further increasing the effective diffusivity within the material does not improve the specific cooling power, while a lower effective diffusivity dramatically decreases performance. This effect is more pronounced for larger particles in fewer layers.

1. Introduction

When microporous materials are exposed to moisture, adsorption of water vapor on the pore surfaces can occur. As water molecules are adsorbed, they go to a lower energy state, by which a significant amount of heat is released. On the other hand, heat needs to be supplied to the water molecules for desorption to occur. Sorption-based processes are used in thermally-driven cooling devices which represent an attractive alternative to traditional vapor compression technology for heating and cooling applications [1,2]. A typical example is the adsorption heat pump, which allows the utilization of low grade waste heat to provide heating or cooling for buildings, vehicles or energy-efficient data centers [3–5].

To make adsorption heat pumps competitive with currently available technologies, their dynamic performance and, more specifically, their heat and mass transport efficiency needs to be improved [6]. A specific challenge is to optimize the adsorption/desorption process. Within such sorption systems, heat and mass transport are strongly coupled during adsorption/desorption: on one hand, the sorption rate is influenced by the temperature via the sorption curve, while, on the other hand, the heat balance is affected by the adsorbed amount and sorption rate via the heat of sorption. Furthermore, the characteristics of the adsorbent, i.e., the material and its geometrical configuration, affect the performance.

Traditionally, two configurations of adsorbent have been used for adsorption heat pumps: (1) consolidated coating, where the adsorbent material, bound in a matrix, is coated on the heat exchanger and (2) fixed bed, consisting of packed adsorbent particles. Consolidated coatings tend to have good heat transfer properties, but are typically applied in thin layers due to mass transfer limitations [7,8]. This study will focus on fixed bed configurations as they offer good mass transfer properties and a simple assembly [9,10]. Despite these favorable characteristics, heat transfer through the bed is thought to be restricted by the points of contact between the adsorbent particles [11]. In order to enhance the heat transfer rate, heat exchangers with metal fins are used and

* Corresponding author.
E-mail address: dominique.derome@empa.ch (D. Derome).

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adsorbent particles are packed between the metal plates, as fins increase the heat transfer area between the adsorbent and the heat transfer fluid, i.e. the fluid of the heat exchanger [12]. The distance between two consecutive fins, thus the thickness of the particle layer, was shown to be one of the main optimization parameters for improving the performance of adsorber heat exchangers [13]. Glaznev and Aristov [14] reported that monolayers of spherical particles resulted in very high specific cooling power (SCP). A major drawback of such a monolayer configuration is that the mass ratio of inert metal of the heat exchanger to absorbent is quite high, resulting in a lower coefficient of performance of the adsorption heat exchanger due to the parasitic heat capacity of the inert metal. Therefore, recently, a higher number of layers, namely 2–8 layers of loose particles, has been proposed for improved efficiency [15,16].

Four operational stages can be distinguished during an ideal thermodynamic cycle within adsorption heat pumps [17]: an isosteric heating phase, an isobaric desorption phase, an isosteric cooling phase and an isobaric adsorption phase. The isosteric phases occur at constant adsorbed amount. During the isobaric adsorption phase, a decrease in temperature is imposed, while the pressure remains constant. The isobaric desorption phase is triggered by an increase of temperature, while the pressure remains constant. In order to assess the adsorption/desorption behavior under conditions relevant for practical operation, temperature swing isobaric conditions need to be considered.

For optimization of sorption-based heat pumps, numerical models are highly complementary to experiments. Modeling is particularly useful for parametric studies in order to derive practical recommendations on desired adsorbent properties, geometries and heat exchanger design [18]. Regarding the particle configuration, most of the modeling work focused on single adsorbent grains [6,19] or on thick adsorbent beds i.e., more than 10–20 layers. These beds are approximated as a porous continuum and mass transfer within the particles is estimated using a linear driving force model [20–22]. For loose grain configurations, a first modeling attempt with discrete adsorbent particles was carried out by Freni et al. [23]. However, the authors only considered a two-dimensional (2D) geometry which actually mimics cylindrical rods, not spherical particles. In order to accurately describe the heat and mass transfer processes for multilayer configurations of spherical particles, a three-dimensional (3D) geometry needs to be considered. 3D numerical studies that investigated stationary heat transfer in adsorption heat exchangers between adsorbent particles and fins did not consider sorption dynamics, but instead assumed a constant heat source due to adsorption [24]. Obviously, 3D calculations have higher computational requirements compared to their 2D counterpart. In addition, another challenge is faced while modeling such particle configurations, namely the contacts between spherical particles. A perfect point contact often leads to discretization problems in terms of meshing of the computational domain. To overcome this, two alternatives are available: reducing the size of the spheres to avoid any contact which results in narrow gaps between particles [25–27], or overlapping the spheres [27,28], resulting in higher contact areas between particles. Such assumptions may, however, have consequences on the sorption behavior. Once a proper model is made, simulations at particle scale can be very useful to better understand the factors which play a role during the adsorption/desorption process. So far, parametric studies from literature have evaluated different material properties and operational parameters. These studies were mostly focused on thick adsorbent beds, where a porous continuum approach was used [22,29].

In this work, we analyze heat and mass transfer for loosely packed adsorbent particles subjected to a temperature swing using a three-dimensional finite element model. To the best of our knowledge, this is the first 3D numerical model considering conjugate heat and mass transport between particles and surrounding vapor, including sorption dynamics. Regular density (RD) silica gel is chosen as the model adsorbent, as it is commercially used for adsorption chillers and its experimental characterization of various properties is available in literature. The proposed model is verified with available experimental data. A comprehensive parametric evaluation of various heat and mass transport properties is carried out for conditions characteristic for the isobaric stage of adsorption. This study provides insights and recommendations for the development of future adsorbents in terms of material properties and configuration as well as for the design of adsorption heat exchangers.

2. Model description

A numerical model is built to investigate the sorption behavior of spherical silica gel particles during the isobaric stages of an adsorption heat pump, when the adsorbent is subjected to a temperature swing. The large temperature drop, or jump, at the metal fin surface caused by the heat transfer fluid in the heat exchanger pipes triggers vapor adsorption or desorption by changing the local moisture equilibrium conditions within the porous adsorbent. The model includes coupled heat and mass transport within the adsorbent particles and in the interparticle space/environment surrounding the adsorbent, where water vapor is present.

2.1. Geometrical model

A three-dimensional geometry is considered in the present study, representative for spherical particles in fixed bed configuration. A typical model geometry is shown in Fig. 1, namely a case with 4 layers of particles of uniform size, with an idealized packing. This packing is obtained by assuming a cubic arrangement of the particles within each horizontal layer i.e., particle centers are aligned over the *y* direction. Furthermore, a rhombic arrangement of two consecutive layers is assumed i.e., particle centers of the second layer are shifted over the *x* direction with respect to the particle centers of the previous layers. The actual size, in terms of height, depth and width, of the representative element is a function of the particle size (d_p) and the number of layers (n) for each configuration. In this study, we consider two particle diameters, $d_p = 0.45$ mm and $d_p = 0.85$ mm and configurations ranging from

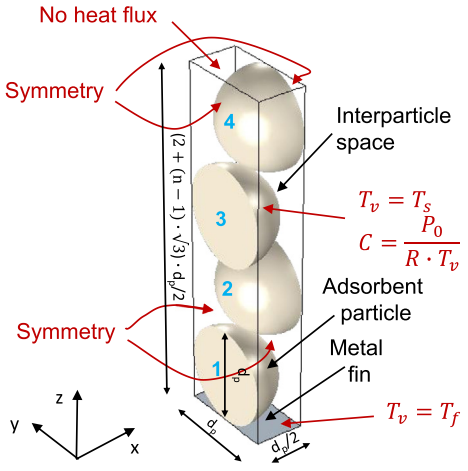

Fig. 1. Computational model with boundary conditions, illustrating a representative element of a multilayer particle configuration on top of a metal fin. The numbers within the spheres indicate the particle layer, counted from the fin surface.