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Optimization of adsorption processes for climate control and thermal energy storage

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ABSTRACT

Adsorption based heat-pumps have received significant interest owing to their promise of higher efficiencies and energy savings when coupled with waste heat and solar energy compared to conventional heating and cooling systems. While adsorption systems have been widely studied through computational analysis and experiments, general design guidelines to enhance their overall performance have not been proposed. In this work, we identified conditions suitable for the maximum utilization of the adsorbent to enhance the performance of both intermittent as well as continuously operating adsorption systems. A detailed computational model was developed based on a general framework governing adsorption dynamics in a single adsorption layer and pellet. We then validated the computational analysis using experiments with a model system of zeolite 13X-water for different operating conditions. A dimensional analysis was subsequently carried out to optimize adsorption performance for any desired operating condition, which is determined by the choice of adsorbent–vapor pair, adsorption duration, operational pressure, intercrystalline porosity, adsorbent crystal size, and intracrystalline vapor diffusivity. The scaling analysis identifies the critical dimensionless parameters and provides a simple guideline to determine the most suitable geometry for the adsorbent particles. Based on this selection criterion, the computational model was used to demonstrate maximum utilization of the adsorbent for any given operational condition. By considering a wide range of parametric variations for performance optimization, these results offer important insights for designing adsorption beds for heating and cooling systems.

1. Introduction

In the past three decades, the total primary energy consumption in the US has increased by ~25% [1], in which the buildings sector account for more than 40% of the overall consumption. In particular, within the buildings sector, heating and cooling applications account for more than half of all the energy consumed. With the significant demand for energy, especially in the building heating ventilation and air-conditioning (HVAC) systems, it is essential to develop new technologies that can improve energy efficiency.

Adsorption-based thermal energy storage, heat-pumps and air-conditioning systems offer numerous advantages including the use of simple construction, reduced number of moving parts, and being environmentally friendly. A schematic diagram illustrating the operation of a basic two-bed adsorption heat pump is shown in Fig. 1. The heat pump operates by pumping a refrigerant from a storage tank or reservoir to the evaporator, where evaporation takes place by absorbing heat, which may be provided by a liquid-based heat exchanger, wherein a coolant enters the evaporator at high temperature and exits at low temperature. The vaporized refrigerant diffuses from the evaporator into one of the adsorption beds, where it is adsorbed by high-capacity adsorptive materials. A significant amount of heat is released due to spontaneous adsorption of vapor, which is dissipated via liquid-cooling as illustrated in the figure. With continuous adsorption of vapor, the bed is gradually transformed from a dry to vapor-saturated state. This can result in a cessation of any further cooling or heating using the adsorption system. Consequently, to facilitate a continuous operation, the system can utilize two beds, as shown in Fig. 1. While one of the beds is saturated with vapor, the other bed is regenerated by heating. A portion of the total heat necessary for regenerating the bed can be supplied by the other bed generating the heat of adsorption. However, additional heating is necessary for complete regeneration. The desorbed vapor is condensed within the condenser and the condensate is subsequently returned to the reservoir. In Fig. 1, the heat of condensation is also shown to be dissipated by liquid cooling. With this simple operational mechanism, adsorption-based heat pumps can provide year-round

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Nomenclature

a, a_o	constant for Toth isotherm [mol/kg Pa]
b, b_o	constant for Toth isotherm [1/Pa]
co	constant for Toth isotherm [K]
C	concentration of vapor phase [mol/m^3]
C_b	concentration of vapor inside the chamber [mol/m^3]
C_i	initial concentration of vapor phase [mol/m^3]
C_{eq}	equilibrium concentration of the adsorbed phase [mol/m^3]
C_μ	concentration of adsorbed phase [mol/m^3]
$C_{\mu b}$	boundary concentration of adsorbed phase [mol/m^3]
$C_{\mu i}$	initial concentration of adsorbed phase [mol/m^3]
c_p	specific heat [J/kg K]
$c_{p,\,c}$	specific heat of the adsorbent crystal [J/kg K]
$c_{p,\,\mu}$	specific heat of the adsorbed vapor phase [J/kg K]
$c_{p,v}$	specific heat of the vapor phase [J/kg K]
d_p	characteristic intercrystalline pore diameter [m]
D_μ	intercrystalline vapor diffusivity [m^2/s]
$D_{\mu 0}$	intercrystalline vapor diffusivity at T_0 [m^2/s]
D_v	intracrystalline vapor diffusivity [m^2/s]
E	constant for Toth isotherm [K]
E_μ	activation energy for vapor diffusion [J/mol]
g, g_0	constant for Toth isotherm
h_{ad}	enthalpy of adsorption [J/mol]
h_v	heat transfer coefficient during adsorption/desorption [W/m^2 K]
k	thermal conductivity [W/m K]
K	permeability of the adsorption bed [m^2]
l	characteristic length [m]
l_s	thickness of a long slab [m]
M	molecular weight of the adsorbate [kg/mol]
p	pressure [Pa]
Pe	Peclet number
p_i	initial vapor pressure [Pa]
p_v	chamber vapor pressure [Pa]
$P(\chi)$	probability of a spherical void of diameter between χ and $\chi + d\chi$
r_c	radius of adsorbent crystal [m]
r_s	radiusof adsorbent sample [m]
$\hat{R}$	universal gas constant [J/mol K]
R_c	radius of a long cylinder [m]
R_s	radius of a sphere [m]
t	time [s]
t_o	total duration of adsorption [s]
T	temperature [K]
T_o	reference temperature [K]
T_i	initial temperature [K]
T_v	chamber vapor temperature [K]
T_w	chamber wall temperature [K]
u	vapor velocity inside the adsorption particle [m/s]
$\bar{u}$	dimensionless vapor velocity
V	volume [m^3]

Greek symbols

γ	dimensionless transport parameter
Γ	dimensionless vapor concentration
Γ_μ	dimensionless adsorbed vapor concentration
δ_m	thickness of the metal substrate [m]
δ_s	thickness or height of the adsorbent sample [m]
ε	porosity of the adsorption bed
ε_{HCP}	porosity of hexagonally closed packed spheres
ϵ_a	emissivity of aluminum surface
ϵ_z	emissivity of adsorbent surface
μ_v	dynamic viscosity of vapor phase, [kg/ms]
ω	vapor adsorbed per unit mass of adsorbent [kg/kg]
ρ	effective density [kg/m^3]
ρ_a	average density of dry adsorption bed [kg/m^3]
ρ_c	dry density of the adsorbent crystal [kg/m^3]
σ	dimensionless parameter
τ	dimensionless time
χ	nondimensional intercrystalline pore diameter
χ_{avg}	nondimensional average intercrystalline pore diameter
∇	gradient operator [m^{-1}]
$\overline{\nabla}$	dimensionless gradient operator

climate control by interfacing liquid-based heat exchangers with the system to deliver both heating and cooling.

Compared to a vapor compression cycle, adsorption systems have the benefit of saving energy if the beds can be regenerated using waste heat or solar energy [2–6]. Furthermore, using novel materials with superior adsorption capacities, such as synthetic zeolites [7] and metal organic frameworks [8,9], adsorption systems have the potential to deliver large energy and power densities. The thermodynamic cycle representing the operation of an adsorption-based heat-pump is shown in Fig. 2(a), wherein Q_{evap} and Q_{cond} are the net heat exchanged in the evaporator and condenser, respectively. Meanwhile, the heat released from the bed during isobaric adsorption at p_{evap} is Q_{ads}, and the heat supplied to regenerate the bed at a constant pressure, p_{cond} is Q_{des}. During continuous operation of the system, the two beds are operated out of phase. This can be seen in Fig. 2(b), which shows the cyclic variation of the temperature of the two beds with a characteristic half-cycle or adsorption time of t_o. It can be seen that a higher switching frequency, while ensuring complete utilization of each bed, can result in a much larger heating and cooling power for a two-bed adsorption system. While the overall energy density delivered by an adsorption-based heat pump is proportional to the adsorption capacity, the overall transport characteristics set the limit on the maximum extractable power density. Consequently, the net rate of heat exchange and vapor diffusion taking place in the characteristic time scale, t_o, is important and controls the maximum power density achievable using the adsorption-based climate control system. In addition to continuously operating multi-bed adsorption systems, thermal energy storage is also feasible using an intermittently operating, single-bed adsorption system, which also relies on efficient transport characteristics to deliver maximum power. Nevertheless, to optimize the overall performance of an adsorption-based thermal system, a detailed analysis of adsorption dynamics is necessary.

Numerical modeling in the form of thermodynamic, lumped-parametric, and full scale heat and mass transfer analysis has been extensively used in the past to predict the performance of adsorption-based heat pumps [10]. However, a thermodynamic model, based solely on first and second-law analysis, does not consider limitations due to heat transfer [11]. A lumped parametric model, although predicts adsorption dynamics, assumes uniform temperature and refrigerant concentration, and therefore neglects the intrinsic heat and mass transfer limitations [12]. A full-scale heat and mass transfer based model, while incorporating transport limitations to determine the overall performance, is complex, where the temperature-dependence of adsorption-capacity, thermophysical and transport properties are incorporated. Consequently, the non-linearity of such coupled phenomenon is generally addressed