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Modeling and computational simulation of adsorption based chemical heat pumps

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HIGHLIGHTS

- ► Performance of a chemical pump reactor is investigated theoretically.
- ► Ethanol adsorption/desorption on active carbon packing is modeled and simulated.
- ► Adsorption/desorption kinetics and equilibrium relations are found experimentally.

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ABSTRACT

In this study a methodology is developed for the design of a packed bed reactor to be used in a Chemical Heat Pump (CHP). Adsorption and desorption of ethanol on active carbon packing in the reactor are investigated. Depending on the cycle, i.e. adsorption or desorption, cooling or heating of the reactor material is modeled through transient energy equation. The parameters associated with the vapor-carbon adsorption kinetics are experimentally determined. Then spatial distribution of temperature and adsorbed vapor amount are obtained with respect to time in adsorption–desorption cycles. These profiles are used to predict heating or cooling powers and COP for different adsorbent bed geometries and adsorption/desorption cycle times. Strong effect of heat transfer resistance of the packing, hence reactor size, on the system performance is observed.

1. Introduction

Despite their limited commercial applications, chemical heat pumps (CHP) have always been considered as an important alternative to conventional heating and cooling systems. The working principle of chemical heat pumps is based on the use of reversible physical–chemical reactions such as vapor adsorption/desorption, the formation of metal hydrides, and reversible chemical reactions [1–7]. The major limitation of vapor adsorption/desorption based CHP applications mainly stems from higher desorption temperatures, lower cooling power per unit adsorbent volume and lower coefficient of performances (COP) compared to conventional compression heat pumps.

An adsorption/desorption based chemical heat pump has three components, which are reactor, liquid reservoir and condenser/cooler [8] as shown in Fig. 1. Cooling/heating cycles are completed in two alternating stages by making use of the temperature dependence of adsorbate equilibrium distribution between vapor phase and solid surface. First, liquid in the reservoir absorbs heat from the surroundings and evaporates. Then vapor is drawn into the reactor where an adsorption reaction takes place. Once the adsorption stage is completed, the flow between the evaporator and adsorption bed is switched off and desorption (regeneration) stage is initiated by heating the reactor. The desorbed vapor is transferred to the condenser where the latent heat is extracted. Flow of the liquid between the condenser and the evaporator is driven by the pressure difference between these components that is maintained by means of an expansion valve or a capillary tube. The system shown in Fig. 1 illustrates a basic CHP and cannot be operated continuously. However, it is possible to arrange this basic unit in terms of multiple stages and effects to achieve continuous operation with improved performance and heating/cooling power by utilizing heat sources at various temperatures [4,9].

In a`bsorption heat pumps the physical quantities including latent heat of the adsorbate (ΔH_v), isosteric heat of adsorption (ΔH_{ads}) and sensible heat of the adsorbate–adsorbent pair determine its COP. For example COP during a cooling cycle can be calculated as

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Nomenclature

COP	coefficient of performance
C_{ads}	concentration of adsorbed vapor in bed (mol/m^3)
C_{bulk}	vapor concentration (mol/m^3)
C_{pc}	specific heat of adsorbent (J/kg K)
C_{peff}	heat capacity of the bed (J/kg K)
C_{pv}	specific heat of vapor (J/mol K)
d_p	particle diameter (m)
h	heat transfer coefficient between adsorbent particles (J/s m^2 K)
h_f	film heat transfer coefficient in the reactor jacket (J/s m^2 K)
ΔH_{ads}	heat of adsorption (J/mol)
ΔH_v	latent heat of vaporization (J/mol)
k_e	effective thermal conductivity (J/s m K)
k_p	thermal conductivity of adsorbent (J/s m K)
$k_s\alpha_v$	mass transfer coefficient (s^{-1})
l	characteristic length, thickness of the packed annular space (m)
L	Reactor length in the axial direction (m)
m_{bed}	mass of the bed (kg)
M	molecular weight of vapor (kg/mol)
n_{ads}	adsorbed vapor amount (mol)
r	radial position
r_i	inner bed radius (m)
r_o	outer bed radius (m)
R_{ads}	Adsorption rate (mol/m^3 s)
t	time
ΔT	temperature difference between adsorption–desorption cycle (K)
$T_{initial}$	initial temperature (K)
T_f	average temperature of cooling/heating fluid (K)
W	vapor adsorption capacity of bed (g vapor/g adsorbent)
w	adsorbed amount of vapor in bed (g vapor/g adsorbent)

Greek letters

ε	porosity
σ	emissivity
μ	viscosity of vapor (Pa s)
ρ_c	density of adsorbent (kg/m^3)
ρ_v	density of vapor (kg/m^3)

$$\mathrm{COP} = \frac{\Delta H_v n_{ads}}{\Delta H_{ads} n_{ads} + C_{peff} m_{bed} \Delta T} \quad (1)$$

where n_{ads} is the total number of moles adsorbed vapor, ΔT is the temperature difference between adsorption–desorption stages, C_{peff} and m_{bed} are the average heat capacity and the mass of the bed (adsorbent + adsorbed vapor), respectively. COP depends strongly on n_{ads} which is a function of adsorption–desorption temperature interval for a selected adsorption pair. It is not meaningful to evaluate COP outside the temperature range at which appreciable adsorption–desorption occur. COPs of the adsorption heat pumps are inherently much lower than those of the conventional heat pumps. However it should be noted that, direct comparison between the COPs of the adsorption heat pumps and the conventional heat pumps can be misleading as no compressor is used in the former one, which is the main advantage.

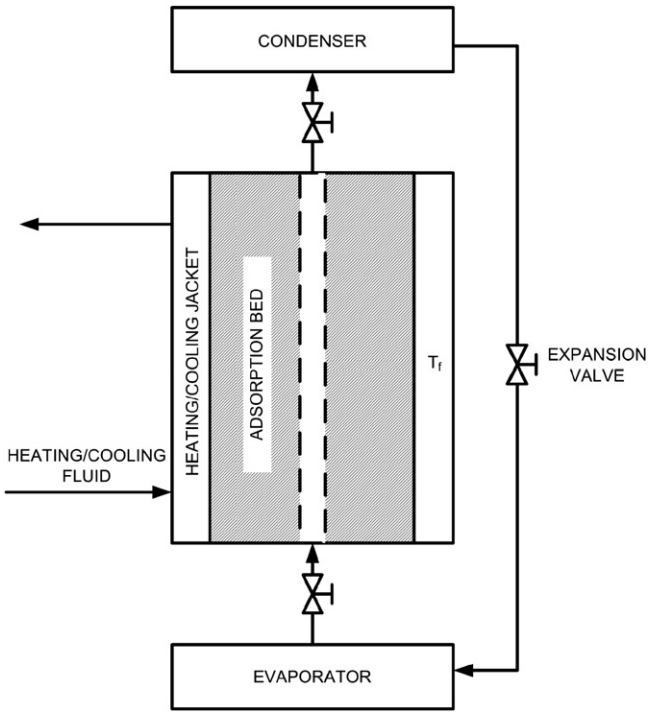

Fig. 1. Single stage adsorption heat pump.

The performance of heat pumps with different vapor-adsorbent pairs has been studied extensively [10–13]. Some of the experimentally studied adsorption pairs are $CaCl_2$–ammonia, activated carbon–methanol, cement–activated carbon composite–methanol, and zeolite–water. The reported COP values are between 0.25 and 0.4 that are lower than the theoretical values [10,11]. Low COP values experienced in a typical chemical heat pump have been attributed to the heat and mass transfer limitations pertinent to the packed bed reactors [12,13]. Heat transfer in the adsorbent bed is critical due to the poor effective thermal conductivity of typical packed beds. The impact of low thermal conductivity of the packing has also been observed in earlier studies in the form of appreciable temperature gradients hence appreciable adsorption capacity variations in the packing leading to poor overall performance of heat pump [14].

In a report by San [15], performance of a multi-bed adsorption heat pump is investigated. Through the developed mathematical model and used numerical scheme, the effects of adsorbent particle size, cycle time, operation temperatures and thermo-physical material properties are computationally investigated. In the transient mass conservation equation, the adsorption/desorption effects are included implicitly through adsorption isotherms by assuming local equilibrium. On the other hand, including the adsorption/desorption rate term directly in the mass equation eliminates use of such assumption in modeling the transient nature of the process.

It is obvious that the impacts of the heat and mass transfer resistances on the heating/cooling performance merit a thorough investigation of adsorption/desorption processes in the reactor. Once the system is modeled accurately in terms of adsorption kinetics, heat and mass transfer in microscopic level, which is the main objective of this study, the process the can be captured realistically by a simulation code. Therefore computer experiments can be done over a wide range of parameters including vapor-adsorption pair, geometry, pressure, temperature, flow rates, etc.

In this study, modeling of adsorption/desorption cycles in a packed reactor of a CHP is presented. In the model, adsorption and desorption cycles in the reactor are handled through the transient