Contents lists available at ScienceDirect



International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Theoretical framework to evaluate minimum desorption temperature for IUPAC classified adsorption isotherms



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ARTICLE INFO

Article history: Received 10 November 2017 Received in revised form 5 January 2018 Accepted 24 January 2018

Keywords: Adsorption Desorption Evaporator Isotherm model Minimum desorption temperature

1. Introduction

International Institute of Refrigeration in Paris [1] estimated that 15% of the total produced electricity of the world is spent on refrigeration and air-conditioning processes of various kinds. Predominantly, vapor compression refrigeration systems are used which are energy intensive, requiring only electricity to drive such systems. Alternative carbon-neutral technologies are needed to reduce the global carbon footprint of refrigeration and air conditioning systems. Thermally driven adsorption chillers have been studied for several decades, primarily as a viable alternate to the conventional vapor compression systems. Several key benefits of adsorption systems based on prior studies are: (i) useful for recovery of low grade thermal energy (<100 °C) which otherwise would go as waste in many processes [2-4]; (ii) can be operated with inexpensive non-concentrating type solar collectors like flat plate or evacuated tube collectors [5–7]; (iii) environmental friendly as they frequently use natural refrigerants like water [8–10], ethanol [11–13], methanol [14–16] with no ozone depletion and global warming potential; (iv) production of multi-effects like cooling

ABSTRACT

An adsorption chiller requires thermal energy to regenerate the adsorbent by desorbing the refrigerant vapor. Minimum desorption temperature is the parameter which defines the lowest possible heat source temperature required for driving adsorption chiller. In this study minimum desorption temperature is evaluated for different types of adsorption isotherms classified by International Union of Pure and Applied Chemistry (IUPAC). For each type, adsorption isotherm model is utilized to estimate the minimum desorption temperature and then compared to the mathematical expression reported in literature derived using Dubinin-Astakhov isotherm model. This allows for critical scrutiny of the universal validity of mathematical expression. It is observed that this expression can estimate the minimum desorption temperature with reasonable accuracy for all isotherm models.

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and desalination [17–19] and even auxiliary power production [20] with suitable system configurations.

The choice of adsorption pair is a primary aspect in designing any thermally driven adsorption chiller. Many studies have focused on the development of adsorbents and their characterization [12.21–25]: theoretical formulation of isotherm models [26–29] as well as thermodynamic analysis of adsorption chillers [18,30-32]. Thermally driven adsorption chiller employs cyclical adsorption desorption processes for compressing refrigerant vapor from evaporator to condenser pressure; utilizing the available energy from temperature swing (difference between heat source and sink temperatures). Typically, single-stage adsorption chillers are known to operate with a temperature swing of about 30-50 °C [13,33,34] for chilled water at 10–14 °C and sink at 30 °C. However, even a temperature swing of 10 °C can be exploited in a multistage adsorption refrigeration system [35]. There are experimental evidences of operation of 3-stage adsorption chiller at a driving heat source temperature as low as 48 °C [36], with the chilled water temperature outlet of 8 °C and ambient at 30 °C. In principle, a ten-stage chiller can be driven with a temperature swing of only 2.2 °C [36]. The above studies highlight that the temperature swing needed for the adsorption chiller is dependent on the ensemble of operating conditions and the number of stages of the chiller. This resulted in the evaluation of a theoretical concept called the "minimum desorption temperature" [31,36-38]. It is defined as the minimum heat source temperature required for successful

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Nomenclature

A A ₀ A ₁	locus of maximum of distribution function (–) constant parameter (–) constant parameter (K)	r R t	adsorbent radius (m) specific gas constant (J mol ^{–1} K ^{–1}) dimensionless parameter in both Tóth and Sips iso-
b	affinity constant (–)	т	therms (-)
D ₀ B	breadth of distribution function (1 T.	reference temperature (K)
D C	constant related to temperature effect $(-)$	v_0	volume adsorbed per unit area of adsorbent surface
с Со	adjusted constant related to temperature effect (-)	v	(nm)
C D	dimensionless parameter (–) constant determined by adsorbent microstructure (K^{-1})	v _m	volume adsorbed when entire adsorbent surface is cov- ered with monolayer (nm)
Eai	molar adsorption energy of gases in the site i (kJ mol ⁻¹)	V	volume (m ³)
H_1	heat of condensation of water vapor at the given tem-	W	equilibrium uptake (kg kg ⁻¹)
	perature (kJ mol ⁻¹)	W_0	adsorption capacity at reference temperature (kg kg $^{-1}$)
ΔH_1	function of heat of sorption of water (kJ mol ⁻¹)	W_m	moisture content corresponding to an adsorbed mono-
ΔH_2	function of heat of sorption of water (kJ mol ⁻¹)		layer (–)
$H_{\rm m}$	heat of sorption of monolayer of water (kJ mol ⁻¹)	Ws	saturation adsorption capacity (kg kg ⁻¹)
H_n	heat of sorption of multilayer of water (kJ mol ⁺)	x	pressure ratio (–)
K	constant related to temperature effect (-)	$x_{i,exp}$	experimental uptake (kg kg ⁻¹)
<i>K</i> ₀	adjusted constant related to temperature effect (-)	X _{i,iso}	uptake obtained from isotherm model (kg kg)
n	number ()		
11 n.	number (-)	Subscripts	
ni N.	density of recentor sites $(\alpha \text{ cm}^{-3})$	aa	adsorption
P Nmi	pressure (kPa)	cona	condensation
p.	pressure at which half of the recentor site <i>i</i> is occupied	des min	
- 1	(kPa)	aes,min	evaporation
0	isosteric heat of adsorption at zero fractional untake	с c	cvaporation
z	$(kj kg^{-1})$	3	Saturation

operation of an adsorption cycle. It is interesting to note that theoretically, minimum desorption temperature only depends on the nature of adsorption isotherm. However, on the account of various sources of thermodynamic irreversibility, an actual chiller needs to be operated at a significantly higher heat source temperature [39]. Nevertheless, the exercise to determine minimum desorption temperature has important implications in the design of an adsorption chiller, as it allows for: (i) choosing the appropriate adsorption pair; (ii) determining the optimum number of stages required.

As mentioned above, minimum desorption temperature depends on adsorption isotherm. In this context, a theoretical equation based on Dubinin-Astakhov (D-A) isotherm model was developed for single-stage [37] and later generalized for n-stage adsorption chillers [36]. A unique feature of the theoretical equation for minimum desorption temperature developed by Saha et al. [36,37] is that it is expressed in terms of adsorption and evaporating temperatures only and thus is device and sorption pair independent. These results were validated with few adsorption pairs like silica gel/water and activated carbon/ethanol pairs. However, the validity of this theoretical framework was not rigorously investigated for other types of adsorption pairs. Based on the nature of adsorption isotherms, IUPAC [40,41] classifies adsorption pairs into six different types. It is widely accepted that the D-A model is not a universal isotherm model to fit all six types of IUPAC classifications. The key interest for undertaking this study is whether the theoretical framework can predict the minimum desorption temperature for all sorption pairs which exhibit other isotherm behaviors. First, we collated few representative adsorption uptake data for describing the six IUPAC isotherm types. All these uptake data were fitted with suitable isotherm models. For each isotherm model, the minimum desorption temperature is derived from the fundamental principle mentioned in the following section. This derived minimum desorption temperature data is compared to the numerical value predicted by the theoretical equation [37]. The investigation is carried out for single-stage adsorption chiller with evaporator temperature and sink temperature varying between 5–25 °C and 20–40 °C respectively. Rigorous error analyses between the derived and calculated results ensue to critically analyze the universal applicability of the theoretical equation.

2. Minimum desorption temperature

2.1. Fundamental principle

In a vapor adsorption refrigeration system, the adsorber bed plays the role of a compressor to thermally compress the vapor in evaporator to condenser pressure. A typical adsorption cycle for thermal compression process is shown in Fig. 1. The refrigerant



Fig. 1. Adsorption-desorption cycle of a typical adsorption refrigeration system.

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