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A thermodynamic analysis of the staged adsorption/desorption with Type-V isotherms#

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ABSTRACT

The staged adsorption/desorption employing adsorbent-adsorbate pairs with “S” shaped isotherms is a promising new concept for achieving efficient and effective mass transfer. This study carried out a thermodynamic analysis, demonstrating the superior regeneration efficiency of the ideal staged wheels compared to the traditional single-stage. Further, three engineering guidelines for the layout design of staged adsorbents along the channel were proposed. Under six classic conditions, the corresponding desiccant wheels with optimized stage configuration exhibited 10~20℃ lower necessary regeneration temperature (T_{reg}) than single-stage wheels.

Keywords: desiccant wheels, adsorption isotherms, adsorbents, staged adsorption/desorption, low-grade energy utilization

NONMENCLATURE

Abbreviations	
MC_{ss}	Average steady-state moisture cycled, kg/kg
RH	Relative humidity
RH_{st}	RH at where the isotherm step rises
Symbols	
T	Temperature, ℃
M	Equilibrium water uptake, kg/kg
G	Mass flow rate, kg/s
X	Absolute humidity, kg/kg
W	Moisture load, kg/s

1. INTRODUCTION

The prospect of desiccants with the Type-V isotherm in adsorptive dehumidification has been highlighted since they maintain high-level mass transfer potential and can be easily regenerated [1]. The relatively weak adsorbate-adsorbent interactions lead to the special S-shaped Type-V isotherm. The single-layer physical adsorption dominates before the step rise of equilibrium uptake. At the higher relative pressure, molecular clustering emerges, leading to self-accelerating pore filling [2-4].

Recent studies [5, 6] reported the concept of counter-flow type staged adsorption/desorption with Type-V isotherm adsorbents, matching the adsorbents featuring various step rise points to the divided stages of the working fluid, which achieves idealized mass transfer efficiency and energy cascade utilization of regenerative medium. The application of the staged adsorption/desorption in the water adsorption cycle is of great interest due to the ubiquity of commercially available adsorbents having Type-V isotherms to water vapour.

However, existing research focused on numerically examining the performance advantages of staged wheels. It necessitates the analysis from the thermodynamics perspective and a method for designing the combination and length distribution of different adsorbents along the channel. Based on the steady-state moisture cycled (MC_{ss}) estimation, this study demonstrated the mechanisms behind the lower necessary T_{reg} of staged wheels compared to traditional single-stage. Further, three criteria for the staged adsorbent design were established and applied to six operational conditions for verification.

2. METHODS

The MC_{ss} analysis allows the estimation of thermodynamic regeneration temperature and the net moisture cycled in the steady-state desiccant air-conditioning cycle under certain operational conditions [7]. Fig. 1 visualizes a simple air-conditioning cycle with desiccant dehumidification. The transition and steady-

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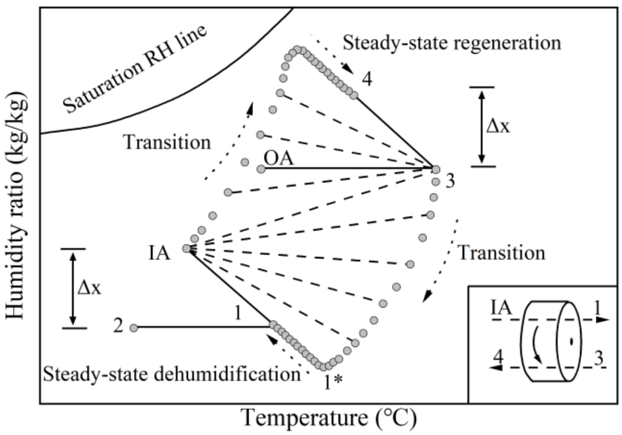

Fig. 1 A simple desiccant air conditioning cycle on psychrometric chart.

state periods of the dehumidification and regeneration processes are indicated by the scattered points representing the outlet air conditions of the wheel. The inlet air (IA) is isenthalpically dehumidified to state 1 and then cooled to state 2 as supply air. In the regeneration process, the outdoor air (OA) is heated to state 3 and humidified to state 4 by desorbing the moisture from the desiccants.

Following the assumptions made by Sultan et al. [1], for given conditions of IA, OA and the desired outlet state of dehumidified air, the MC_{ss} can then be estimated by the equilibrium adsorption at the left/right desiccant ends as Eq. 1:

$$MC_{ss} = \frac{M_{IA} + M_1}{2} - \frac{M_3 + M_4}{2} \tag{1}$$

where *M* [kg/kg] represents the water uptake equilibrium with the local air. MC_{ss} indicates the net dehumidification potential of the adsorbents to process the specific amount of air at a particular T_{reg} and is not directly responsible for the system's dynamic performance. In addition, a minimum T_{reg} for the steady-state cycle can be decided since the equilibrium adsorption uptake for desiccant in state 3 has to be less than in state 1.

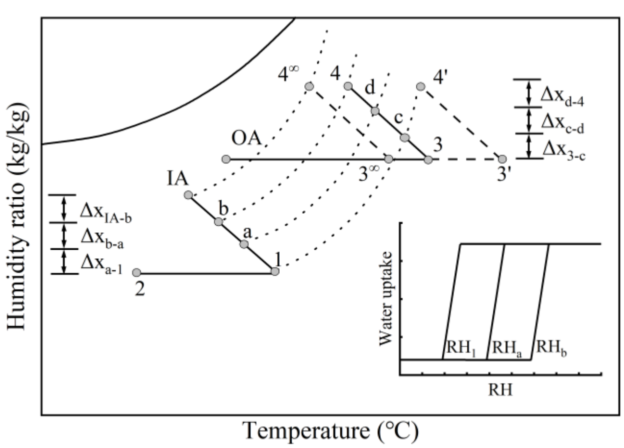

Fig. 2 The ideal staged cycle on psychrometric chart.

3. MC_{SS} ANALYSIS FOR THE STAGED WHEELS

In most applications, the maximum outlet humidity of product air is specified. The adsorbent is supposed to possess a Type V isotherm with a high saturation capacity above this humidity and a low capacity below it for efficient and effective dehumidification. Consequently, the comparison analysis between staged and single-stage wheels mainly concerned the use of desiccants with Type-V isotherm.

3.1 For the ideal staged cycle

An ideal three-staged adsorption/desorption process is plotted in Fig. 2 as an example of the staged cycle's MC_{ss} analysis, which differs slightly from that of a single stage. Additional assumptions have been made along with those from [1]:

1) The ideal Type-V isotherms are unrelated to temperature and have nearly vertical slop of step rise.

2) The moisture cycled during the adsorption and desorption process for each desiccant in its stage is equal based on mass conservation, which means:

$$\begin{aligned} \Delta x_{IA-b} &= \Delta x_{d-4} \\ \Delta x_{b-a} &= \Delta x_{c-d} \\ \Delta x_{a-1} &= \Delta x_{3-c} \end{aligned} \tag{2}$$

The subscripts IA-b, b-a, and a-1 denote the three stages in the dehumidification process, whereas 3-c, c-d, and d-4 are for the regeneration process.

3) The states of OA, IA and required supply air (state 2) remain unchanged.

4) Neglects the relation between the specific moisture capacity of dry air and temperature.

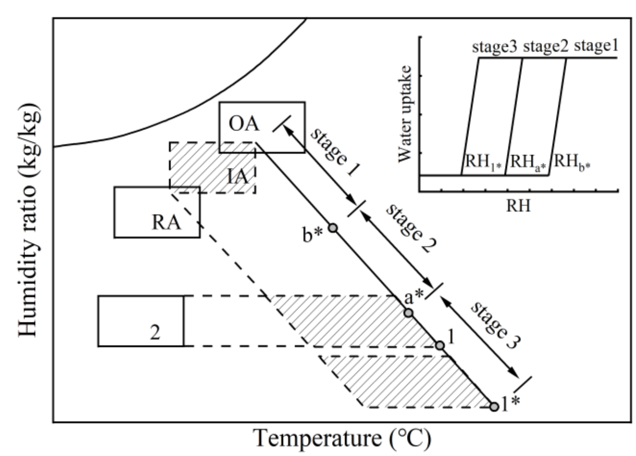

Fig. 3 A practical staged cycle.

First, the subscripts of RH and *T* in the context below represent the corresponding state points on the psychrometric chart, except for "st" which stands for the isotherm step rise's threshold. In a single-stage process, one desiccant with an isotherm having the RH_{st} no more than RH_1 at T_1 is necessary to reach state 1 during the adsorption, leading to the theoretical highest necessary T_{reg} ($T_{3'}$). Suppose the dehumidification process is divided into three stages. In that case, the air should be dehumidified from state IA to 1 by three desiccants with RH_{st} equal to RH_b, RH_a, and RH_1, respectively. The necessary T_{reg} would then decline to T_3 since the regeneration air flows reversely, and the RH of each staged point c, d, and 4 needs to be less than RH_1, RH_a, and RH_b accordingly. Benefiting from the staged adsorption/desorption, the highest moisture transfer potential remains in this ideal cycle for a wide range of process air humidity with a decreased necessary T_{reg} than the single-stage cycle. Interestingly, if there are infinite stages, point b goes to point IA, and the T_{reg} can be the theoretical minimum as $T_{3\infty}$.

3.2 For the staged cycle in engineering practice

The former subsection clarifies how staged adsorption/desorption improves energy efficiency. However, it is based on idealized assumptions. A further consideration of the engineering practice and the dynamic performance of wheels is essential.

For simplification, Fig. 3 draws a three-stage dehumidification process. The 1:1 mixed inlet air (IA) by outdoor air (OA) and return air (RA) is dehumidified in three stages to the humidity according to the required supply air state 2. In reality, the conditions of OA, RA, and 2 constantly shift, which was assumed to be within the solid line square. Three guidelines for the design of staged wheels can be suggested and explained:

1) The "Most unfavourable design conditions":

Taking into account the product air's dynamically increasing humidity during the steady-state dehumidification process, the designed product air in the "worst-case scenario" should be at the state 1 in Fig. 1. Since then, in Fig. 3, the state IA with the highest enthalpy (the most latent cooling load) and state 2 with the lowest humidity (the most difficult to be reached) give the state of point 1 for the design of staged adsorbents. In the case of the constant air volume system with varying supply air conditions, the staged cycle may not be necessary since one advantage is the dehumidified air's stable humidity [5]. In the VAV (Variable Air Volume) system where the condition of supply air is fixed within a specific range, the equations below model the mass conservation of air conditioning, showing that a minimum humidity of RA and a maximum moisture load give the lowest humidity for state 2:

$$\begin{aligned} &G_E + G_R = G_S \\ &X_E = X_R \\ &W = W_{room} + W_{OA} \\ &W = X_R G_R + X_E G_E - X_S G_S \\ &X_S = X_R - W / G_S \end{aligned} \quad (3)$$

The W [kg/s], G [kg/s], and X [kg/kg] denote the moisture load, airflow volume, and humidity of air, respectively, where the subscripts E, R, and S are the exhaust air, return air, and supply air.

2) The "Deepest dehumidification":

Fig. 3 shows the possible designed range of states IA, 1, and 1* by shaded areas: Once located point 1 in the "worst-case scenario", state 1*, representing the driest product air at the beginning of the steady-state dehumidification (equivalent to the point 1* in Fig. 1), can be pinpointed by defining the limited fluctuation range of product air's humidity. The "Deepest dehumidification" means that the water uptake equilibrious with state 1* of the appropriate desiccant in stage 3 should be at its isotherm's step rise threshold, ensuring the mass transfer potential during the whole dehumidification process.

3) The "Evenly staged process line":

The distance between the two endpoints for any staged process line is expected to be short to avoid regeneration difficulty, leading to the "Evenly staged process line". Consequently, as seen in Fig. 3, the staged points a* and b* could be located since their relative distance to point 1* settles. The rest of the desiccants should be selected according to points a* and b* in the same way as stage 3. An example gives a better understanding: After deciding the desiccant for stage 3 by a presumed point 1*, the difference between this desiccant's RH_{st} and the RH of process air widens from point 1* to point a*. This gap should not be too large on the way away from 1*, as the desiccant set for stage 3 becomes increasingly replaceable by another hydrophobic one with a higher RH_{st}. The explanation above illustrates the significance of the staged cycle idea from a new perspective and makes the "Evenly staged process line" reasonable. To be clear, the width of the process line does not represent the actual coating length.

In brief, the "Most unfavourable design conditions" decides the design conditions of IA and product air in engineering practice. The high moisture transfer driving force is assured by the "Deepest dehumidification" during the dehumidification process. The "Evenly staged process line" reduces the regeneration difficulty and locates the staged point for adsorbent selection.

Table. 1: Working conditions

	Cool&Humid	Hot&Humid
T_{OA} (℃)	20	30
Y_{OA} (g/kg)	12.34(85%RH)	22.89(85%RH)
Thermal comfort zone	18~25℃, 40~70%RH	
Mix ratio of OA and RA	1:0, 0:1, 1:1	

In order to verify the feasibility of the guidelines, the dynamic desiccant air-conditioning process was simplified into the steady-state cycle with fixed state points to estimate the dehumidification performance of wheels. The classic thermal comfort range was regarded, i.e., 18∼25℃ and 40∼70% RH for residential buildings. The most unfavourable conditions, 25℃/70% RH and 18℃/40% RH, were chosen as the return and supply air states, respectively. Three air supply modes (full return air, full fresh air, and mixed ratio 1:1 of fresh air to return air) were considered under two ambient environments: Cool&Humid and Hot&Humid.

The engineering criteria proposed above determined the combination of desiccants of six staged wheels under the working conditions shown in Table. 1. To emphasize the significance of isotherms, other adsorbent properties, such as density, thermal conductivity, and adsorption capacity, have been neglected and should be screened in practice. The hysteresis loop phenomenon was not considered since the design only referred to the dehumidification process line.

Table. 2 Adsorption models of studied desiccants

	Model Type	Reference
Silica gel	S-B-K	[1]
MIL-160	CMMS	[8]
MIL-125		[9]
FAM-Z01	D-A	[10]
FAM-Z05		[10]
CMS		[11]
MSC3K-162	D-A, I/V model	[12]

Table. 2 concludes the adsorption models of desiccants involved in this study. To eliminate the effect of maximum adsorption capacity, $MC_{ss}\%$ as the evaluation index was taken to compare the dehumidification potential between the staged cycle and single-stage cycle:

$$\mathrm{MC_{ss}}\% = \frac{\mathrm{MC_{ss}}}{W_{\mathrm{eq,in}}} \tag{4}$$

where $W_{eq,in}$ [kg/kg] is the equilibrium water uptake of each adsorbent at its endpoint near to the process air inlet. Staged desiccants' MC_{ss} can be calculated by:

$$\begin{aligned} \mathrm{MC_{ss1}} &= \frac{M_{\mathrm{IA}}+M_{\mathrm{b}}}{2} - \frac{M_{\mathrm{d}}+M_{4}}{2} \\ \mathrm{MC_{ss2}} &= \frac{M_{\mathrm{a}}+M_{\mathrm{b}}}{2} - \frac{M_{\mathrm{d}}+M_{\mathrm{c}}}{2} \\ \mathrm{MC_{ss3}} &= \frac{M_{\mathrm{a}}+M_{1}}{2} - \frac{M_{3}+M_{\mathrm{c}}}{2} \end{aligned} \tag{5}$$

4. RESULTS AND DISCUSSION

Fig. 4 compares the $MC_{ss}\%$ of each desiccant in staged and single-stage cycles at various T_{reg} under the six conditions. The presented $MC_{ss}\%$ values for the single stage included silica gel and the third-stage adsorbent. This is because, in contrast to the hydrophilic desiccant in the third stage, the other two cannot independently dehumidify air to state 1*. Under all the conditions, it can be observed that the potential moisture removal ability of the staged cycle exhibited significantly higher advantages than the single stage.

For the hot&humid condition in full fresh air mode, the staged desiccants must have RH_{st} not exceeding 2.14%, 8.9%, and 28.16% at 74.69℃, 59.79℃, and 44.9℃, respectively, as guided by the criteria. A two-staged cycle was designed as no perfectly matched adsorbent combinations was found in references. In such case, the superior $MC_{ss}\%$ of FAM-Z01 required a T_{reg} around 120℃. Explanation follows: As the fresh air under hot&humid condition brought the increased absolute humidity to be processed, the state of regenerative airflow would easily enter the range where FAM-Z01 has a high equilibrium adsorption capacity. Therefore, increased circulating moisture necessitates staged adsorption/desorption.

As for the $MC_{ss}\%$ reaching 70% of S-MSC3K-162 in Fig. 4-d and of S-MIL-160/S-MIL-125 in Fig. 4-f, those desiccants' slightly lower RH_{st} at the corresponding temperature than the RH of design state resulted in the enhanced adsorption with higher required T_{reg}.

The arrangement of adsorbents in the staged cycle remained the same in Fig. 4-a and Fig. 4-b, as the process line IA → 1 was unchanged with varying ambient conditions in the full return air mode. The trends of $MC_{ss}\%$ with temperature were remarkably similar under the two outdoor conditions, proving that the engineering design of staged wheels should consider the dehumidification process line only.

In the single-stage cycle, MIL-160 presented improved $MC_{ss}\%$ under sufficiently high T_{reg}. This can be understood as MIL-160, an extremely hydrophilic material, implying a relatively low humidity flow to dehydrate it. The superiority of the staged cycle was confirmed since this difficult-to-regenerate desiccant

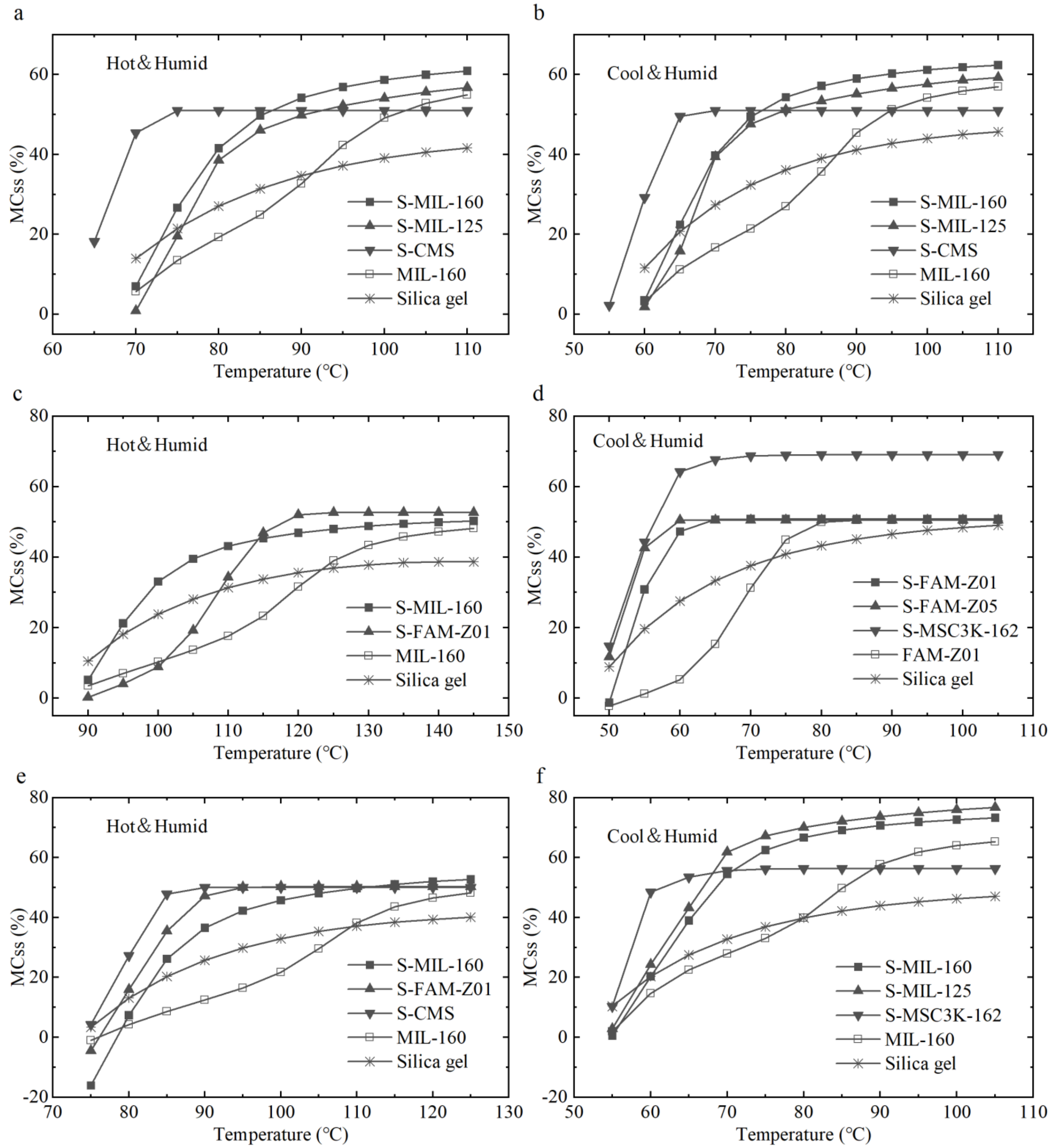

Fig. 4 The MC_{ss}*% comparison between multi-stage cycle and single-stage cycle:* a&b- *full return air mode,* c&d-*full fresh air mode,* e&f-*1:1 mixed inlet air mode. (“*S-*” represents staged cycle)*

achieved high-level MC_{ss}% with a 10～20℃ lower T_{reg} in the staged cycle.

Further, unlike the others that took MIL-160 in the third stage out of its hydrophilicity, the cycle under Cool&Humid in full fresh air mode used FAM-Z01, which is less hydrophilic than MIL-160 in terms of RH_{st}. Apparently, due to the lowest enthalpy of state IA in this condition (corresponds to 20℃/85% RH), FAM-Z01 is able to replace the MIL-160 for drying air to the state of point 1* with easier regeneration. Hereby the concept of matching the appropriate desiccants with the right stage of process airflow has been roughly realized through the proposed design method.

To summarize, the engineering criteria successfully addressed the difficulty of the screen and arrangement of multi-desiccant along the channel. The designed staged wheels had amplified dehumidification potential with reduced T_{reg} compared to the conventional single stage. Due to the ensured moisture transfer driving force at the highest temperature within the whole period, the internal cooling to compensate for the adsorption heat may not be necessary for the staged cycle, bringing interest in the recovery of adsorption heat.

5. CONCLUSIONS

This paper elaborated on the advantages of the ideal staged adsorption/desorption cycle in a counter-flow type desiccant wheel. Then, three engineering guidelines for staged wheel design were demonstrated through a comparison study. The results and discussion indicate that the staged adsorption/desorption improves the adsorption efficiency, alleviates the regeneration difficulty, and facilitates the utilization of low-grade heat sources.

The main conclusions follow:

1) Considering the varying conditions, especially those affecting the state variation of dehumidified airflow along the channel, is indispensable for the design of the staged wheels. The engineering design conditions obey the “Most unfavourable design conditions” principle.

2) The “Deepest dehumidification” and the “Evenly staged process line” should be referred to arrange the appropriate desiccants in each stage, guaranteeing the mass transfer efficiency and system performance.

3) If no adsorbent perfectly satisfies the design requirements by one of the stages, alternatives with more hydrophilicity will cause regeneration difficulty.

4) The suggested design method conforms to processing different airflow stages along the channel using appropriate desiccants. The discussed staged wheels showed more than doubled dehumidification potential under 10～20℃ reduced T_{reg} compared to the single stage.

5) The necessity of the staged cycle grows with the increasing moisture load. Interestingly, a theoretical minimum necessary T_{reg} exists for an ideal infinitely staged cycle.

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