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A CFD approach to investigate the effect of the flow field on thermal and moisture transport enhancement of a small-scale MOF dehumidifier

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SUMMARY

Solid desiccant dehumidification can achieve efficient moisture control in air-conditioning systems. A small-scale dehumidifier can quickly regulate the moisture load of a specific space, such as drug storage, cultural relics preservation, etc. Although many mathematical models have been proposed to predict the performance of desiccant-coated air-conditioning systems, only a few of them can be applied to such a small-scale device. And many existing models take advantage of the empirical correlations to calculate the heat and mass transfer coefficients, which are infeasible to new desiccants and new system design and its optimization. In this work, we used the CFD method to investigate thermal and moisture transport performance on a small-scale Metal-organic Framework (MOF) based heat sink (SDCHS). The model built up the relationship among humid air, desiccant, and heat sink and then coupled the subdomains of the fluid flow, heat transfer, and specie transport. The reliability of this model was validated by the experimental tests of SDCHS under different operation conditions. Based on the measured results of humidity ratio and temperature, the discrepancies were maintained below 15%. A parametric optimization was subsequently carried out on the flow field of SDCHS to enhance the heat and mass transfer, and various performance indexes were calculated to demonstrate the maximum utilization efficiency under the given operating condition. This dimensional analysis provides some simple guidelines to the design of SDCHS with the most suitable geometry

INTRODUCTION

Under the background of the energy crisis, energy-saving buildings have become a general trend. However, the increasing demand on the comfortable living environment has prompted the installation of the air conditioning systems, leading to the increase of the building energy consumption [1]. In this regard, an air conditioning system that features high energy efficiency and compact structures gained much more attention [2]. As a promising method, solid desiccant-based system can efficiently reduce the latent load of the indoor air, overcome the high energy consumption for the traditional systems and even have a flexible system structure [3,4].

In the past decades, people attempted to coat the heat exchangers (e.g., condenser and evaporator) with the solid desiccant, and the performance of the humidity management has been greatly improved [3,5]. As a classic working principle (dehumidification) in a solid desiccant system, solid desiccant can solely deal with the latent load of the process air, supported by a cooling source to keep the isothermal conditions. This allows the desiccant to work to its fullest potential. However, the drawbacks of the early solid desiccant system include the bulky size and low operation efficiency, which primarily rely on the selection of materials and the system structure [6]. In this case, some novel materials, i.e., metal-organic framework (MOF), have been studied due to their remarkable sorption performance and milder regeneration conditions. On the other hand, the system structure design and optimization should consider the selected materials and the local climate. All these methods considered will help to overcome the drawbacks of the early solid desiccant systems.

Herein, a small-scale MOF dehumidifier was fabricated. To better the hygrothermal transfer performance of this device, a CFD approach was used to investigate the correlation between the fluid flow and the heat and mass transfer for a MOF dehumidifier. More specifically, we hope to observe the effect of different geometric parameters on the system performance. In this case, MIL-160(Al) was coated at the surface of fins, and the parameter study was conducted to optimize the geometry of the flow channel.

METHODS

System analysis

Figure. 1 shows the schematic of the flow channel. It is clear that the flow channel consisted of many uniform unit channels. Based on the symmetry principle, it is feasible to simplify the whole flow channel, and take one unit channel as the target [7]. This work is to investigate the correlation between the flow conditions and heat and mass transfer on the humidity management capability under different geometric parameters of the unit channel. In this regard, the single unit channel considers the coupling of heat transfer, mass transport and fluid flow to do the geometric optimization of the flow channel.

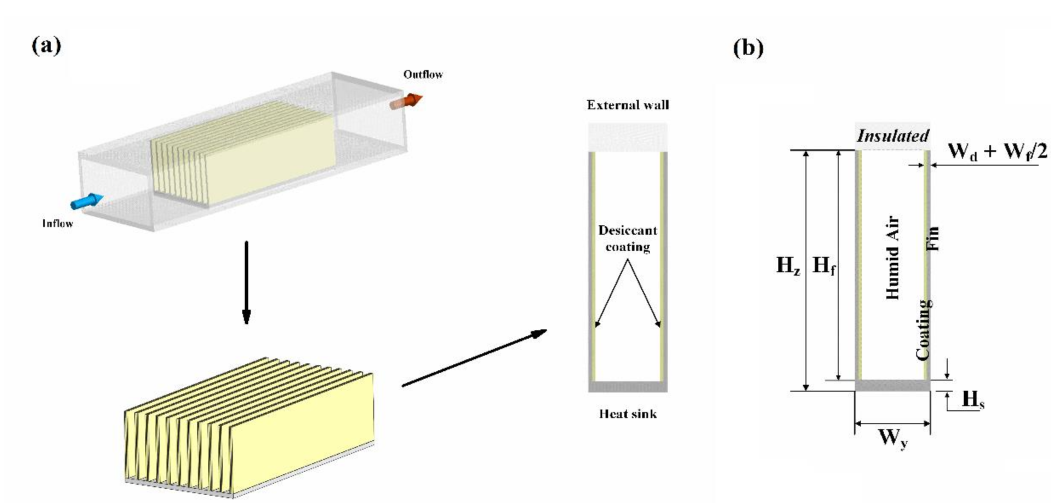

Figure 1. Schematic of the flow channel. a) Flow channel; b) Single unit channel

Mathematical model

The flow state of the air inside the channel was in laminar flow, and Figure. 1(b) shows the framework of the computational model. The single unit channel with the geometric size of L_x*W_y*H_z was investigated. The MOF coating with a thickness of W_d was coated at the surface of fins (L_x*W_f*H_f). Multiphysics fields including fluid flow, heat and mass transfer were built based on a 3D model to describe the whole physical process in COMSOL v.5.4 software. The governing equations can be described as:

Desiccant domain:

$$\frac{\partial c_d}{\partial t} = -\nabla \cdot \vec{\boldsymbol{J}} \tag{1}$$

$$(\rho C_p)_d \frac{\partial T_d}{\partial t} = -\nabla \cdot \overrightarrow{\boldsymbol{q_d}} \tag{2}$$

Air domain:

$$\nabla \cdot (\rho \overrightarrow{\boldsymbol{u_a}}) = 0 \tag{3}$$

$$\rho_a \frac{\partial \overrightarrow{\boldsymbol{u_a}}}{\partial t} + \rho_a (\overrightarrow{\boldsymbol{u_a}} \cdot \nabla) \overrightarrow{\boldsymbol{u_a}} = \nabla \cdot (-p\vec{\boldsymbol{I}} + \overrightarrow{\boldsymbol{K}}) \tag{4}$$

$$\frac{\partial c_v}{\partial t} + \overrightarrow{\boldsymbol{u_a}} \cdot \nabla c_v = -\nabla \cdot \vec{\boldsymbol{g}} \tag{5}$$

$$(\rho c_p)_a \left(\frac{\partial T_a}{\partial t} + \overrightarrow{\boldsymbol{u_a}} \cdot \nabla T_a \right) = -\nabla \cdot \overrightarrow{\boldsymbol{q_a}} \tag{6}$$

Heat sink domain:

$$(\rho C_p)_{Al} \frac{\partial T_{Al}}{\partial t} = -\nabla \cdot \overrightarrow{\boldsymbol{q_{Al}}} \tag{7}$$

Noted that the adsorption heat during the adsorption process of coatings was regarded as the boundary conditions, not in the above equations. And the mass flux at the interface between the desiccant and the air adopted the same approach. Vivekh et al. [8, 9] have proved this method.

RESULTS

Table 1 provided the inlet air conditions for the tests, and it was used to help measure the dehumidification capacity under the middle level humidity level. Table 2 showed different operation parameters including mass flowrate, equivalent heat flux at the bottom of the heat sink and cycle time. There are four different test cases. All the test cases were used to validate our developed multi-physic model. Figure 2 described the basic operation principles of the flow channel, which is controlled by the heat flux at the bottom side of the heat sink. There are cooling mode to provide the isothermal dehumidification condition and heating mode to regenerate the coating layer. In other words, one complete cycle consisted half cycle of dehumidification process and half cycle of regeneration process.

According to the test conditions, Figure 3 showed the overall discrepancy between the measured and simulated results for all the cases. It is clear that the discrepancy was maintained around 15% for both the temperature and humidity ratio of the outlet air.

Table 1 Operation conditions.

Parameters	Values
Inlet air temperature	21°C
Inlet air relative humidity	65%

Table 2. Operating parameters of different experimental cases.

	Mass flow rate (kg/h)	Equivalent heat flux (W/cm^2)	Cycle time (min)
Case 1	8.17	-0.6(AD)/2.4(De)	5
Case 2	16.35	-0.3(AD)/2.7(De)	5
Case 3	8.17	-0.15(AD)/2.4(De)	10
Case 4	8.17	-0.34(AD)/1.3(De)	5

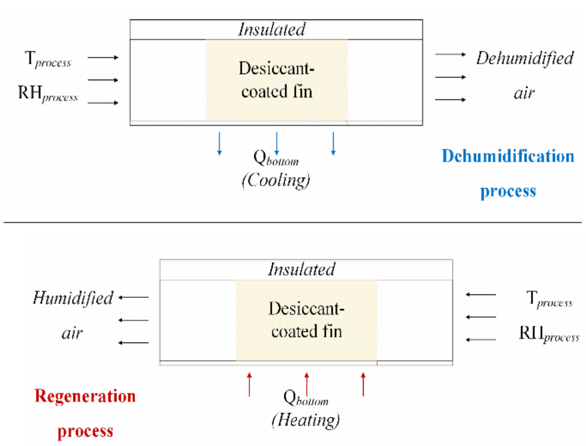

Figure 2. Operation principles of the flow channel.

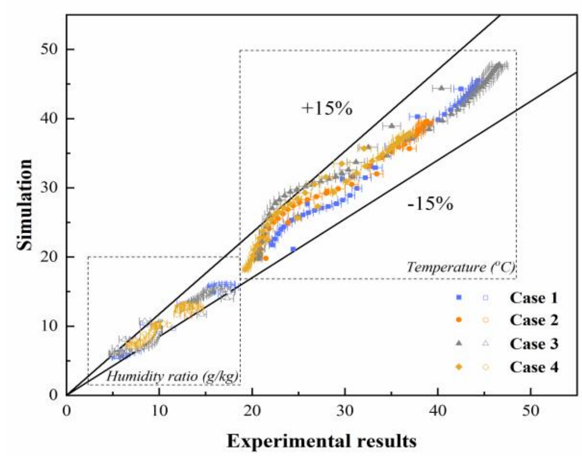

Figure 3. The overall discrepancy between the measured and simulated results.

DISCUSSION

To better analyse the operation performance under different geometry of the single unit channel, we defined two indexes:

Dehumidification rate (D_r): It represents the moisture removal over a period of time.

$$\overline{D_r} = \frac{\int_{t_s}^{t_e} \dot{m}_a(d_{in} - d_{out})\, dt}{(t_e - t_s) * NUM} \quad (34)$$

*Dehumidification coefficient of performance (DCOP):*It is the ratio of air enthalpy change to the consumed energy during the regeneration process.

$$\Omega_m = \int_{t_s}^{t_e} \dot{m}_a(h_{in} - h_{out})\, dt \quad (31)$$

$$\mathrm{DCOP} = \frac{\Omega_m}{\int_{t_s}^{t_e} Q_{bottom} A\, dt} \quad (32)$$

Where $\dot{m}_a$ is the mass flowrate [kg/s]; d the humidity ratio [kg/kg]; t_e and t_s the start and end time of the dehumidification process [s]; NUM the number of fins; h the enthalpy of the air [J/kg]; Q_{bottom} the equivalent heat flux [W/m^2].

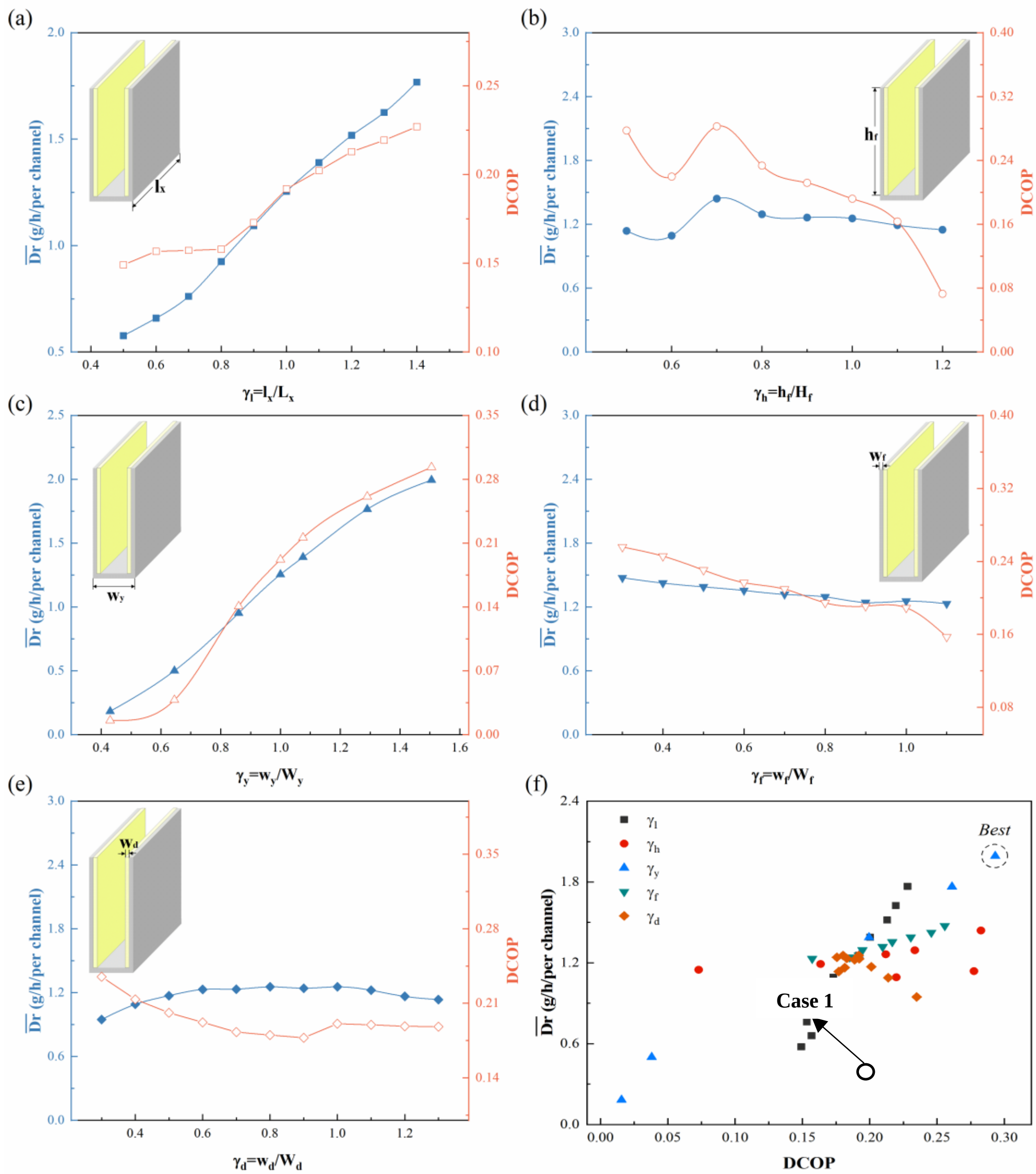

Figure 4. Effect of the geometry of the single unit channel on $\overline{D_r}$ and DCOP.

Figure 4 indicated that the change of the geometry for the single unit channel has quite different effect on the operation performance ($\overline{D_r}$ and DCOP). From Figure 4(a) and (c), the increase of the length and width of the unit channel will have more prominent effect on $\overline{D_r}$ and DCOP. Taking Case 1 as the reference, it can be found that the $\overline{D_r}$ and DCOP of the optimized case can have 1.59

and 1.51 times larger than the reference group. In this regard, the optimization of the geometry has significant effect on the operation performance, that includes the improved dehumidification capacity and energy-saving potential.

CONCLUSIONS

Solid desiccant system can efficiently overcome the drawbacks of traditional air conditioning systems, i.e., high energy consumption, but is highly relied on the selection of the desiccants and the system structure. In this paper, a MOF-coated dehumidifier has been fabricated, and the geometry of the flow channel has been optimized. The measured results have proved the high fidelity of our developed 3D model. From the following parameter study, the operation performance can be greatly improved by optimizing the geometry of the unit channel. The future work will focus on developing a model for the prediction of the full-scale device, and investigating the advanced control strategy.

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