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Optimal Placement of Heat Exchangers in a Carbon Capture-Based Ventilation System

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Abstract. Achieving acceptable air quality levels in indoor spaces by regulating the concentrations of H_2O and CO_2 is important for occupant health. Conventional techniques rely on supplying dehumidified outdoor air to dilute these species to within their healthy ranges. Typically, the outdoor air dehumidification is conducted using vapor compression cooling either as standalone systems or integrated with desiccant dehumidifiers. These methods are known to be energy intensive, especially in hot and humid climates. Ventilation systems using indoor air with adsorption-based CO_2 capture are thus proposed. These systems use adsorbent packed beds to dehumidify and decarbonize the indoor air before it is sensibly cooled and supplied to the space. For energy efficient operation of these systems, heat recovery units are necessary. In this work, heat and mass balance models were developed and used to determine the optimal placement location of the heat recovery units. It was found that a heat exchanger preceding the decarbonization bed increased the MOFs capacity, resulting in 33 % lower mass requirements. This was accompanied by a reduction in the thermal and electrical energy consumption by 43.5 % and 25 %, respectively, with respect to the configuration where the heat exchanger was placed after both air treatment systems.

Key words. Carbon capture, adsorption-based ventilation, heat recovery.

1. Introduction

Providing occupant in indoor spaces with acceptable air quality is of crucial importance to protect their physical and cognitive heath especially since they tend to spend more than 90 % of their time in enclosed spaces [1]. Such breathable indoor quality (IAQ) is ensured by maintaining the indoor generated species such as H_2O, CO_2 and VOCs to below their healthy thresholds [2]. Among these species, a special attention must be given to the levels of indoor humidity and CO_2 levels due to their high generation rates from the occupants compared to the other species. Moreover, these species have direct impact on the occupants health [3, 4]. Conventionally, ventilation systems are used to pump dehumidified outdoor to dilute these species, where the outdoor air is dried using vapor compression cooling. However, this technique is energy intensive, especially in hot and humid climates [5]. For this reason, thermally driven dehumidification system are proposed as an energy-efficient alternative since they rely on low grade thermal energy such as solar energy instead of electrical energy [6]. Such systems suffer from large footprint due to the need to treat large amounts of outdoor air [7].

Recent efforts are directed to reduce the reliance on outdoor air and increase the fractions of recirculated indoor air. This is especially beneficial since the indoor air is characterized by lower temperature and humidity levels than that of the outdoor air. This reduces the sensible and latent cooling needs imposed on the ventilation system [8]. Nonetheless, this comes at the expense of jeopardizing the air quality by increasing the indoor CO_2 levels beyond the recommended threshold of 1000 ppm set by ASHRAE [9]. Accordingly, indoor air treatment for carbon removal by adsorption has been suggested as a novel ventilation strategy [10]. However, most adsorbents suffer from reduced and even abolished capacity for CO_2 in presence of H_2O, especially at the dilute levels [11]. Accordingly, the indoor air requires dehumidification prior to the carbon removal, which can be achieved using the thermally driven desiccant dehumidifiers. Such system has been proposed by many researchers [12, 13]. Nonetheless, no one considered the effect of the pre-dehumidification on the carbon capture performance. This is especially critical since the dehumidified air is characterized by an elevated temperature that could hinder or reduce the CO_2 adsorbent temperature. However, heat recovery units can be used to benefit from the energy of the discharged cool air to enhance the system performance.

Therefore, the objective of this work is to evaluate the placement of the heat recovery unit to determine the optimal location that minimized the system size and energy consumption. For this reason, mathematical models for the heat and mass transfers are developed and applied for a case study of a typical high occupancy classroom located in the hot and humid climate of Doha, Qatar.

2. System description

The proposed system is implemented in a classroom space located in a hot and humid climate. The proposed system is operated to meet the students thermal comfort conditions by maintaining a temperature of 24 °C and a relative humidity ranging between 40 % and 60 % [14]. To provide the student with acceptable IAQ, the system should maintain CO_2 levels below 1000 ppm, O_2 concentration above 19.5 % and formaldehyde level below 8 ppb [10, 15-17]. Formaldehyde is chosen as the representative species of the VOCs family since it is commonly found in occupied spaces [17]. The proposed system consists of two packed beds in series that handle the dehumidification and decarbonization of the indoor air, an air-to-air heat exchanger that acts as a heat recovery unit from the discharged indoor air and a cooling coil of a vapor compression cooling systems to provide the space with the necessary supply temperature. Two configurations of this system are proposed in this work where the placement of the heat recovery unit is varied with respect to the decarbonization bed as shown in Fig. 1.

In the first configuration (Fig. 1(a)), the heat exchanger is placed before the decarbonization bed. The indoor air at state (2) is extracted from the classroom at a flowrate $\dot{m}_{sa}$ and divided into airstreams. One airstream at flowrate $\dot{m}_{ta}$ is first dehumidified to state (3) before it is cooled in the heat recovery unit to state (4). The air is then decarbonized to state (5) before it is mixed with the recirculated indoor air $\dot{m}_{ra}$ and outdoor air at flowrate $\dot{m}_{oa}$ and state (1). The resulting air at state (6) is sensibly cooled to state (7) before it is resupplied back to the space. The corresponding states of the ventilation air are shown on the psychrometric chart (Fig. 1(a)).

In the second configuration (Fig. 1(b)), the heat recovery unit is placed after the decarbonization bed. In this case, the indoor air at state (2) is dehumidified to state (3), decarbonized to state (4) before it is sensibly cooled in the heat recovery unit to state (5). The remainder of the process is as in the previous configuration.

3. Methodology

Mathematical models are developed for the heat and mass transfers in the packed adsorption beds as well as inside the classroom space. These models are used to size and operate the packed beds for the two different configurations of the proposed system to determine the optimal placement of the heat exchanger with respect to the decarbonization bed.

A. Packed bed model

The adsorbent for both H_2O and CO_2 are loosely packed in fixed beds to selectively capture the targeted species. In addition, heat is also exchanged between the adsorbent and the air due to the exo- and endothermic nature of the adsorption/desorption processes [18]. Accordingly, coupled heat and mass transfers are needed to accurately model the packed bed operation and accurately determine the outlet air conditions [19]. For this reason, a transient one-dimensional model is adopted with axially dispersed flow and constant velocity along the airflow direction [20]. Moreover, the adsorption rate (mass exchange) between the adsorbent and air is modelled using the linear driving force assumption, where the mass exchange is proportional to the difference between the equilibrium uptake $\bar{q}_i^*$ (kg/kg) and the actual uptake $\bar{q}_i$ (kg/kg).

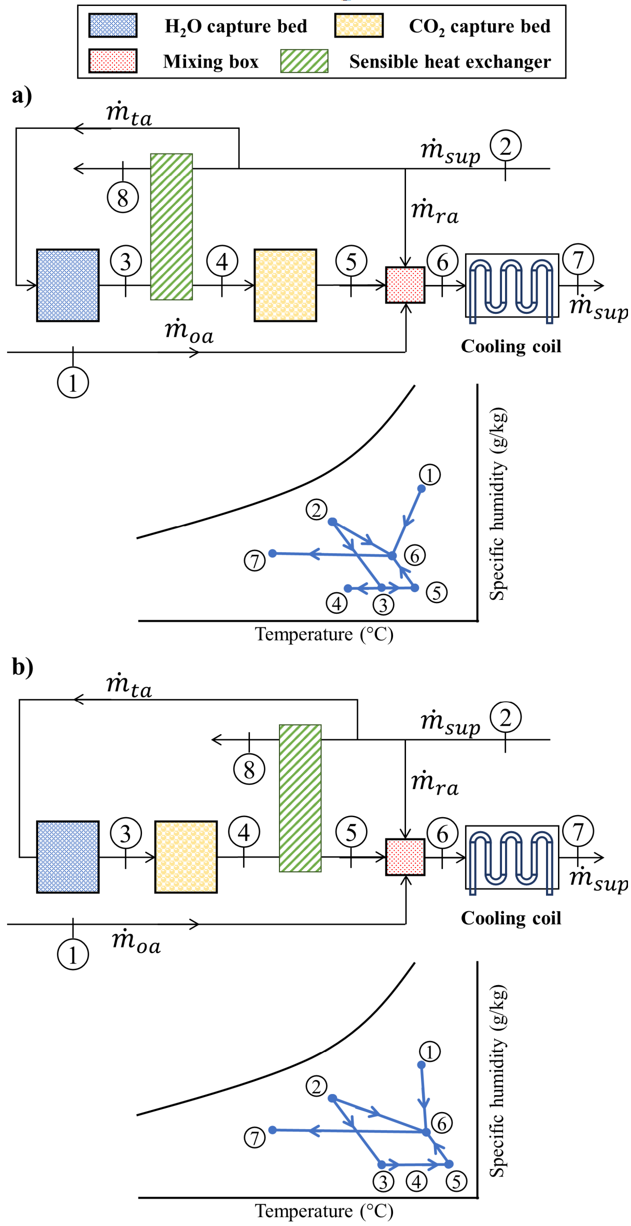

Fig. 1. Schematic of the proposed system with the two considered placement of the heat recovery unit a) before and b) after the decarbonization bed.

The equilibrium uptake is calculated at the adsorbent temperature and the species concentration in the air using the isotherm model of the adsorbent. The species mass balance on the air side is thus given by

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial z} - D_{zi}\frac{\partial^2 C_i}{\partial z^2} + \left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)\rho_s k_i(\bar{q}_i^* - \bar{q}_i) = 0 \quad (1)$$

where C_i (kg/m^3) is the concentration of species "i" (H_2O or CO_2) in the air, u (m/s) is the flow velocity, ρ_s (kg/m^3) and ρ_a (kg/m^3) are the adsorbent and air density, respectively. ε_t (-) is the bed porosity, and D_{zi} (m^2/s) is the axial diffusion coefficient. k_i (s^{-1}) is the linear driving force assumption time constant. The detailed model is presented by Harrouz et al. [21] and not reported here for conciseness.

B. Space model

To determine the air conditions of temperature and species concentrations in terms of the supplied air conditions, heat and mass balances were developed for the inside of the classroom space. The model of Yassine et al is [22] adopted, where the balances are carried out for a control volume consisting of the whole classroom air, which is assumed to be well mixed (homogeneous). The lumped transient heat and mass balances are thus given by

$$\rho_a V_{CR} C_{p,a} \frac{dT_{CR}}{dt} = \dot{m}_{sup} C_{p,a}\left(T_{sup} - T_{CR}\right) + Q_e + Q_i \quad (2)$$

$$\rho_a V_{CR} \frac{d y_{CR,i}}{dt} = \dot{m}_{sup}\left(y_{i,sup} - y_{CR,i}\right) \pm \dot{Y}_i \quad (3)$$

where ρ_a (kg/m^3) and $C_{p,a}$ (J/kg·K) are the air density and specific heat capacity of the indoor classroom space of volume V_{CR} (m^3), temperature T_{CR} (K), and species concentration $y_{CR,i}$. $\dot{m}_{sup}$ (kg/s), T_{supp} (K) and $y_{i,sup}$ are the supply air flowrate, temperature and species concentration, respectively. Q_e (W) and Q_i (W) are the heat gains into the space from the envelope and internal sources, respectively, and $\dot{Y}_i$ is the species generation rate.

C. Numerical solution

The different models of heat and mass balances are solved using the finite volume approach with implicit scheme for the time derivative (transient term) and the first order upwind scheme for the first order spatial derivative (convection term) while the second order spatial derivative (diffusion term) was solved using the central difference scheme. A time step independence test yielded a time step of 10^{-3} s that is adopted to ensure accurate results with acceptable computational time. The convergence reached when the difference in the calculated parameters between two consecutive iterations is smaller than 10^{-8}.

4. Case study

The developed models are applied for a case study of a typical high occupancy classroom of dimensions (5 m × 10 m × 3.5 m) with 33 students, located in Doha on the coastal region of Qatar facing the Persian Gulf. The prevailing climate conditions in this region is characterized by extreme hot and humid conditions, where peak outdoor air conditions of dry bulb and dew point temperatures reach 44.3 °C and 30.2 °C, respectively [23]. The space envelop is selected to abide by the Qatar Construction Standard 2014 and the detailed properties are presented by Harrouz et al. [24]. The students are assumed to be conducting a sedentary activity at rest with a metabolic rate of 1.2 met resulting each in a CO_2 emissions rate of 10.8 mg/s, a H_2O emission rate of 11.57 mg/s and a consumption rate of O_2 of 9.92 mg/s [25]. In addition, the classroom is characterized by an emission rate of formaldehyde of 10.2 mg/h. the sizing of the different beds depends on the amount of the water vapor and CO_2 to be removed from the treated indoor air flowrate $\dot{m}_{ta}$. This mass depends on the cycle time, inlet air conditions of temperature and species concentration and regeneration temperature and flowrate. A fixed cycle time operation mode is chosen due to its simple control, and for the current work, a cycle time of 1800 s is adopted with 70:30 ratio of adsorption to regeneration duration [26]. The inlet conditions consist of the indoor air conditions as presented in section 2. However, the outlet air conditions are determined to ensure that the supplied treated air can offset the species generation. Moreover, the outlet humidity from the dehumidification should ensure that the indoor air is dry enough to eliminate the competitive selectivity of H_2O over CO_2. Such dryness level depends on the selected adsorbent for carbon capture. For the CO_2 outlet concentration, a 20-ppm level was adopted for practical reasons as adopted by Cheng et al. [27]. Finally, to determine the packed bed diameter, an airflow velocity between 1 – 3 m/s is considered [28, 29].

For the proper operation of the proposed system, the adsorbing material should be adequately chosen. For indoor air dehumidification, the conventional silica gel is selected due to its commercial availability at low prices, moderate regeneration temperature (<80 °C). Silica gel is also characterized by a moderate H_2O capacity reaching a maximum of 0.3 kg/kg at 25 °C temperature [30]. For the carbon capture, the selected adsorbent should present high capacity at dilute levels of CO_2, moderate selectivity of H_2O over CO_2, low regeneration temperature, hygrothermal and cycling stability. For this reason, MOF-74-Mg is selected since it exhibits a CO_2 capacity of 6.3 g/kg at outdoor CO_2 levels [11] and a regeneration temperature of 60 °C [31]. Moreover, for the selected adsorbent MOF-74-Mg, an inlet humidity must not exceed 4 g/kg [32].

5. Results and discussion

The developed mathematical models were validated for the adsorption of both water vapor on silica gel and CO_2 on MOF-74-Mg with published data in literature. It was found that the maximum discrepancy on the calculated outlet air temperature and species concentration from the packed bed model were less than 9.5 % [24].

Using the classroom space model, it was found that the supply, treated and outdoor air flowrates needed at the peak humidity conditions were found to be 1.02 kg/s, 0.26 kg/s, and 0.078, respectively [24]. These flowrates were required to offset the different species generation/consumption rates and ensure acceptable IAQ in the classroom and meet the required indoor air temperature that provided thermal comfort for the students.

The validated packed bed model was then used to properly size the packed beds for dehumidification and decarbonization following the approach presented in the previous section for both system configurations. Since the heat exchanger location was varies with respect to the decarbonization bed only, the size of the dehumidification bed remained the same. It was found that 15 kg of silica gel were needed in each bed to handle the peak latent load of the indoor air that ensure an airstream that is dry enough before entering the CO_2

capture bed. On the other hand, the size of decarbonization bed was drastically changed as can be seen in Table 1. For the first configuration, the heat exchanger was placed before the carbon capture bed. This resulted in pre-cooling of the dehumidified air that reduced the temperature of the MOFs and increased its CO_2 capacity to 10 g/kg at 34 °C. This resulted in peak thermal and electrical energy consumption of 0.39 kWh and 0.88 kWh, respectively. For the second configuration, the decarbonization bed was sized while considering the temperature of the dehumidified air leaving the dehumidification bed. For the current case study, it was found that the dried air reached a temperature of 39 °C at the outlet of the bed. At this temperature, the MOFs capacity for CO_2 was reduced to 7.5 g/kg. This caused the increase of the needed adsorbent mass to 38.6 kg for each bed, which was equivalent to a rise of 33 % in the system size with respect to the first configuration. Consequently, the thermal energy for the adsorbent regeneration and the electrical energy required for the fan operation increased to 0.56 kWh and 1.1 kWh, respectively. This configuration resulted thus in 43.5 % and 25 % lower thermal and electrical energy consumption compared to the previous configuration. Therefore, the placement of the heat exchanger before the decarbonization bed was the optimal solution for energy efficient operation of the proposed system.

Table 1. The obtained packed bed dimensions for the considered system configurations.

Heat exchanger placement	*Before decarbonization bed*	*After decarbonization bed*
Dehumidification bed		
Silica gel mass (kg)	14.6	
Bed height (m)	0.20	
Bed diameter (m)	0.35	
Carbon capture bed		
MOF-74-Mg mass (kg)	29.0	38.6
Bed height (m)	0.30	0.40
Bed diameter (m)	0.60	0.60

6. Conclusion

This research work investigated the placement of heat recovery units in an adsorption-based carbon capture ventilation system. Depending on their locations, these units affect both the adsorption packed beds, their energy consumption as well as the energy consumption of the vapor compression cooling system. Mathematical models for the heat and mass balances in the adsorption beds were developed to determine the optimal configuration that minimized the investment and operating costs of the novel ventilation system. The models were applied for a case study of a high occupancy classroom located in the hot and humid climate of Qatar. For the peak outdoor air conditions of humidity, the configuration with the heat recovery preceding the decarbonization bed showed a reduction of 33 % in the carbon capture bed size along with 43.5 % and 25 % lower thermal and electrical energy consumption.

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References

[1] N. E. Klepeis *et al.*, "The National Human Activity Pattern Survey (NHAPS): a resource for assessing exposure to environmental pollutants," *Journal of Exposure Science & Environmental Epidemiology,* vol. 11, no. 3, pp. 231-252, 2001.

[2] R. Pitarma, G. Marques, and B. R. Ferreira, "Monitoring indoor air quality for enhanced occupational health," *Journal of medical systems*, vol. 41, no. 2, p. 23, 2017.

[3] U. Satish *et al.*, "Is CO2 an Indoor Pollutant? Direct Effects of Low-to-Moderate CO2 Concentrations on Human Decision-Making Performance," *Environmental Health Perspectives,* vol. 120, no. 12, pp. 1671-1677, 2012/12/01 2012, doi: 10.1289/ehp.1104789.

[4] A. V. Arundel, E. M. Sterling, J. H. Biggin, and T. D. Sterling, "Indirect health effects of relative humidity in indoor environments," *Environmental health perspectives,* vol. 65, pp. 351-361, 1986.

[5] L. Pérez-Lombard, J. Ortiz, and C. Pout, "A review on buildings energy consumption information," *Energy and Buildings,* vol. 40, no. 3, pp. 394-398, 2008/01/01/ 2008, doi: https://doi.org/10.1016/j.enbuild.2007.03.007.

[6] J. Pillai and R. Desai, "Dehumidification Strategies and Their Applicability (C105)(P)," in *2018 Building Performance Analysis Conference and SimBuild*, 2018: ASHRAE.

[7] J. Taweekun and V. Akvanich, "The experiment and simulation of solid desiccant dehumidification for air-conditioning system in a tropical humid climate," 2013.

[8] S. A. Batterman and H. Burge, "HVAC systems as emission sources affecting indoor air quality: a critical review," *HVAC&R Research,* vol. 1, no. 1, pp. 61-78, 1995.

[9] *ANSI/ASHRAE Standard 62.1-2010. Ventilation for acceptable indoor air quality*, ASHRAE, 2010.

[10] M. K. Kim, L. Baldini, H. Leibundgut, J. A. Wurzbacher, and N. Piatkowski, "A novel ventilation strategy with CO2 capture device and energy saving in buildings," *Energy and Buildings,* vol. 87, pp. 134-141, 2015/01/01/ 2015, doi: https://doi.org/10.1016/j.enbuild.2014.11.017.

[11] A. Kumar *et al.*, "Direct air capture of CO2 by physisorbent materials," *Angewandte Chemie*

International Edition, vol. 54, no. 48, pp. 14372-14377, 2015.
[12] A. Sinha, H. Thakkar, F. Rezaei, Y. Kawajiri, and M. J. Realff, "Direct Air Capture of CO2 in Enclosed Environments: Design under Uncertainty and Techno-Economic Analysis," in *Computer Aided Chemical Engineering*, vol. 44, M. R. Eden, M. G. Ierapetritou, and G. P. Towler Eds.: Elsevier, 2018, pp. 2179-2184.
[13] A. Sinha, H. Thakkar, F. Rezaei, Y. Kawajiri, and M. J. Realff, "Reduced building energy consumption by combined indoor CO2 and H2O composition control," *Applied Energy*, vol. 322, p. 119526, 2022.
[14] *ANSI/ASHRAE Standard 55-2017: Thermal Environmental Conditions for Human Occupancy*, ASHRAE, 2017.
[15] N. R. Council, "Formaldehyde-an assessment of its health effects," 1980.
[16] L. Zhang, *Formaldehyde: exposure, toxicity and health effects*. Royal Society of Chemistry, 2018.
[17] T. Salthammer, S. Mentese, and R. Marutzky, "Formaldehyde in the indoor environment," *Chemical reviews*, vol. 110, no. 4, pp. 2536-2572, 2010.
[18] T. L. Dantas *et al.*, "Adsorption of carbon dioxide onto activated carbon and nitrogen-enriched activated carbon: surface changes, equilibrium, and modeling of fixed-bed adsorption," *Separation Science and Technology*, vol. 45, no. 1, pp. 73-84, 2009.
[19] S. Murathatunyaluk, K. Srichanvichit, A. Anantpinijwatna, and P. Kitchaiya, "Modeling of Non-Isothermal Adsorption Process in a Silica Gel Desiccant Packed Bed," in *Computer Aided Chemical Engineering*, vol. 43: Elsevier, 2018, pp. 49-54.
[20] K. S. Hwang and W. K. Lee, "The adsorption and desorption breakthrough behavior of carbon monoxide and carbon dioxide on activated carbon. Effect of total pressure and pressure-dependent mass transfer coefficients," *Separation science and technology*, vol. 29, no. 14, pp. 1857-1891, 1994.
[21] J. P. Harrouz, E. Katramiz, K. Ghali, D. Ouahrani, and N. Ghaddar, "Comparative analysis of sustainable desiccant–Evaporative based ventilation systems for a typical Qatari poultry house," *Energy Conversion and Management*, vol. 245, p. 114556, 2021.
[22] B. Yassine, K. Ghali, N. Ghaddar, I. Srour, and G. Chehab, "A numerical modeling approach to evaluate energy-efficient mechanical ventilation strategies," *Energy and Buildings*, vol. 55, pp. 618-630, 2012/12/01/ 2012, doi: https://doi.org/10.1016/j.enbuild.2012.08.042.
[23] B. R. Hughes, H. N. Chaudhry, and S. A. Ghani, "A review of sustainable cooling technologies in buildings," *Renewable and Sustainable Energy Reviews*, vol. 15, no. 6, pp. 3112-3120, 2011.
[24] J. P. Harrouz, K. Ghali, M. Hmadeh, N. Ghaddar, and S. Ghani, "Feasibility of MOF-based carbon capture from indoor spaces as air revitalization system," *Energy and Buildings*, vol. 255, p. 111666, 2022.
[25] M. Mossolly, K. Ghali, and N. Ghaddar, "Optimal control strategy for a multi-zone air conditioning system using a genetic algorithm," *Energy*, vol. 34, no. 1, pp. 58-66, 2009.
[26] L. Chai *et al.*, "Ventilation rates in large commercial layer hen houses with two-year continuous monitoring," *British Poultry Science*, vol. 53, no. 1, pp. 19-31, 2012.
[27] H.-H. Cheng and C.-S. Tan, "Removal of CO2 from indoor air by alkanolamine in a rotating packed bed," *Separation and purification technology*, vol. 82, pp. 156-166, 2011.
[28] A. A. Pesaran and A. F. Mills, "Moisture transport in silica gel packed beds—I. Theoretical study," *International Journal of Heat and Mass Transfer*, vol. 30, no. 6, pp. 1037-1049, 1987.
[29] J.-Y. San and G.-D. Jiang, "Modeling and testing of a silica gel packed-bed system," *International journal of heat and mass transfer*, vol. 37, no. 8, pp. 1173-1179, 1994.
[30] X. Wang, W. Zimmermann, K. Ng, A. Chakraboty, and J. Keller, "Investigation on the isotherm of silica gel+ water systems," *Journal of thermal analysis and calorimetry*, vol. 76, no. 2, pp. 659-669, 2004.
[31] J. Wang *et al.*, "Direct capture of low-concentration CO2 on mesoporous carbon-supported solid amine adsorbents at ambient temperature," *Industrial & Engineering Chemistry Research*, vol. 54, no. 19, pp. 5319-5327, 2015.
[32] S. Mukherjee *et al.*, "Trace CO2 capture by an ultramicroporous physisorbent with low water affinity," *Science Advances*, vol. 5, no. 11, p. eaax9171, 2019.