

Investigating Combined Effect of Air Temperature, Humidity, and Velocity on the Thermal Comfort of Poultry Birds

Shahzad, Khawar

Department of Agricultural Engineering, Bahauddin Zakariya University

Sultan, Muhammad

Department of Agricultural Engineering, Bahauddin Zakariya University

<https://doi.org/10.5109/4739234>

出版情報 : Proceedings of International Exchange and Innovation Conference on Engineering & Sciences (IEICES). 7, pp.279-289, 2021-10-21. Interdisciplinary Graduate School of Engineering Sciences, Kyushu University

バージョン :

権利関係 :



Investigating Combined Effect of Air Temperature, Humidity, and Velocity on the Thermal Comfort of Poultry Birds

Khawar Shahzad ¹, Muhammad Sultan ^{1*}

¹Department of Agricultural Engineering, Bahauddin Zakariya University, Multan 60800, Pakistan

*Corresponding author email: muhammadsultan@bzu.edu.pk

Abstract: The study presents the combined effects of temperature, humidity, and velocity upon the thermal comfort of poultry birds. The months of April, May, June, and July pose challenges for the well-being of these vulnerable birds. The average daily variations as depicted by the figures show how the temperature synchronizes with the corresponding humidity value at a certain period in the day. The minimal rise in the relative humidity against the subsequent fall in dry bulb temperature wreaks havoc on the poultry birds. Apart from energy-efficient evaporative cooling techniques, the present study depicts the importance of the velocity factor to mitigate heat stress. Temperature-Humidity-Velocity index (THVI) is introduced synergistically to check and balance the thermal comfort of poultry birds. According to the results, the THVI index indicates the efficiency of optimal velocity limits to dissipate moisture heat production in the poultry sheds. The results indicate that the rise in velocity value synergistically increases the thermal exposure time (ET) against the THVI value. The increase in velocity elongates the normal zone for the one-degree rise in temperature.

Keywords: Temperature-Humidity index, Temperature-Humidity-Velocity index, thermal Comfort of poultry birds, thermal exposure time

1. INTRODUCTION

The agriculture and livestock sector contributes appreciably to the economy of Pakistan in terms of production and employment [1], [2]. Among livestock species, poultry birds are considered the cheapest source of protein. The below-given figures are the display of statistics drawn from the economic survey of Pakistan. Figure 1 displays the meat production among different categories of livestock [1], [3]. The data represents that poultry meat production is on the continuous rise among goat, camel, mutton, and beef. This value is also at a peak while compared with the counterparts. Poultry has proved to be the part and parcel of mankind in their daily calorie intake.

All such development of poultry is indebted to technological advancement. The control sheds are built to provide an efficient environment for the birds to nurture. Poultry birds are highly susceptible once the relative humidity is concerned [4]–[6]. Any small amount of rising in humidity invites disasters to the poultry sector. The appropriate handling of the Temperature-Humidity index (THI) with the help of efficient evaporative air-conditioning options (DEC, IEC, MEC) has ameliorated the condition [3]. In this way, the mortality rate of poultry birds against thermal stresses has been significantly controlled [7]. Thus, meat production has trumpeted the past year's records so far. The THI value is incorporated with velocity to devise THVI for satisfying the thermal comfort zone of poultry birds [8], [9].

These birds are sensitive to thermal stresses because their physical composition lacks sweat glands [8]. Unlike humans, the poultry birds undergo the panting process to release their moisture heat whereas the sweat glands in humans release water vapors from the pores of the skin. The below figure represents the comparative analysis for temperature rise and the thermal stress in poultry birds. The thermoneutral zone is the initial portion of this bar

where the birds act normally [7]. As the temperature rise, the slow panting (release of moisture production) process exaggerates to the peak of thermal stress. Once this limit is crossed, the poultry birds start perishing [10].

This thermal regulation of body temperature by these birds happens to be a strenuous effort. For this purpose, various air-conditioning options have been devised by the researchers. Direct Evaporative Cooling (DEC) is the running practice of poultry control sheds where the water vapors are directly added into the stream of dry air [11]–[13]. Indirect Evaporative Cooling (IEC) is the technique by which a dry air stream is passively cooled from the wet channel aligned together [14]. Maisotsenko-based Evaporative Cooling (MEC) is an advanced technique by which dry air stream is cooled actively and passively intermittently [15]–[17]. Among these three techniques, MEC is presented as the most efficient one by the researchers as it cools the air stream without raising the relative humidity above the optimal value [18]. Whereas the DEC cools the air stream rich in humidity as compared to the IEC and MEC. IEC is relatively less efficient than the MEC in terms of thermal efficiency and dew-point effectiveness [15], [19]–[21].

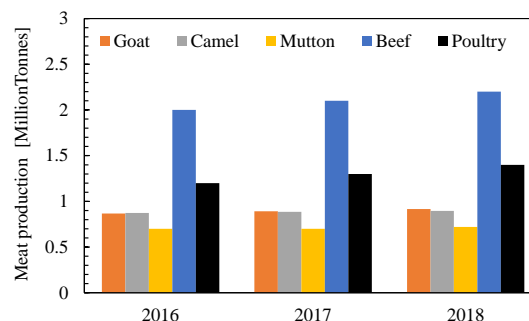


Fig. 1 Comparison of livestock species against year-wise meat production in Pakistan.

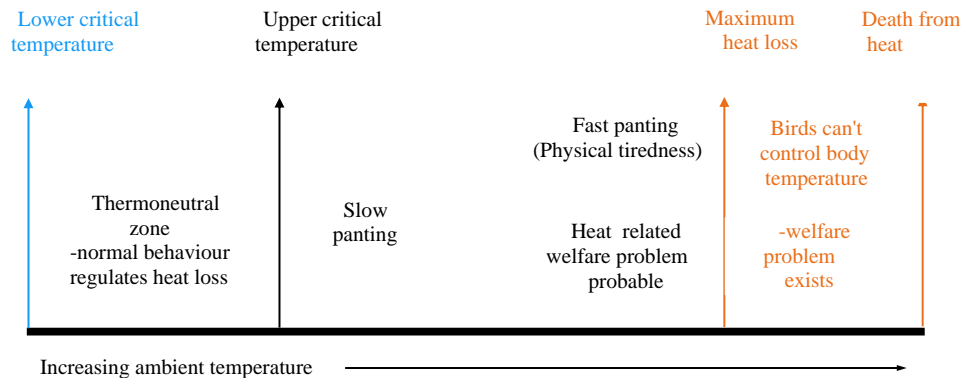


Fig. 2 A comparative analysis of Thermal stress versus increasing temperatures in poultry birds [2].

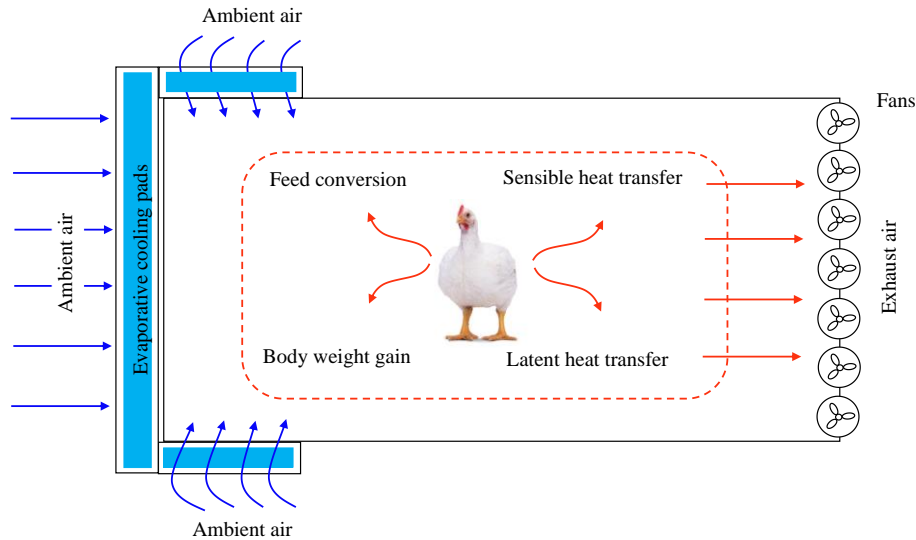


Fig. 3 Schematic of poultry air-conditioning.

The figure given below is the depiction of real-life control shed where a dry air stream is being cooled directly. The suction pressure generated by the fans produces the chilling effect in the control chamber. The placement of poultry birds is ideally arranged in between the water channels and fans to make the most out of the cooling medium. The exhaust air is thrown out of the fans with a foul smell. Future studies may explore the options to utilize this exhausted cool air stream for cold storage of agricultural products. This air-conditioning cum cold storage could be the feasible option of harnessing the energy efficiently.

This paper aims to address the issues of poultry thermal comfort. For this purpose, the insight of poultry air-conditioning is sketched out. The Temperature-Humidity-Velocity Index (THVI) is studied further with the demonstration of synergistic effect over the poultry birds.

2. RESEARCH METHODOLOGY

From the literature study, the THI value for broilers is calculated by using the values of dry bulb temperature and relative humidity into the equation [22], [23]. The equation for wet-bulb temperature is also employed to assist the THI equation for the desired values of relative

humidity. For THI value wet-bulb temperature is calculated by equation (2) [24]. Further, the THVI is calculated from the equation by putting the values of THI and assumed velocity into this equation to understand the synergistic effect [2], [3], [23]. For distinguishing the normal, alert, and danger zones, thermal exposure time ET is calculated by the equations (4-6) for each degree temperature rise with the help of THVI [23].

$$THI = 0.85T_{db} + 0.15T_{wb} \quad (1)$$

$$T_{wb} = T \tan^{-1} \left[0.151977 + (RH + 8.313659)^{\frac{1}{2}} \right] + \tan^{-1}(T + RH) - \tan^{-1}(RH - 1.676331) + 0.00391838RH^{\frac{3}{2}} \tan^{-1}(0.023101RH) - 4.686035 \quad (2)$$

$$THVI = (0.85t_{db} + 0.15t_{wb}) \times V^{-0.058} \quad (0.2 \leq V \leq 1.2) \quad (3)$$

$$\text{For } 1^\circ\text{C temperature rise,} \\ ET = (2 \times 10^{29}) \times THVI^{-17.68} \quad (4)$$

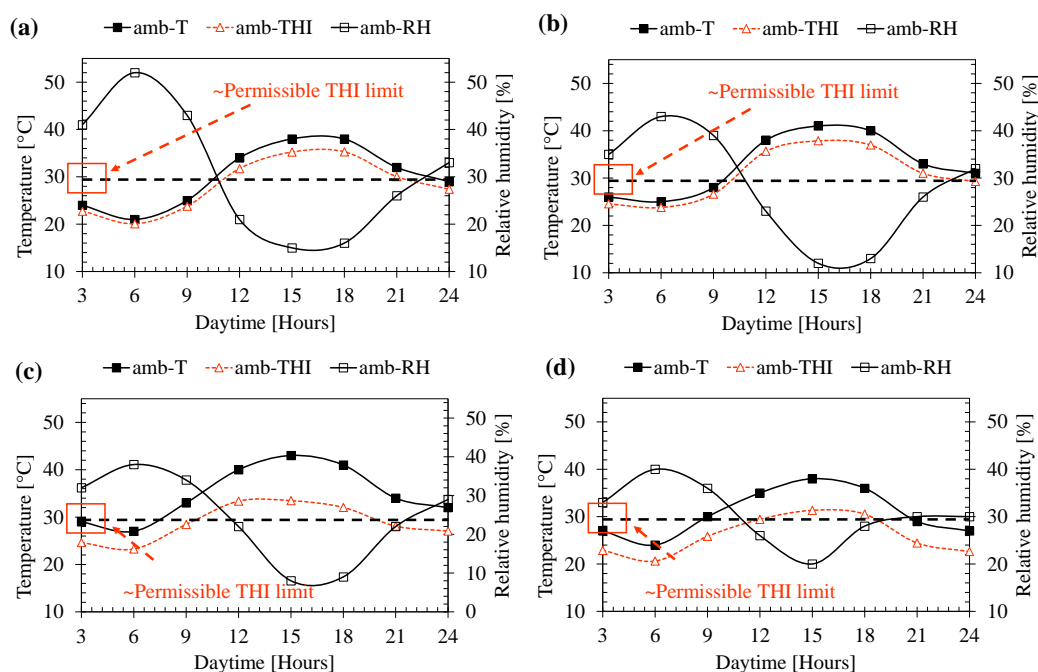


Fig. 4 Daily weather analysis as a function of dry-bulb temperature and relative humidity.

For 2.5°C temperature rise,

$$ET = (4 \times 10^{13}) \times THVI^{-7.38} \quad (5)$$

For 4°C temperature rise,

$$ET = (3 \times 10^{11}) \times THVI^{-5.91} \quad (6)$$

where THI represents temperature-humidity index °C, T_{db} is dry bulb temperature [°C], T_{wb} is wet-bulb temperature [°C], RH is relative humidity [%], THVI represents temperature-humidity-velocity index °C, and ET stands for exposure time in minutes.

3. RESULTS AND DISCUSSION

The average daily temperature and relative humidity for the whole day are plotted down against the day hours. The weather data so obtained for the monsoon season is plotted to visualize the daily temperature and relative humidity values at a certain point in time. The month of May in fig 4 part (b) shows the lowest curve of relative humidity values throughout the day against other months. The month of July in fig 4 part (d) gives the nearest possible relation between temperature and humidity in the day hours. It means that humidity increases with increasing temperatures in June and July as compared to the decreasing humidity values with the increasing temperatures of April and May. The literature study and manual for poultry production suggest the permissible limit of THI equal to 30. Any slight deviation up or down this line deteriorates the situation for the thermal comfort of poultry birds.

The broiler chickens are under observation in figure 5 given below where the values of dry bulb temperature are plotted against THI values. For conditional analysis, a range of dry-bulb temperatures is drawn against the THI

values obtained so. The condition is understood as the temperature is increased while the corresponding THI value goes up in a period. The values of THI are ticked at a certain point before moving to the next temperature range. This elongation in THI and temperature range is the representation of some resistance to thermal stress by the poultry birds. As the temperature goes up, these THI values are less condensed and get agitated to warn the coming stress position for the birds beyond the threshold limit.

The THVI is thus another parameter to understand the synergistic effect at the nexus of temperature, humidity, and velocity. The given below figure 6 is plotted from the empirical model equations by multiplying the THI value with the exponential value of suitable velocity to forecast the effect. Initially, the lower velocity limits dragged the normal zone upward. As the velocity values increase further, the normal zone crosses up the alert

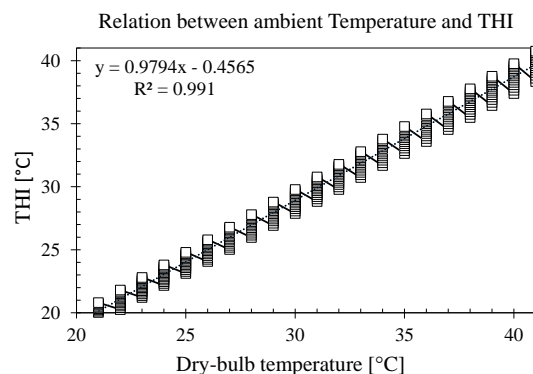


Fig. 5 Dry-bulb temperature and THI as a correlating factor for broiler chickens [3].

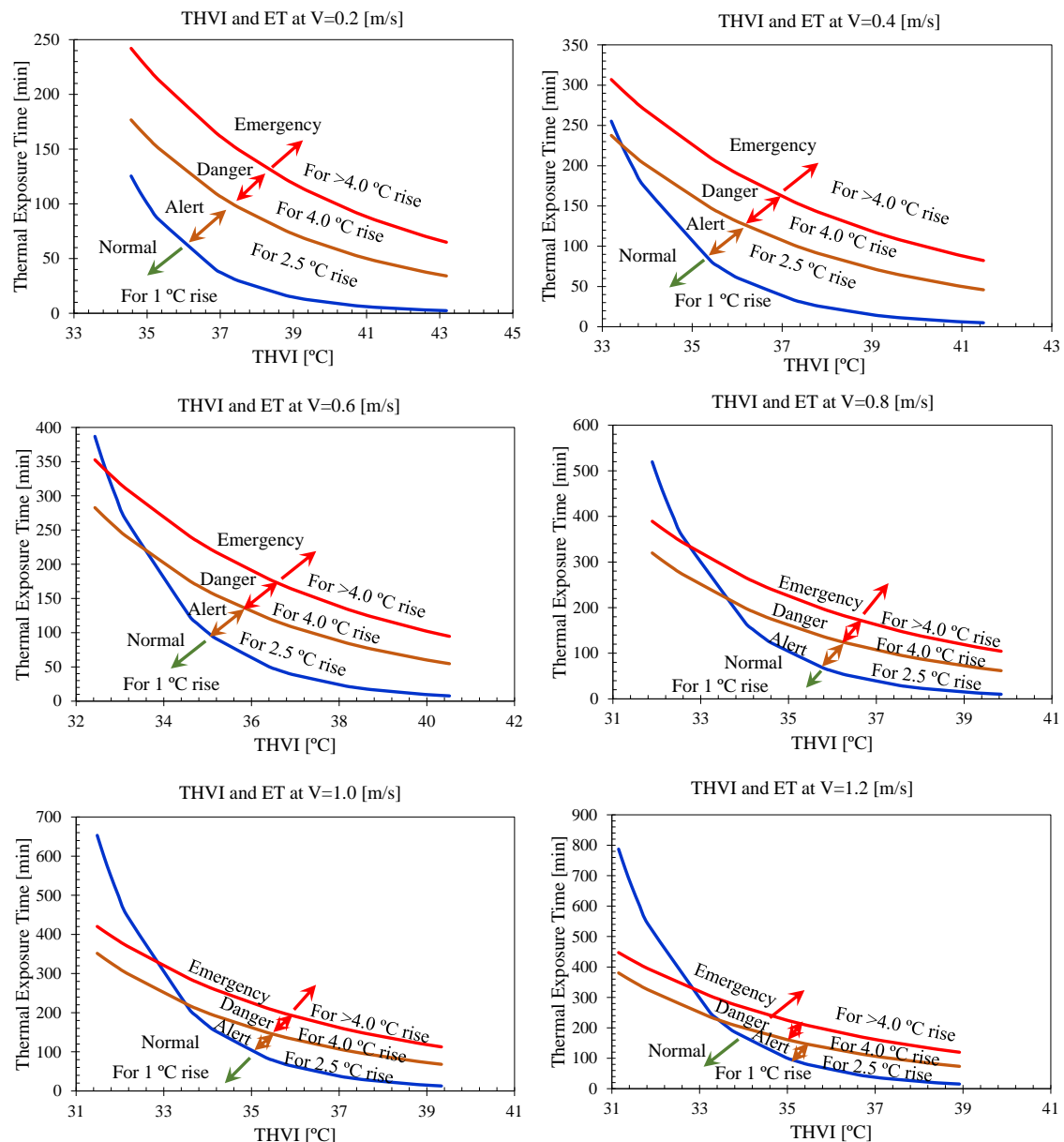


Fig. 6 Thermal comfort zone for poultry birds for THVI index and Thermal Exposure Time (ET) [2].

and danger zone to show the developed resistive action in the environment. The more the velocity in the air, the more is the thermal exposure time (ET) for the poultry birds.

The velocity values are assumed from the range of 0.2 to 1.2 ms^{-1} . At velocity 0.2 ms^{-1} , the normal zone is less elongated as compared to the one developed at 1.2 ms^{-1} . As a result, it is conceived that the velocity parameter is equally significant as other parameters of air conditioning are considered for the welfare of poultry birds.

4. CONCLUSIONS

The paper pitched rightly from the significance of poultry birds in the agriculture and livestock sector in the country. The increasing demand and supply of poultry meat as the cheapest source is dependent upon intelligent and efficient air-conditioning options. In this regard, a short story is put forth regarding the Evaporative Cooling (EC) systems. Further, the physiological composition of poultry birds is dissected to explore the lacking sweat

glands. The humidity factor is also explained in comparing EC systems. Then came the interval point where the significance of THI is explained from the day hours against fluctuating temperature and humidity values.

The case study for the THI value of broiler chickens against dry-bulb temperature is narrated to understand the thermal resistance of these birds. Finally, the THVI value is explained as a summation of the poultry thermal exposure time across the rising temperature line. The objective of the study represented that the thermal exposure time is increased with increasing values of velocity. Similarly, the thermal resistivity in the poultry birds is also developed positively. For future studies in this regard, the simulation tools are recommended as the accurate ones against empirical model equations to assess the same situation precisely.

ACKNOWLEDGMENTS

All this work is part of the Ph.D. research of Mr. Khawar Shahzad (1st Author). This research work has been

carried out in the Department of Agricultural Engineering, Bahauddin Zakariya University, Multan-Pakistan. The Bahauddin Zakariya University, Multan-Pakistan funded this research under the Director Research/ORIC grant titled “Development and performance evaluation of prototypes of direct and indirect evaporative cooling-based air-conditioning systems” awarded to Principal Investigator Muhammad Sultan.

5. REFERENCES

- [1] “Pakistan economic survey 2018-19 | Ministry of Finance | Government of Pakistan.” https://www.finance.gov.pk/survey_1819.html (accessed Jun. 30, 2021).
- [2] H. M. U. Raza *et al.*, “Investigating Applicability of Evaporative Cooling Systems for Thermal Comfort of Poultry Birds in Pakistan,” *Appl. Sci.*, vol. 10, no. 13, p. 4445, Jun. 2020, doi: 10.3390/app10134445.
- [3] K. Shahzad *et al.*, “Experiments on Energy-Efficient Evaporative Cooling Systems for Poultry Farm Application in Multan (Pakistan),” *Sustainability*, vol. 13, no. 5, p. 2836, Mar. 2021, doi: 10.3390/su13052836.
- [4] H. Xin, I. L. Berry, G. T. Tabler, and T. L. Barton, “Temperature and Humidity Profiles of Broiler Houses with Experimental Conventional and Tunnel Ventilation Systems,” *Appl. Eng. Agric.*, vol. 10, no. 4, pp. 535–542, 1994, doi: 10.13031/2013.25883.
- [5] S. Pedersen and M. Gaardbo Thomsen, “Heat and Moisture Production of Broilers kept on Straw Bedding,” *J. Agric. Eng. Res.*, vol. 75, no. 2, pp. 177–187, Feb. 2000, doi: 10.1006/jaer.1999.0497.
- [6] Joseph L Purswell, William A Dozier III, Hammed A Olanrewaju, Jeremiah D Davis, Hongwei Xin, and Richard S Gates, “Effect of Temperature-Humidity Index on Live Performance in Broiler Chickens Grown From 49 To 63 Days of Age,” presented at the 2012 IX International Livestock Environment Symposium (ILES IX), 2012. doi: 10.13031/2013.41619.
- [7] T. Yanagi, Jr., H. Xin, and R. S. Gates, “a research facility for studying poultry responses to heat stress and its relief,” *Appl. Eng. Agric.*, vol. 18, no. 2, 2002, doi: 10.13031/2013.7787.
- [8] S. T. Nascimento, A. S. C. Maia, K. G. Gebremedhin, and C. C. N. Nascimento, “Metabolic heat production and evaporation of poultry,” *Poult. Sci.*, vol. 96, no. 8, pp. 2691–2698, Aug. 2017, doi: 10.3382/ps/pex094.
- [9] H. J. Chepete and H. Xin, “Heat and Moisture Production of Poultry and Their Housing Systems - A Literature Review,” presented at the Livestock Environment VI, Proceedings of the 6th International Symposium 2001, 2001. doi: 10.13031/2013.7089.
- [10] X. Hui *et al.*, “New control strategy against temperature sudden-drop in the initial stage of pad cooling process in poultry houses,” *Int. J. Agric. Biol. Eng.*, vol. 11, no. 1, pp. 66–73, 2018, doi: 10.25165/j.ijabe.20181101.2479.
- [11] H. M. U. Raza, M. Sultan, M. Bahrami, and A. A. Khan, “Experimental investigation of evaporative cooling systems for agricultural storage and livestock air-conditioning in Pakistan,” *Build. Simul.*, vol. 14, no. 3, pp. 617–631, Jun. 2021, doi: 10.1007/s12273-020-0678-2.
- [12] S. Noor, H. Ashraf, M. Sultan, and Z. M. Khan, “Evaporative Cooling Options for Building Air-Conditioning: A Comprehensive Study for Climatic Conditions of Multan (Pakistan),” *Energies*, vol. 13, no. 12, p. 3061, Jun. 2020, doi: 10.3390/en13123061.
- [13] S. Noor *et al.*, “spatiotemporal investigation of evaporative cooling options for greenhouse air-conditioning application in Pakistan,” *Fresenius Environ. Bull.*, vol. 30, no. 03, p. 13.
- [14] M. Sultan and T. Miyazaki, “Energy-Efficient Air-Conditioning Systems for Nonhuman Applications,” in *Refrigeration*, O. Ekren, Ed. InTech, 2017. doi: 10.5772/intechopen.68865.
- [15] M. H. Mahmood, M. Sultan, T. Miyazaki, S. Koyama, and V. S. Maisotsenko, “Overview of the Maisotsenko cycle – A way towards dew point evaporative cooling,” *Renew. Sustain. Energy Rev.*, vol. 66, pp. 537–555, Dec. 2016, doi: 10.1016/j.rser.2016.08.022.
- [16] H. Ashraf *et al.*, “Dynamic Evaluation of Desiccant Dehumidification Evaporative Cooling Options for Greenhouse Air-Conditioning Application in Multan (Pakistan),” *Energies*, vol. 14, no. 4, p. 1097, Feb. 2021, doi: 10.3390/en14041097.
- [17] M. Kashif *et al.*, “Study on Desiccant and Evaporative Cooling Systems for Livestock Thermal Comfort: Theory and Experiments,” *Energies*, vol. 13, no. 11, p. 2675, May 2020, doi: 10.3390/en13112675.
- [18] M. H. Mahmood, M. Sultan, and T. Miyazaki, “Significance of Temperature and Humidity Control for Agricultural Products Storage: Overview of Conventional and Advanced Options,” *Int. J. Food Eng.*, vol. 15, no. 10, Oct. 2019, doi: 10.1515/ijfe-2019-0063.
- [19] M. W. Shahzad, M. Burhan, D. Ybyraiymkul, S. J. Oh, and K. C. Ng, “An improved indirect evaporative cooler experimental investigation,” *Appl. Energy*, vol. 256, p. 113934, Dec. 2019, doi: 10.1016/j.apenergy.2019.113934.
- [20] J. Lin, R. Wang, C. Li, S. Wang, J. Long, and K. J. Chua, “Towards a thermodynamically favorable dew point evaporative cooler via optimization,” *Energy Convers. Manag.*, vol. 203, p. 112224, Jan. 2020, doi: 10.1016/j.enconman.2019.112224.
- [21] Y. Al Horr, B. Tashtoush, N. Chilengwe, and M. Musthafa, “Operational mode optimization of indirect evaporative cooling in hot climates,” *Case Stud. Therm. Eng.*, vol. 18, p. 100574, Apr. 2020, doi: 10.1016/j.csite.2019.100574.
- [22] X. Tao and H. Xin, “Acute Synergistic Effects of Air Temperature, Humidity, and Velocity on Homeostasis of Market-Size Broilers,” vol. 46, p. 10.
- [23] Xiuping Tao and Hongwei Xin, “Temperature-Humidity-Velocity Index for Market-size Broilers,” presented at the 2003, Las Vegas, NV July 27–30, 2003, 2003. doi: 10.13031/2013.14094.
- [24] R. Stull, “Wet-Bulb Temperature from Relative Humidity and Air Temperature,” *J. Appl. Meteorol. Climatol.*, vol. 50, no. 11, pp. 2267–2269, Nov. 2011, doi: 10.1175/JAMC-D-11-0143.1.

Study on Metal and Covalent Organic Frameworks for Adsorption-Based Atmospheric Water Harvesting

Muhammad Bilal¹, Muhammad Sultan^{1*}, Muhammad Aleem¹

¹Department of Agricultural Engineering, Bahauddin Zakariya University, Multan 60800, Pakistan

*Corresponding author email: muhammadsultan@bzu.edu.pk

Abstract: Atmospheric water harvesting (AWH) using adsorbent materials holds a great potential to supply drinking water in water-stressed regions. The adsorbents with a maximum working capacity, relative pressure range with multiple adsorption-desorption cycles, and vibrant temperature response are suitable for this application. In this regard, this paper outlines the significance of reticular chemistry of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) which have been emerged as the unique class of adsorbents capable of extracting atmospheric water even at low relative humidity levels and perform with fast water uptake and release kinetics. The historical advancements along with the design of porosity, building units, and reticular designs of MOFs and COFs are reviewed in this study. Recently developed MOFs have been successfully synthesized and utilized as the adsorbents in AWH devices specifically in the desert areas. The number of porous MOFs and COFs have been synthesized and tested at various conditions.

Keywords: metal-organic frameworks, covalent organic frameworks, reticular chemistry, atmospheric water harvesting

1. INTRODUCTION

Human society depends on the availability of freshwater, but it represents only 2.5% of the total water available on the globe. Out of this, only 0.4% is the most useful part which is divided into lakes (67.4%), soils (12.2%), swamps (8.5%), rivers (1.6%), and atmospheric water vapor (9.6%). Water scarcity has been experiencing by many countries and this projection is increasing day by day due to climate change, water pollution, and global population [1,2]. In this situation, humidity in the earth's atmosphere can be considered as an alternative resource to access fresh drinking water. Providing drinkable water by the liquification of water vapors is a unique way to overcome the water scarcity issues. In this regard, MOFs and COFs have emerged as the possible candidates for this application. The understanding of the reticular chemistry of these materials is very important to increase the adsorption and desorption capacities [1,3–9]. Therefore, this study presents the historical advancements along with the design of porosity, building units, and reticular designs of MOFs and COFs.

2. METAL ORGANIC FRAMEWORKS (MOFs)

2.1. History of MOFs

In most of the twentieth century, it was believed that linking molecules with strong bonds to form extended structures is a "waste of time" because "it doesn't work". However, these state of affairs were changed when germanium sulfide clusters (with a negative charge) were linked with manganese ions (with a positive charge) to develop an extended structure [10]. Fig. 1 shows the crystalline inorganic extended structure. This was the first successful attempt in the field to develop solid-state materials by linking molecular building blocks. With time, attention was made to the development of organic molecules as building units with the advantage of being charged to improve the metal ion's bonding strength. Therefore, in 1995 a layered MOF (crystalline form) was developed by linking the carboxylate organic molecules (1,3,5-benzotricarboxylate) with cobalt ions [11]. Fig. 2(a) represents the metal ions linked by charged organic linkers to develop MOFs in crystalline form. Immediately after this development, some examples

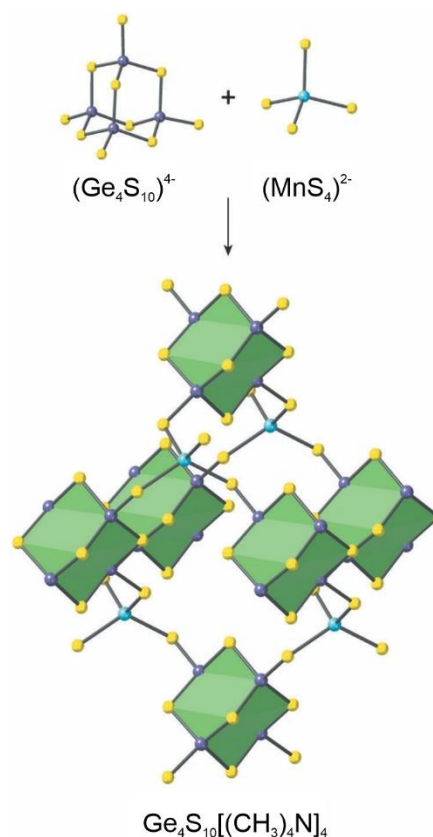


Fig. 1. Illustration of crystalline inorganic extended structure (germanium sulfide clusters linked with manganese ions) [10].

came into the limelight which showed that the carboxylate linkage formed multi metallic clusters called secondary building units (SBUs) which were rigid, robust, and proved as the excellent objects to combine with organic linkers and develop porous MOFs [12,13]. Conclusively, in 1998, an illustration of 1,4-benzene dicarboxylate linking with zinc ions came into the field in which pores filled with N, N-dimethylformamide molecules, later this structure was named as MOF-2 [14]. Fig. 2(b) shows the structure of carboxylate linkers which formed secondary building units to develop porous MOF.

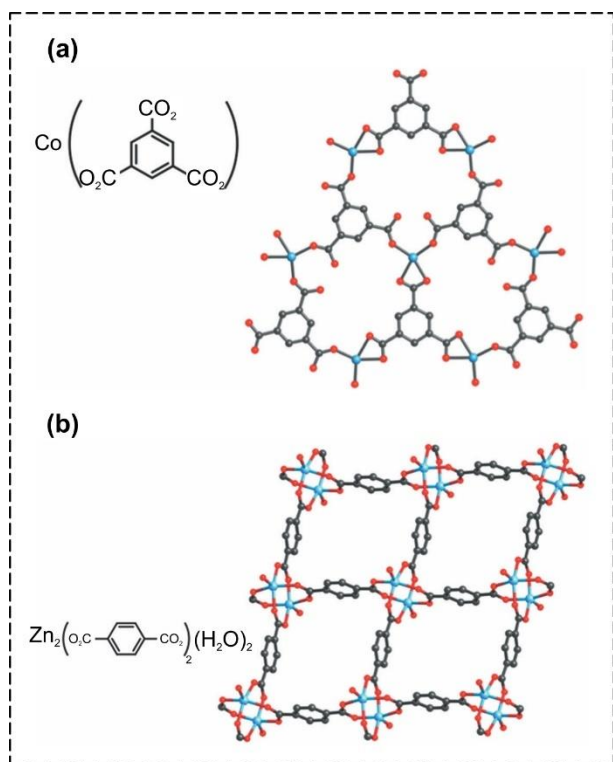


Fig. 2. Metal-Organic Frameworks (a) metal ions linked by charged organic linkers to develop MOFs in the crystalline form [11] (b) structure of carboxylate linkers which formed secondary building units to develop porous MOFs [14].

2.2. Porosity design of MOFs

Pore size has a direct impact on the adsorption properties of MOFs. Without changing the underlying topology of solid-state materials, the alteration of matrices and functionality of any given structure has proven to be a challenging task. In case of MOFs chemistry, isorecticular frameworks (with different pore sizes and the same underlying topology as the parent structure) can be developed by the functionalization of the linker and without changing its general shapes. Isorecticular structures can be developed by prior knowledge of the synthetic conditions where SBUs have been formed. This strategy was first implemented by the information of isorecticular structures based on MOF-5. Fig. 3 shows the isorecticular MOFs series based on MOF-5 (IRMOF-1). In fig. 3, a variety of ditopic carboxylate linkers were reticulated with Zn^{2+} ions under those conditions which were used in the synthesis of parent MOF-5 (IRMOF-1) [15]. This results in the frameworks with the same structures but with either added substituents or modified pore sizes.

2.3. Building units of MOFs

The building units of metal-organic frameworks are the organic and inorganic components, named secondary building units (SBUs) and linkers, respectively. In the 1990s, bipyridines and nitriles which were the neutral donor linkers were used to prepare the coordination networks. But later, these were replaced by the charged chelating linkers with binding groups of carboxylates.

The advantages of these linkers are (i) these charged carboxylates neutralize the positive charges of the metal

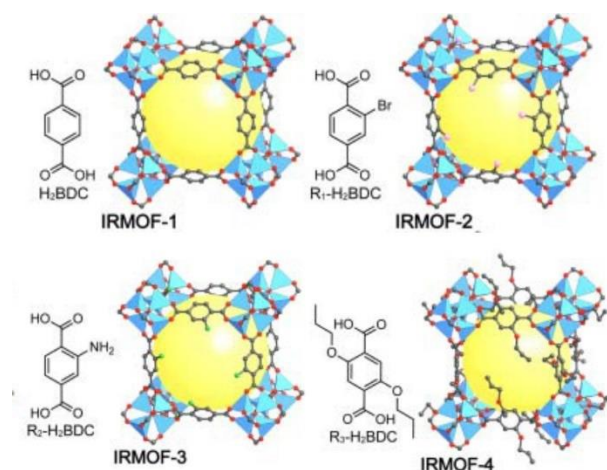


Fig. 3. Illustration of Isorecticular IRMOF series based on MOF-5 [6].

nodes and developed the neutral frameworks thus removing the need for counter ions, (ii) structural rigidity and directionality increases due to their chelating ability, (iii) because of fixed coordination geometry and connectivity, the formation of polynuclear clusters increases, and (iv) highly stable (thermal, chemical, and mechanical) MOFs will be developed with the strong bonding of linkers and the metal centers of SBUs. It was seen that linkers used in the synthesis of MOFs were possessing high symmetry and were usually built from unsaturated hydrocarbon fragments. Finally, these specifications will allow the preparation of chemically and mechanically stable frameworks.

2.4. Reticular design of MOFs

Reticular chemistry is the study of linking chemical molecules and clusters with strong bonds to develop extended structures such as MOFs. MOFs were honored to be developed as the first class of crystalline solids in the field of reticular chemistry. Fig. 4 shows the main achievements of the reticular design of MOFs for water harvesting from the air. Hydrolytic stability is considered a fundamental requirement for a water harvesting material. Till now, many MOFs have been developed through carboxylate coordination bonds, but may not show long-term water stability. Therefore, azolate based linker molecules having stronger metal linker coordination bonds has been presented as a viable strategy to design hydrolysis resistant MOFs [16]. Furthermore, MOFs should exhibit high architectural stability to resist the capillary forces behaving on the pore walls during water release [17]. It was observed that the step-shaped isotherms are suitable for AWH because the high amount of water (high water uptakes and releases) can be collected through small pressure or temperature gradients [18]. The step-shaped isotherms can be explained by the formation of water molecule networks (hydrogen-bonded) within the MOF material during the adsorption process. In previous studies [1,19–23], at low partial pressures, water molecules first adsorb at the primary adsorption sites, and with increasing vapor

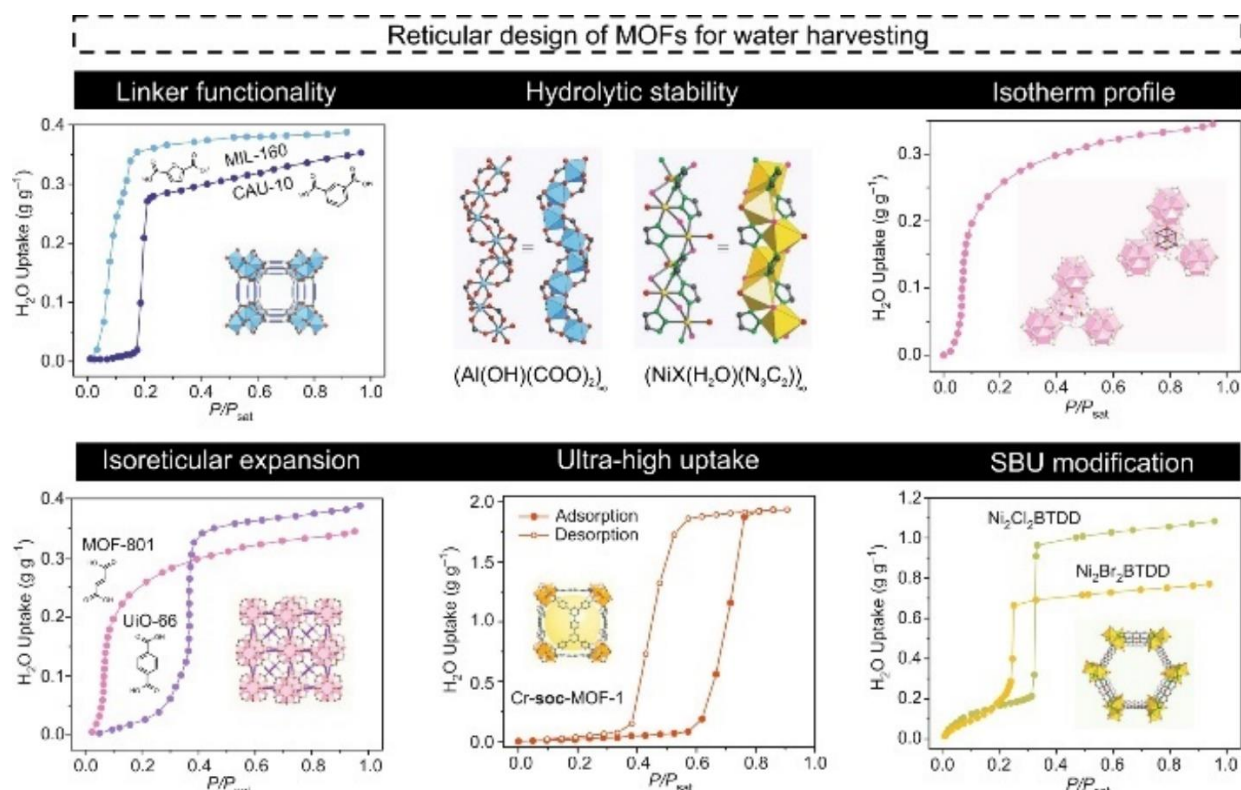


Fig. 4. Features of reticular design of MOFs for water harvesting from air reproduced from [4,18,24,25].

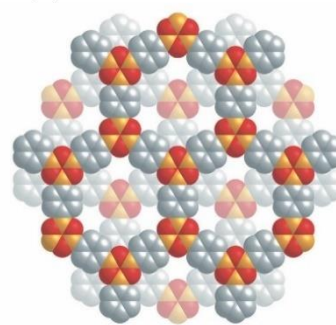
pressure, more molecules will bind to create clusters within the MOF pores. Isoreticular expansion is considered as one of the unique characteristics of reticular chemistry, once the synthetic conditions for the development of MOFs with specific SBUs have been found then these can be reused (slight modification of linkers, for the same modality but different size, length, same underlying net, different pore size, and the environmental conditions) [26]. It was found that an isoreticular expansion of any MOF materials will become unstable in cyclic conditions and therefore this strategy cannot always be used to develop MOFs with higher water uptake capacity [17]. In case of uptake, the highest water uptake was achieved by MOF (Cr-soc-MOF-1 ($\text{Cr}_3\text{O}(\text{TCPT})_{1.5}(\text{H}_2\text{O})_2\text{Cl}$, where TCPT^{4-} is 3,3',5,5'-tetrakis(4-carboxylatephenyl)-p-terphenyl) and showed 1.95 g g^{-1} with a pore volume of $2.1 \text{ cm}^3 \text{ g}^{-1}$ [4]. For AWH, it was obvious to use hydrophilic groups ($-\text{COOH}$, $-\text{OH}$) to shift the steep water uptake region to low relative humidities regions. It was found that the use of heterocycles in MOF backbones can significantly increase the hydrophilicity and can retain the pore volume. Various methods have been developed and used for SBUs modifications to increase the water sorption properties [27]. One of these methods is to exchange the metal cations that exist in the SBU with the solution which contains the different cations of the same valency and size [28]. Similarly, anions in SBUs can be exchanged with the replacement of Cl^- by Br^- anions in $\text{Ni}_2\text{Cl}_2\text{BTDD}$ (BTDD^{2-} , bis (1H-1,2,3-triazolato[4,5-b],[4',5'-i])dibenzo[1,4]dioxin) to obtain $\text{Ni}_2\text{Br}_2\text{BTDD}$.

3. COVALENT ORGANIC FRAMEWORKS

3.1. History of COFs

The formation of crystalline solids can be understood by the combination of organic building units through covalent bonds in between the elements (H, B, C) into covalent organic frameworks (COFs). In 2005 and 2007, the first COFs were developed and later examined for various applications [29,30]. Fig. 5 shows the illustrations of the first COFs that were synthesized. It was seen that the COFs have to be chemically, and thermally robust. COF-1 was developed from the self-condensation of BDDBA at 120°C . In addition, the COF-1

(a) 2D structure of COF-1



(b) 3D structure of COF

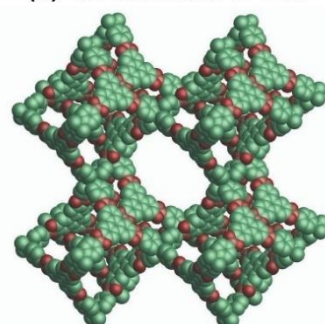


Fig. 5. Covalent organic frameworks (a) COF-1 composed entirely of light atoms linked with covalent bonds to develop 2D frameworks (b) 3D COF whose structure is the lightest one of all solid compounds [29,30].

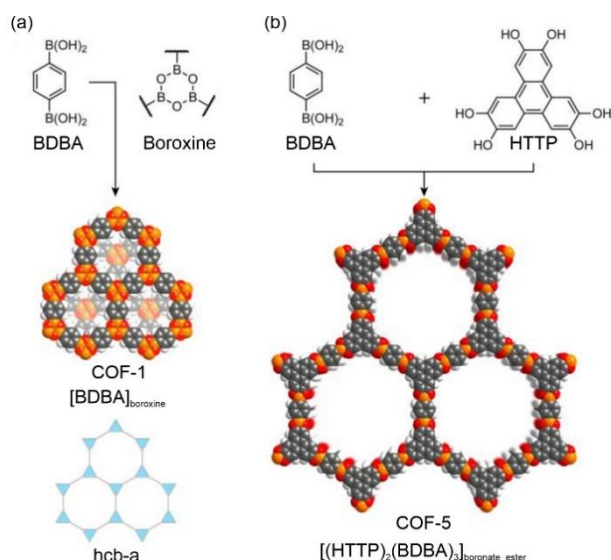


Fig. 6. Formation of COF-1 and COF-5 (a) BDBA results in boroxine linkages to develop COF-1 (b) reticulation of BDBA with HHTP results to COF-5 [29].

layers have openings of 15.1 Å and are arranged in a staggered confirmation. Fig. 6 (a) shows the BDBA results in boroxine linkages to develop COF-1. Later, COF-5 was developed by the reticulation of BDBA with HHTP and the resulting framework was also of hcb topology as shown in fig. 6(b).

1 3.2. Reticular design of COFs

The approach of the reticular design of COFs is very complex and divided into five steps. Fig. 7 shows the general approach for the synthetic synthesis of COFs. From step 1, first, a target framework topology will be identified, and the highest symmetry of this topology will be dissected into the vertices by breaking the edges. Then vertices will be evaluated based on their number of points and suitable angles in step 2. The precise knowledge of geometry is very crucial. Then in step 3, molecular equivalents of the vertices will be identified. In step 4, covalent organic frameworks will be formed by stitching together the covalent bonds with molecular buildings units [6]. In step 5, characterization by crystallographic techniques will be done to confirm the development of

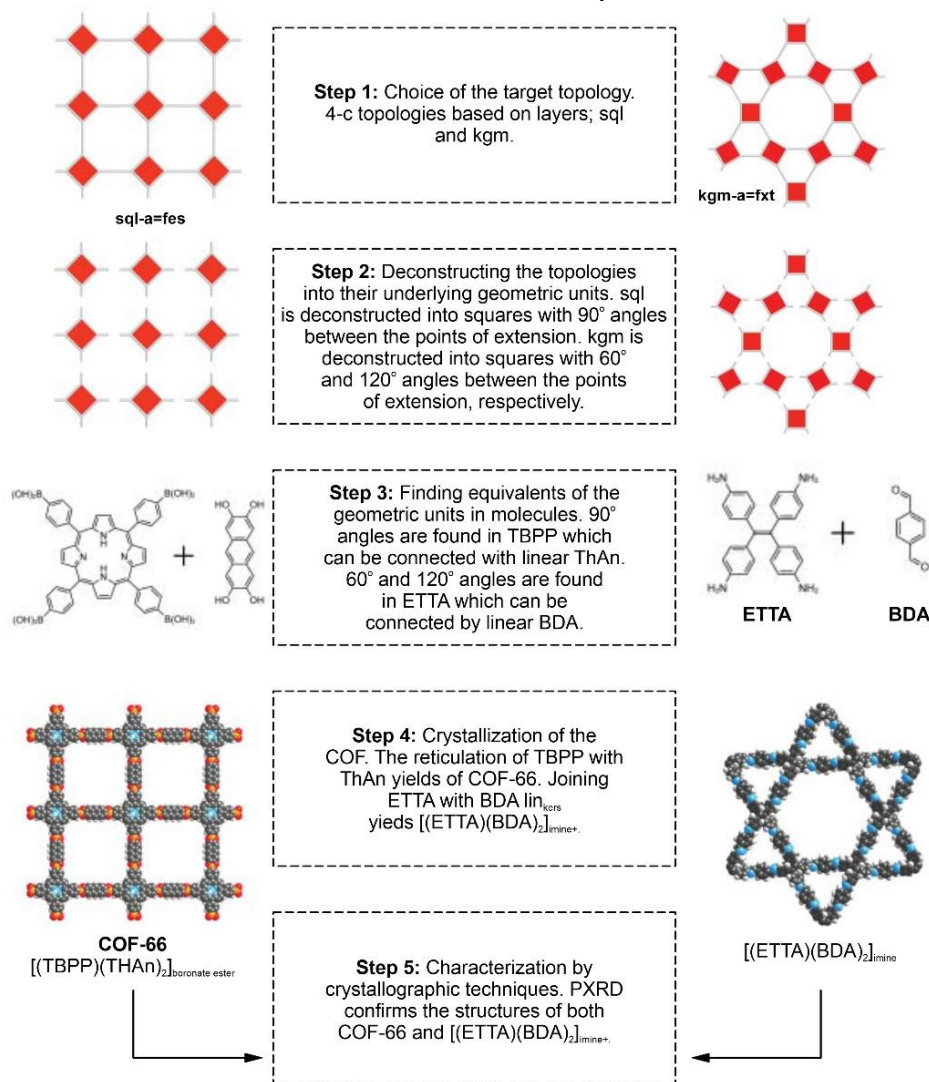


Fig. 7. Approach for the reticular synthesis of covalent organic frameworks [6].

the expected framework structure. To date, five edge-transitive 2D topologies and four 3D topologies have been synthesized. The 2D layered topologies are hcb, sql, kgm, hxl, and kgd whereas the 3D topologies are dia, ctn, bor, and pts nets. It was concluded that to develop 3D frameworks, polyhedral linkers rather than polygonal should be used.

4. CONCLUSIONS

In this study, the historical progress and development of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) are discussed from the AWH standpoint. Recently developed MOFs are promising due to their structural diversity and hydrophilicity. Porosity designs and building units of MOFs are presented in this paper. Furthermore, the importance of reticular designs of MOFs and COFs is highlighted. Numerous MOFs have been synthesized and developed with different topologies, pore sizes, and structures. In the case of COFs, only five 2D topologies (hcb, sql, kgm, hxl, and kgd), and four 3D topologies (dia, ctn, bor, and pts) have been reported. It is clear from the discussion that the insights of the chemistry of MOFs and COFs are very crucial in terms of maximum working capacity, relative pressure range with multiple adsorption-desorption cycles, and vibrant temperature response. It is concluded that if carefully designed and synthesized the MOFs and COFs materials then these could well be the answer to address the water scarcity conditions in the future.

5. REFERENCES

- [1] Kalmutzki MJ, Diercks CS, Yaghi OM. 2018 Metal-Organic Frameworks for Water Harvesting from Air. *Adv Mater* 30:1–26. <https://doi.org/10.1002/adma.201704304>.
- [2] Singha B, Eljamal O. 2020 A Review on Water Conservation and Consumption Behavior: Leading Issues, Promoting Actions, and Managing the Policies. *Proc. Int. Exch. Innov. Conf. Eng. Sci.*, vol. 6, p. 171–8. <https://doi.org/10.5109/4102484>.
- [3] Ploetz E, Engelke H, Lächelt U, Wuttke S. 2020 The Chemistry of Reticular Framework Nanoparticles: MOF, ZIF, and COF Materials. *Adv Funct Mater*:1909062. <https://doi.org/10.1002/adfm.201909062>.
- [4] Towsif Abtab SM, Alezi D, Bhatt PM, Shkurenko A, Belmabkhout Y, Aggarwal H, et al. 2018 Reticular Chemistry in Action: A Hydrolytically Stable MOF Capturing Twice Its Weight in Adsorbed Water. *Chem* 4:94–105. <https://doi.org/10.1016/j.chempr.2017.11.005>.
- [5] Nguyen TTM, Le HM, Kawazoe Y, Nguyen HL. 2018 Reticular control of interpenetration in a complex metal-organic framework. *Mater Chem Front* 2:2063–9. <https://doi.org/10.1039/c8qm00368h>.
- [6] Yaghi OM, Kalmutzki MJ, Diercks CS. 2019 Introduction to Reticular Chemistry. <https://doi.org/10.1002/9783527821099>.
- [7] Abtab SMT, Alezi D, Bhatt PM, Shkurenko A, Belmabkhout Y, Aggarwal H, et al. 2018 Reticular chemistry in action: A hydrolytically stable MOF capturing twice its weight in adsorbed water. *Chem* 4:94–105.
- [8] Sultan M, El-Sharkawy II, Miyazaki T, Saha BB, Koyama S, Maruyama T, et al. 2015 Insights of water vapor sorption onto polymer based sorbents. *Adsorption* 21:205–15.
- [9] Bilal M, Sultan M, Miyazaki T. 2020 Spatiotemporal Investigation of Atmospheric Water Harvesting Potential Using Response Surface Methodology for Multan (Pakistan) and Fukuoka (Japan). *Proc Int Exch Innov Conf Eng Sci* 6:128–33. <https://doi.org/10.5109/4102477>.
- [10] Yaghi OM, Sun Z, Richardson DA, Groy TL. 1994 Directed Transformation of Molecules to Solids: Synthesis of a Microporous Sulfide from Molecular Germanium Sulfide Cages. *J Am Chem Soc* 116:807–8. <https://doi.org/10.1021/ja00081a067>.
- [11] Yaghi OM, Li G, Li H. 1995 Selective binding and removal of guests in a microporous metal-organic framework. *Nature* 378:703–6. <https://doi.org/10.1038/378703a0>.
- [12] Li H, Davis CE, Groy TL, Kelley DG, Yaghi OM. 1998 Coordinatively Unsaturated Metal Centers in the Extended Porous Framework of Zn₃ (BDC) 3⊙ 6CH₃OH (BDC= 1, 4-Benzenedicarboxylate). *J Am Chem Soc* 120:2186–7.
- [13] Rahman MM, Pal A, Saha BB. 2020 Simulation-based Optimum Models for Type-I (a) and Type-I (b) IUPAC Classified Adsorption Isotherms.
- [14] Li H, Eddaoudi M, Groy TL, Yaghi OM. 1998 Establishing microporosity in open metal-organic frameworks: gas sorption isotherms for Zn (BDC)(BDC= 1, 4-benzenedicarboxylate). *J Am Chem Soc* 120:8571–2.
- [15] Desiraju GR, Parshall GW. 1989 Crystal engineering: the design of organic solids. *Mater Sci Monogr* 54.
- [16] Choi HJ, Dincă M, Dailly A, Long JR. 2010 Hydrogen storage in water-stable metal-organic frameworks incorporating 1, 3-and 1, 4-benzenedipyrazolate. *Energy Environ Sci* 3:117–23.
- [17] Mondloch JE, Katz MJ, Planas N, Semrouni D, Gagliardi L, Hupp JT, et al. 2014 Are Zr 6-based MOFs water stable? Linker hydrolysis vs. capillary-force-driven channel collapse. *Chem Commun* 50:8944–6.
- [18] Hanikel N, Prévot MS, Yaghi OM. 2020 MOF water harvesters. *Nat Nanotechnol* 15:348–55. <https://doi.org/10.1038/s41565-020-0673-x>.
- [19] Kim H, Yang S, Rao SR, Narayanan S, Kapustin EA, Furukawa H, et al. 2017 Water harvesting from air with metal-organic frameworks powered by natural sunlight. *Science* (80-) 356:430.
- [20] Tu Y, Wang R, Zhang Y, Wang J. 2018 Progress and Expectation of Atmospheric Water Harvesting. *Joule* 2:1452–75. <https://doi.org/10.1016/j.joule.2018.07.015>.
- [21] Kim H, Rao SR, Kapustin EA, Zhao L, Yang S, Yaghi OM, et al. 2018 Adsorption-based atmospheric water harvesting device for arid climates. *Nat Commun* 9:1–8. <https://doi.org/10.1038/s41467-018-03162-7>.
- [22] Liu X, Wang X, Kapteijn F. 2020 Water and Metal-Organic Frameworks: From Interaction toward Utilization. *Chem Rev*.

- <https://doi.org/10.1021/acs.chemrev.9b00746>.
- [23] Kim H, Rao SR, LaPotin A, Lee S, Wang EN. 2020 Thermodynamic analysis and optimization of adsorption-based atmospheric water harvesting. *Int J Heat Mass Transf* 161:120253. <https://doi.org/10.1016/j.ijheatmasstransfer.2020.120253>.
 - [24] Furukawa H, Gándara F, Zhang YB, Jiang J, Queen WL, Hudson MR, et al. 2014 Water adsorption in porous metal-organic frameworks and related materials. *J Am Chem Soc* 136:4369–81. <https://doi.org/10.1021/ja500330a>.
 - [25] Cadiau A, Lee JS, Damasceno Borges D, Fabry P, Devic T, Wharmby MT, et al. 2015 Design of Hydrophilic Metal Organic Framework Water Adsorbents for Heat Reallocation. *Adv Mater* 27:4775–80. <https://doi.org/10.1002/adma.201502418>.
 - [26] Eddaoudi M, Kim J, Rosi N, Vodak D, Wachter J, O’Keeffe M, et al. 2002 Systematic design of pore size and functionality in isorecticular MOFs and their application in methane storage. *Science* (80-) 295:469–72.
 - [27] Kalmutzki MJ, Hanikel N, Yaghi OM. 2018 Secondary building units as the turning point in the development of the reticular chemistry of MOFs. *Sci Adv* 4:eaat9180.
 - [28] Brozek CK, Dincă M. 2014 Cation exchange at the secondary building units of metal–organic frameworks. *Chem Soc Rev* 43:5456–67.
 - [29] Cote AP, Benin AI, Ockwig NW, O’Keeffe M, Matzger AJ, Yaghi OM. 2005 Porous, crystalline, covalent organic frameworks. *Science* (80-) 310:1166–70.
 - [30] El-Kaderi HM, Hunt JR, Mendoza-Cortés JL, Côté AP, Taylor RE, O’Keeffe M, et al. 2007 Designed synthesis of 3D covalent organic frameworks. *Science* (80-) 316:268–72.