CFD Analysis of Carbon Capturing MOF with Chimney for Urban Areas

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***Abstract*— In this project, the adsorption of CO_2 on metal organic frameworks (MOFs) is comprehensively reviewed. First of all, the problems caused by greenhouse gas emissions are addressed, and different technologies used in CO_2 capture are briefly introduced. The aim of this chapter is to provide a comprehensive overview of CO_2 adsorption on solid materials with special focus on an emerging class of materials called metal organic frame works owing to their unique characteristics comprising extraordinary surface areas, high porosity, and the readiness for systematic tailoring of their porous structure. Recent literature on CO_2 capture using MOFs is reviewed, and the assessment of CO_2 uptake, selectivity, and heat of adsorption of different MOFs is summarized, particularly the performance at low pressures which is relevant to post combustion capture applications. Different strategies employed to improve the performance of MOFs are summarized along with major challenges facing the application of MOFs in CO_2 capture. The last part of this chapter is dedicated to current trends and issues, and new technologies needed to be addressed before MOFs can be used in commercial scales.**

In this project, we provide a short review on the most recent advances in using MOFs for CO_2 adsorption and separation that are directly related to CO_2 capture. Some of the important properties of MOF adsorbents which are crucial for practical applications but are largely overlooked in research carried out so far are discussed.

***Keywords*— carbon dioxide capture, metal-organic frameworks (MOFs), solid sorbent.**

I. INTRODUCTION

The Earth's global climate system is continually facing devastating changes due to various human-made and natural factors. Smithson mentioned that the increase in greenhouse gas concentrations in the atmosphere directly impacts the global climate system, which is known as global warming. These greenhouse gases trap the sun's radiation in the Earth's atmosphere; this phenomenon is known as the greenhouse effect, causing global warming. Carbon dioxide gas is blamed for being the main factor that causes the greenhouse effect because it is the most important anthropogenic greenhouse gas (Intergovernmental Panel on Climate Change (IPCC), 2007). Rochelle stated that more than 85% of the world's energy demand is based on burning fossil fuels; this will result in massive emissions of CO_2 into the atmosphere. There are natural and anthropogenic sources for carbon dioxide gas emissions into the atmosphere. Chemical engineering industries are considered one of the primary anthropogenic sources of CO_2 into the atmosphere in which natural gas and fossil fuels are burned for various purposes. As a result of the industrial revolution and the rapid increase in the population growth rate, more fossil fuels are burnt to satisfy the population's needs and demands. Hence, more carbon dioxide is emitted into the atmosphere. Consequently, the separation and capture of CO_2 became a necessity.

CO_2 can be separated and captured using five leading technologies, including absorption, adsorption, cryogenics, membrane, and microbial or algae. In the meantime, the research trend has been focusing on three main types of technology for carbon capture, namely oxy-fuel combustion, pre-combustion, and post-combustion. Omoregbe (2020) investigated those main types of technology by using publications retrieved from the Web of Science database from the year 1998 to 2018. The results of the authors' investigations presented that from the year 1998 to 2007 there was almost no research output on carbon capture, until the year 2008, in which climate change abatement was first introduced, and the industrial and public awareness of clean, greener fossil energy options grew. The authors also stated that among the commonly studied carbon capture technologies, the post-combustion capture technology was the most referenced technology for carbon capture, with approximately 80.9% of total publications retrieved. On the other hand, the technology with the lowest number of publications is oxy-fuel combustion, with approximately 3.4% of total publications retrieved. Several porous materials can be incorporated into these carbon capture technologies to allow and enhance the separation or the capture of CO_2. One of the best-used porous materials in carbon capture technologies are metal-organic frameworks (MOFs).

During the last two decades, a new crystalline porous materials class has emerged. This class of materials is known as MOFs. As a result of the MOFs' unique properties, this class has gained remarkable attention across the globe. The main limitation of the application of MOFs in the carbon capture processes is the high cost. The synthesis process of MOFs is very costly, which makes them economically unviable. This project investigates MOFs' applications in the CO_2 capture, adsorption, separation, conversion, and reduction processes. It aims to draw and provide general guidelines and conclusions for the MOFs' importance as a porous material for carbon dioxide gas-related process.

II. Design Of Chimney

A. Software Used

The design of a chimney contains several complexes and attempt has been made to meet the requirements of original chimney by using SolidWorks.

SolidWorks is a solid modelling computer-aided design and computer-aided engineering computer program published by Dassault Systemes.

B. Dimension of Chimney

- The height of the chimney is 5000mm.
- The lower diameter of the chimney is 1500mm.
- The higher diameter of the chimney is 600mm.
- The thickness of the chimney is 100mm.

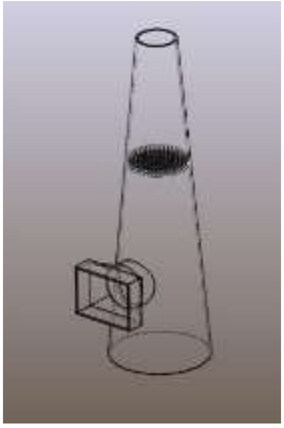
C. Tools Used

In the SolidWorks modelling software there are some tools such as

- 2d Sketch
- Plane
- Loft
- Revolve
- Extrude
- Extrude Cut
- Fillet
- Chamfer

D. Chimney Design

The pictographic representation of the design of chimney with duct as per the given dimensions is shown below.



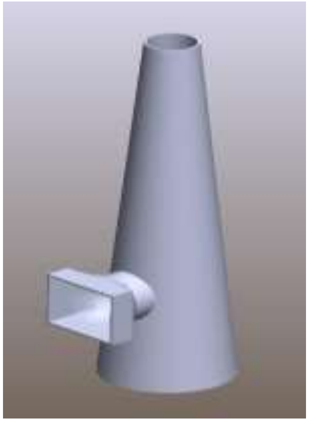


Fig. 1 Chimney Design

Also the wireframe view of the design of chimney with duct at same dimension is shown above.

III. Design Of MOF

A. Software Used

The design of a chimney contains several complexes and attempt has been made to meet the requirements of original chimney by using CATIA.

CATIA is a solid modelling computer-aided design and computer-aided engineering computer program published by Dassault Systemes.

B. Dimension of Chimney

- The length of the MOF is 150mm.
- The height of the MOF is 100mm.
- The breadth of the MOF is 15mm

C. Tools Used

In the SolidWorks modelling software there are some tools such as

- 2d Sketch
- Plane
- Extrude
- Extrude Cut
- Sweep
- Sweep Cut
- Linear Pattern
- Fillet
- Chamfer

Are used to complete this design in the solidworks software.

D. MOF Design

The pictographic representation of the design of MOF as per the given dimensions is shown below.

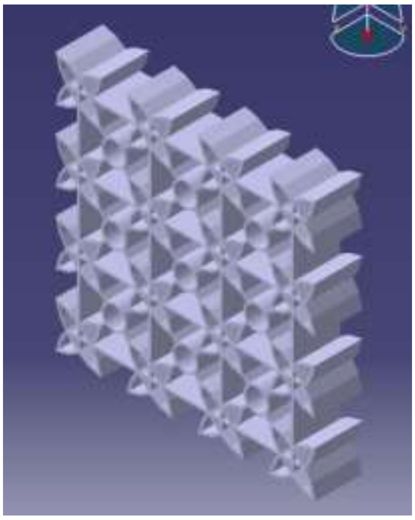


Fig. 2 MOF Design Model 1

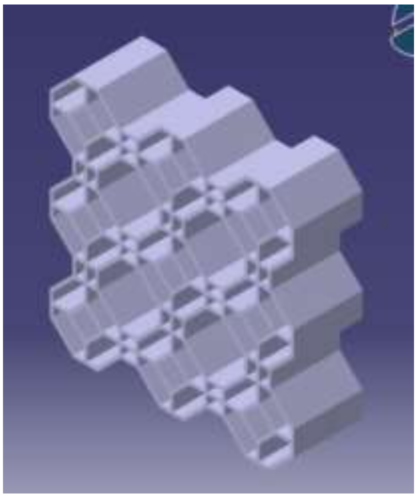


Fig. 3 MOF Design Model 2

IV. Design Of Fan & Duct

A. Software Used

The design of a chimney contains several complexes and attempt has been made to meet the requirements of original chimney by using SolidWorks.

SolidWorks is a solid modelling computer-aided design and computer-aided engineering computer program published by Dassault Systemes.

B. Dimension of Duct

- The height of the rectangular duct is 1000mm.
- The length of the rectangular duct is 750mm.
- The extrude length of the rectangular duct is 300mm.
- The diameter of the circular duct is 600mm.
- The extrude length of the circular duct is 200mm.
- The breadth of the duct is 30mm.

C. Tools Used

In the SolidWorks modelling software there are some tools such as

- 2d Sketch
- Plane
- Extrude
- Circular Pattern
- Linear Pattern
- Extrude Cut
- Loft
- Revolve
- Sweep
- Sweep Cut
- Surface Cut
- Fillet
- Chamfer

D. Fan & Duct Design

The pictographic representation of the design of fan and duct as per the given dimensions is shown below.

Fig. 4 Fan Design

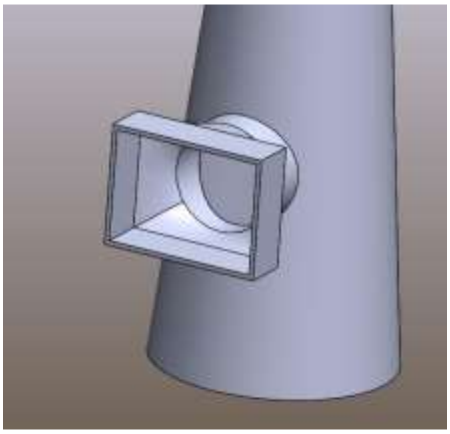


Fig. 5 Duct Design

V. Analysis Of MOF

A. Model 1

1) *Mass Flow Analysis*:

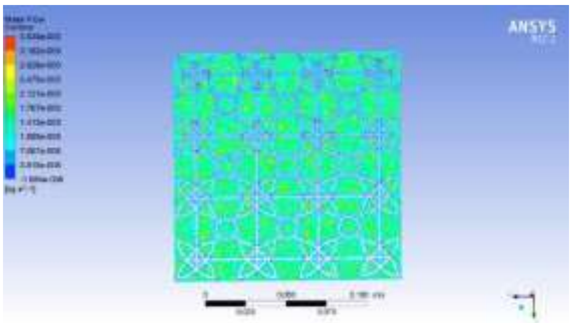


Fig. 6 Mass Flow Analysis (Model 1)

2) Force Analysis:

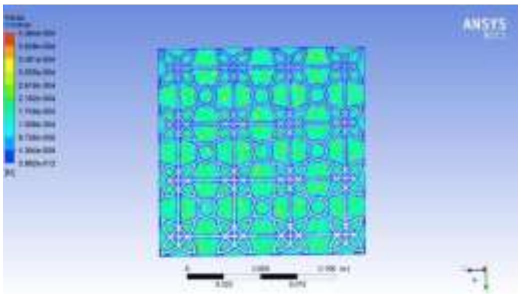


Fig. 7 Force Analysis (Model 1)

3) Pressure Analysis:

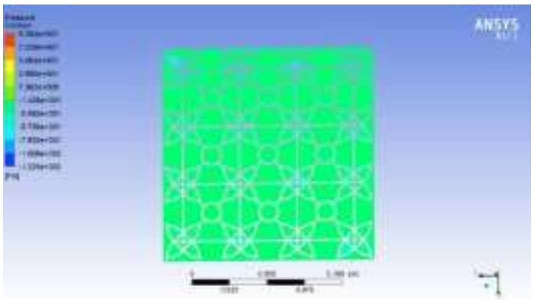


Fig. 8 Pressure Analysis (Model 1)

4) Velocity Analysis:

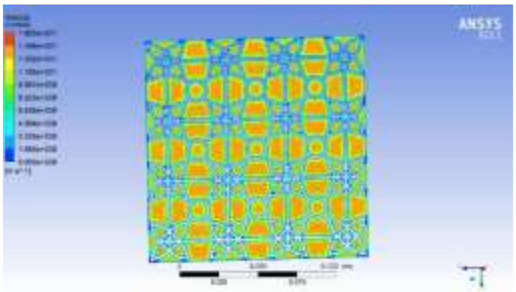


Fig. 9 Velocity Analysis (Model 1)

5) Density Analysis:

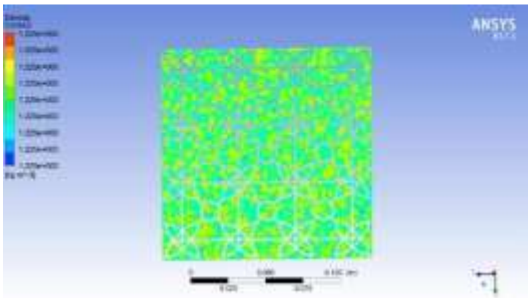


Fig. 10 Pressure Analysis (Model 1)

B. Model 2

1) Pressure Analysis:

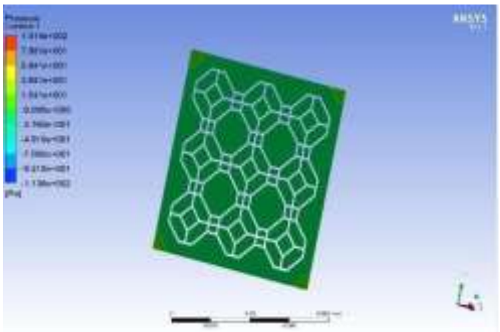


Fig. 11 Pressure Analysis (Model 2)

2) Velocity Analysis:

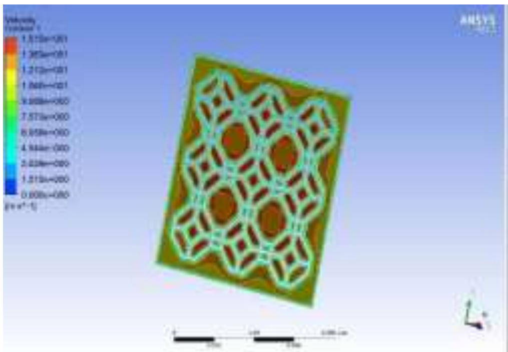


Fig. 12 Velocity Analysis (Model 2)

3) Velocity Rendering Analysis:

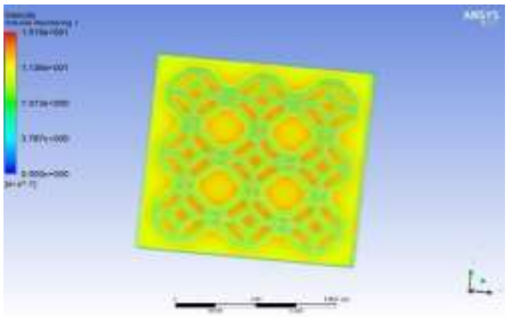


Fig. 13 Velocity Rendering Analysis (Model 2)

IV. Conclusions

Capture of CO_2 either from flue-gas or directly from air presents a challenge but also an opportunity to play a significant role in tackling greenhouse gases such as CO_2 over the coming century. In this contribution, we examine the use of benchmark MOMs for their potential use in CO_2 adsorption processes under humid conditions, particularly DAC and moist-simulated flue-gas. Competition with water vapour was found to significantly reduce the CO_2 adsorption performance of the physisorbent materials compared with anhydrous conditions. However, there was quite a wide range in performance, with both pore size and pore chemistry affecting the performance of physisorbents studied herein. Humid conditions exacerbated the situation and even wider ranges of uptakes and selectivity were observed. The functionalization of organic ligands with hydrophobic decoration, such as methyl groups in the case of **ZIF-8**, may be an approach that could be used to improve S_{CW} of physisorbents. However, our results indicate that increased electrostatics generated by inorganic pillars in HUMs or grafted amines are most effective at improving Q_{st} and overall CO_2 adsorption performance. In conclusion, competition with water vapour is a significant challenge for implementation of physisorbent materials in CO_2 capture, either from DAC or from flue-gas. Control of pore size and pore chemistry through crystal engineering may be a successful strategy to improve CO_2 capture performance even in the presence of water vapour and must be further addressed if physisorbents are to compete with chemisorbents in terms of uptake.

However, the best physisorbents studied herein were found to be much easier to recycle than the benchmark chemisorbent **TEPA-15-SBA**, suggesting that faster and less energy intensive recycling of physisorbents could compensate for the lower uptake values.

Future Scope

Using alternative renewable energy is a viable option to circumvent the CO_2 problems, but the industrial process required for the realisation of these technologies contributes to the carbon footprint. So, what can be done about this?

One of the most efficient strategies would be to capture and store the CO_2 (the process referred to as carbon capture and sequestration) so that it can be converted to valuable products such as chemical fuel or industrial raw materials. This approach allows us to achieve a carbon-neutral lifestyle without compromises.

The need to capture large quantities of CO_2 efficiently is associated with exxagerated costs which act as a barrier to the industrial realisation of carbon capture and storage technologies (CCS).

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