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# Metal-Organic Frameworks for Carbon Capture – Modelling the Manufacture through Life Cycle Assessment

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**Abstract**

With the acceptance from governing bodies that the future of decarbonisation requires CCUS as a key component [1,2], the need for carbon capture technologies that can remove $CO_2$ from industrial emission sources in an energy efficient manner has never been greater. This has led to a stronger research focus on innovative solutions to the carbon capture challenge. Currently, amine-based technologies are more widely deployed than any other technology [3,4], though the environmental concerns and high regeneration energy usage show their deficiencies [5,6], which provides a target for research into alternative technologies to improve upon.

Metal organic frameworks (MOFs) are solid sorbent materials that represent a promising alternative technology to amines. MOFs have demonstrated efficiency at $CO_2$ capture [7]. MOF structures are highly tunable, with limitless options for the type and combination of input materials. Research is being conducted to evaluate their effectiveness in reducing environmental impact and energy usage across their entire lifetime, from manufacture to use, to recycling and disposal. However, there are still many gaps that need filling, especially with regard to applying real experimental data to influence their manufacture and use.

Life-Cycle Assessment (LCA) is a recognized framework allowing for a complete cradle-to-cradle overview of a product's life-cycle [8], using real-world data to inform computer simulations of the processes involved in manufacturing, using, disposing and recycling materials. The output evaluates their environmental impact against a number of characterization factors, including global warming potential (GWP) and ozone depletion. It is an ideal method to assess $CO_2$ capture technologies, but there are very few that have been conducted for MOF-based technologies. Understanding how each process stage can be refined and improved is crucial to implement the materials on an industrial scale.

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LCA studies on MOF manufacture have been conducted in SimaPro, using the ecoinvent v3.11 database and ReCiPe 2016 Midpoint (H) impact assessment method. This process involves finding the relevant input quantities (materials, energy etc) in the available databases, constructing each process step, then extrapolating the data to determine the environmental impact. This allows the emissions from manufacturing these materials to be assessed and compared with mature technologies alongside variants of input materials. It also poses numerous questions to consider for further development of techniques and compositions of these materials. A number of these are detailed below:

*Input variations:* By analysing the emissions from a 'starting' material, certain hotspots can be identified, either from specific parts of the process or from an input material. Investigating where this impact comes from and finding an alternative material to reduce emissions is where LCA comes into its own. For example, the use of a 'transition metal' was causing great impact, so finding an alternative 'group 2 metal' to replace it reduced that considerably, and removing the need for the material entirely further reduced the emissions. Swapping solvents was another element that saw a reduction. A combination of these substitutions showed that emissions could be effectively cut by nearly two-thirds.

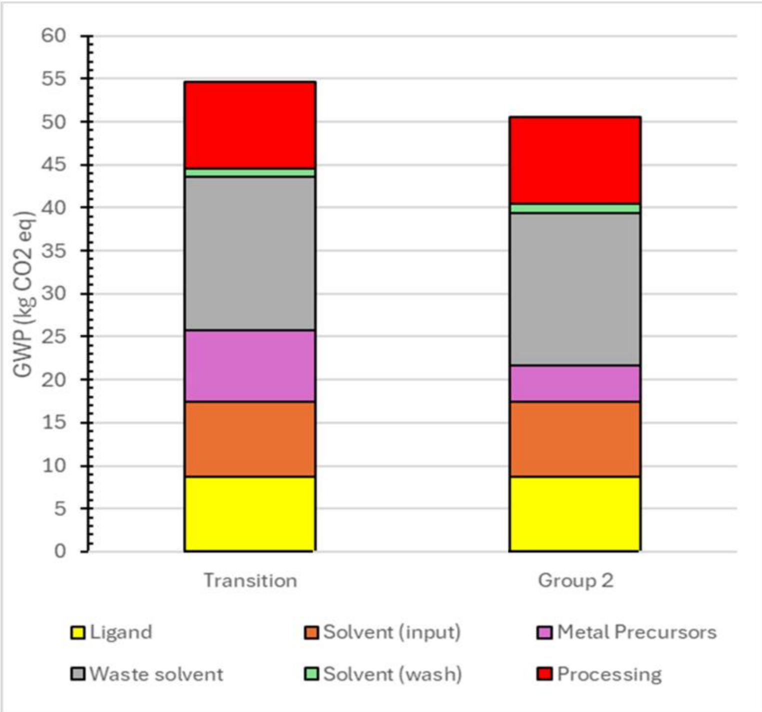


**Figure 1: Comparison of GWP (kg $CO_2$ eq/kg MOF manufactured) for original and varied compositions**

*Region of origin:* A number of input materials are available as an averaged 'global' value, but also broken up into different streams from a variety of sources. A common MOF precursor is sourced from China, which has a far greater environmental impact than the averaged 'global' or Europe equivalents. Changing region of origin would greatly reduce the overall process impact. This is an example of where LCA can show beneficial pathways for commercialization, by looking at how changes in material/energy sourcing can impact emissions.

*Waste treatment streams:* The definition of waste treatment options in ecoinvent is limited by the industries that have provided data, and thus are either very specific or don't cover numerous elements. While the waste out of each process for MOF manufacture can be broken up between each material, there is less differentiation between components in the database. As such, we must try to find the most applicable endpoint for each, taking into account type of material (e.g. inert or hazardous waste) and final destination (e.g. landfill or incineration). Investigating these different streams and proposing alternatives is an element in emission reduction that would otherwise be disregarded when discussing the environmental impacts.

*Impact Categories:* While reducing the carbon emissions is a high priority for these technologies, there are numerous other environmental concerns that can be assessed for these materials. Using the ReCiPe 2016 method in SimaPro allows the assessment of not only GWP, but also elements such as ozone depletion, freshwater eutrophication and ecotoxicity. Consideration of all the affected elements is important for future improvements in the manufacture of this technology. Water consumption is a particularly big concern, with worries about water scarcity through large-scale industrialisation increases in future years. This provides a push for processes to be more economical with their water use, which is an element that can be measured and reduced through this study.

Overall, the research conducted involves modelling the manufacture of the MOF, using real data from large-scale production for the quantities of input materials and energy consumptions, with assumptions made for outsourced processes. The emissions calculated can be exported and compared against other mature technologies, and variations in input quantities and composition of the MOF are compared to show the reduction in emissions from making these variations. This has been done for MOFs produced in solvent-based and water-based methods, and will continue to be refined and updated as new information is provided from experimentation and industry-scale testing.

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