Life Cycle Assessment of Producing the Metal-Organic Framework MIL-101(Fe)

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Abstract

Metal-organic frameworks (MOFs) have emerged as a captivating class of materials at the forefront of materials science and chemistry due to their remarkable structural diversity and wide-ranging applications in gas adsorption, photocatalysis, drug delivery, and energy storage. Among the myriad of MOFs, MIL-101(Fe) stands out as a particularly intriguing and versatile member of this family. In order to achieve sustainable use of these well-liked materials, they need to be examined and analyzed in terms of economic, technical, and environmental effects. In this study, the metal-organic framework nanomaterial MIL-101(Fe) was synthesized using the solvothermal method. We have shown that it is feasible to employ a Life Cycle Assessment (LCA) to ascertain that the utilization of solvents during the synthesis process has a significant impact. To confirm the synthesized structure, the physicochemical properties of the nanomaterial were examined using scanning electron microscopy (SEM), X-ray diffraction (XRD) analysis, and Fourier-transform infrared spectroscopy (FTIR). we delve into the application of SimaPro using the ReCiPe H method at both Midpoint and Endpoint levels. We aim to underscore how this integration enables environmental analysts, researchers, and decision-makers to acquire a more profound understanding of the ecological impacts associated with diverse activities and decisions.

Keywords: Life Cycle Assessment, Photo catalyst, Metal-Organic Framework, MIL-101(Fe).

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1-Introduction

Metal-organic frameworks are crystalline hybrid organic-inorganic structures formed by the coordination of metal ions with organic compounds [1] Since metal-organic frameworks have a very high specific surface area and numerous pores, they find applications in various fields such as energy storage[2], gas adsorption[3], sensors[4], drug delivery[5], magnetic materials[6], and pollutant adsorption in aqueous environments[7]. As the utilization of MOFs continues to grow, understanding their environmental impact becomes crucial. The inherent versatility of MOFs, stemming from their unique structure and tunable properties, necessitates a systematic examination of their environmental implications[8]. Life Cycle Assessment (LCA) serves as a comprehensive methodology to evaluate the environmental footprint of MOFs throughout their entire life cycle, from raw material extraction to synthesis, utilization, and eventual disposal. Life Cycle Assessment (LCA) stands out as a standardized methodology for gauging the environmental footprint of a product. Identifying environmental issues through traditional methods is not comprehensive and often focuses on one aspect, Therefore, life cycle assessment is an appropriate method for assessing all environmental impacts of a product, leading to the quantification and examination of the resources and energy used, as well as the emissions and pollutants released into the environment. The International Organization for Standardization (ISO) has provided guidelines for the examination and study of environmental impacts, including ISO 14041, ISO 14040, and ISO 14042. These guidelines consist of four general stages, including goal definition, system boundary, impact assessment, and ultimately result interpretation[9]. This approach encompasses the entire life cycle of the product, commencing with the extraction of metals, minerals, power, etc. (cradle) essential for chemical production in its manufacturing process. It also considers the product's usage and includes accounting for its disposal (grave)[10]. This study delves into the complexities of LCA methodology applied to MIL-101(Fe), considering factors such as precursor production, synthesis methods, and end-of-life scenarios. Through a rigorous life cycle perspective, we aim to contribute valuable information to researchers, industries, and policymakers working towards sustainable materials development. and the environmental impact of this study was assessed using SimaPro 9 software and the ReCiPe H method at two levels, Endpoint and Midpoint. As MOFs play a pivotal role in various technological advancements, understanding and mitigating their environmental impact is integral to fostering a more sustainable future.

2-Methodology

2.1. Materials

Iron (III) chloride hexahydrate extra pure 98.0% assay ($FeCl_3 \cdot 6H_2O$, Sinochem, China), dimethylformamide extra pure 99.9% (DMF, Daejung, Korea), terephthalic acid for synthesis (H_2BDC), tetra-*n*-butyl orthotitanate for synthesis (TBOT, Merck, Germany) were utilized without further purification and of analytical grades. Deionized water was used for both the synthesis and the procedures.

2.2. Method

In this study, the environmental impacts of synthesized metal-organic framework nanomaterial MIL-101(Fe) were investigated at the laboratory scale, considering a functional unit of producing 1 kilogram of MIL-101(Fe) nanomaterials. The environmental impacts of the synthesized nanomaterials were assessed and evaluated using the ReCiPe H method. This method encompasses both midpoint and endpoint modeling approaches. By comprehensively assessing these factors, we aim to identify opportunities for improving the sustainability of MOF applications and guiding the development of eco-friendly synthesis and utilization practices. To synthesize the metal-organic framework, initially, 1.32 grams of iron (III) chloride hexahydrate were dissolved in 30 milliliters of dimethylformamide under constant magnetic stirring for half an hour at room temperature until a clear, slightly yellow solution was obtained. Subsequently, 0.50 grams of terephthalic acid were added to the solution, and it was stirred for another half an hour with a magnetic stirrer until the white particles of terephthalic acid were completely dissolved and no longer visible in the solution. Finally, the resulting mixture was transferred to a 50-milliliter Teflon container and placed in an autoclave, which was heated to 110 degrees Celsius for 20 hours. After the specified time, the Teflon container was removed from the autoclave and allowed to cool to room temperature. The final precipitate was transferred to another container and washed 7 times with dimethylformamide and 3 more times with ethanol using a centrifuge. Finally, it was dried under vacuum at 80 degrees Celsius. The resulting cream-colored powder with a slight orange tint was stored in a desiccator for use in subsequent stages [11].

3-Results and Discussion

The findings of this study and the SimaPro software output using the ReCiPe H method were analyzed at two levels. To confirm the structure of the synthesized nanomaterial, characterization techniques including SEM, XRD, and FTIR were employed.

3.1. Characterization

According to “Figure 1”, the average particle size of MIL-101(Fe) is around 1 μm, and their surface structure is octahedral, which is in line with previous research findings [12].

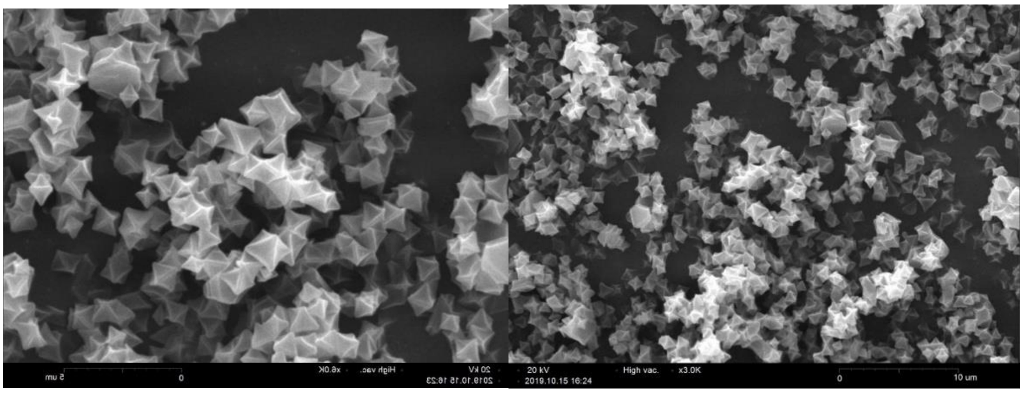

Figure. 1. SEM micrograph of MIL101(Fe)

The XRD analysis of MIL-101(Fe) depicted in “Figure 2”, revealed prominent diffraction peaks occurring at 2θ values of 1.00 (111), 2.40 (220), 4.55 (311), 8.45 (753), and 8.60 (822), thus providing confirmation of the successful creation of well-crystalline MIL-101(Fe) which are consistent with those found in a previous study[12].“Figure 3” The FT-IR spectrum of MIL-101(Fe) MOF displays distinctive peaks in its spectrum specifically, the peaks at 1656 cm-1 and 1506 cm-1 correspond to the asymmetric and symmetrical stretching vibrations of the carbonyl bond (C–O) found in the carboxyl groups (-COOH) within the MOF particle's structure. Furthermore, the peak at 1396 cm-1 can be attributed to the stretching vibrations of C–C groups present in the aromatic rings, while the sharp peak at 3400 cm-1 is a result of the stretching vibration of hydroxyl groups (-OH), indicating the adsorption of water molecules on the

surface. Furthermore, we can observe the bending vibration of the C–H bond linked to the benzene ring around the 749 cm-1 range. Lastly, the stretching vibration of the Fe–O bond in MIL-101(Fe) is detected at 550 cm-1[12].

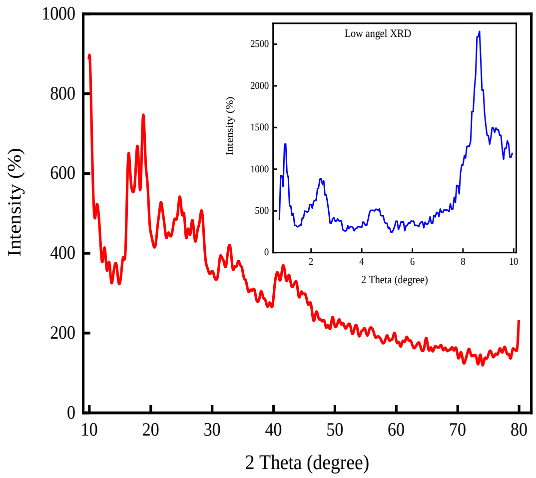

Figure 2. XRD spectra of MIL-101(Fe)

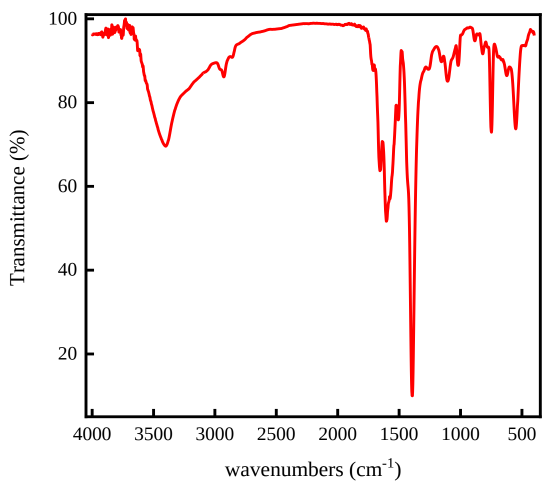

Figure. 3. FT-IR spectra of MIL-101(Fe)

3.2. LCA Results

The results of the environmental impact assessment obtained from the SimaPro software using the ReCiPe H method at two levels, Endpoint and Midpoint, are shown in “Figure 4”. Based on this, at the Endpoint level, the system has three impact categories, including human toxicity, ecosystem, and resources. The production process of one kilogram of MIL-101(Fe) metal-organic framework has the greatest impact on human toxicity, accounting for 49.86%, and has the least impact on the ecosystem. The ReCiPe H method at the Midpoint level includes 18 impact categories, which are displayed in “Figure.5” These impact categories are ranked from the highest to the lowest. According to the results obtained from the ReCiPe H method at the Midpoint level, the highest impact is attributed to Terrestrial Ecotoxicity and Marine Ecotoxicity, respectively. The most influential factors on Terrestrial Ecotoxicity and Marine Ecotoxicity include the use of dimethylformamide in the synthesis of the metal-organic framework structure.

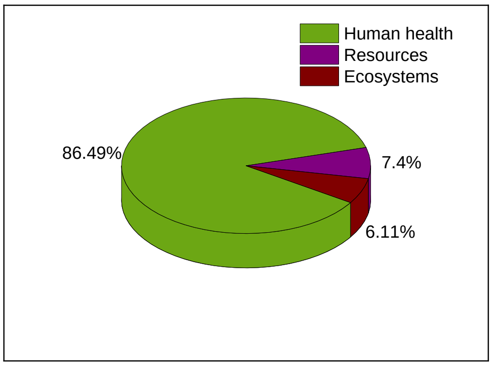

Figure 4.

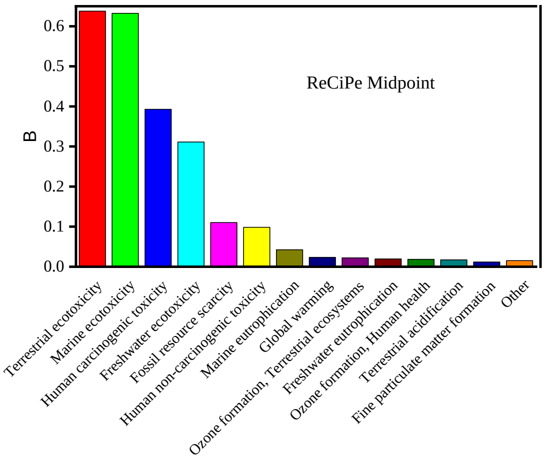

Figure 5

4. Conclusion

Based on the findings of this study, it can be concluded that the amount of dimethylformamide used for the synthesis of the metal-organic framework has the greatest environmental impact in all 18 impact categories. Based on the results, it is advisable to minimize the use of solvents when feasible, or to consider strategies for reusing them if complete elimination is not possible.

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