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

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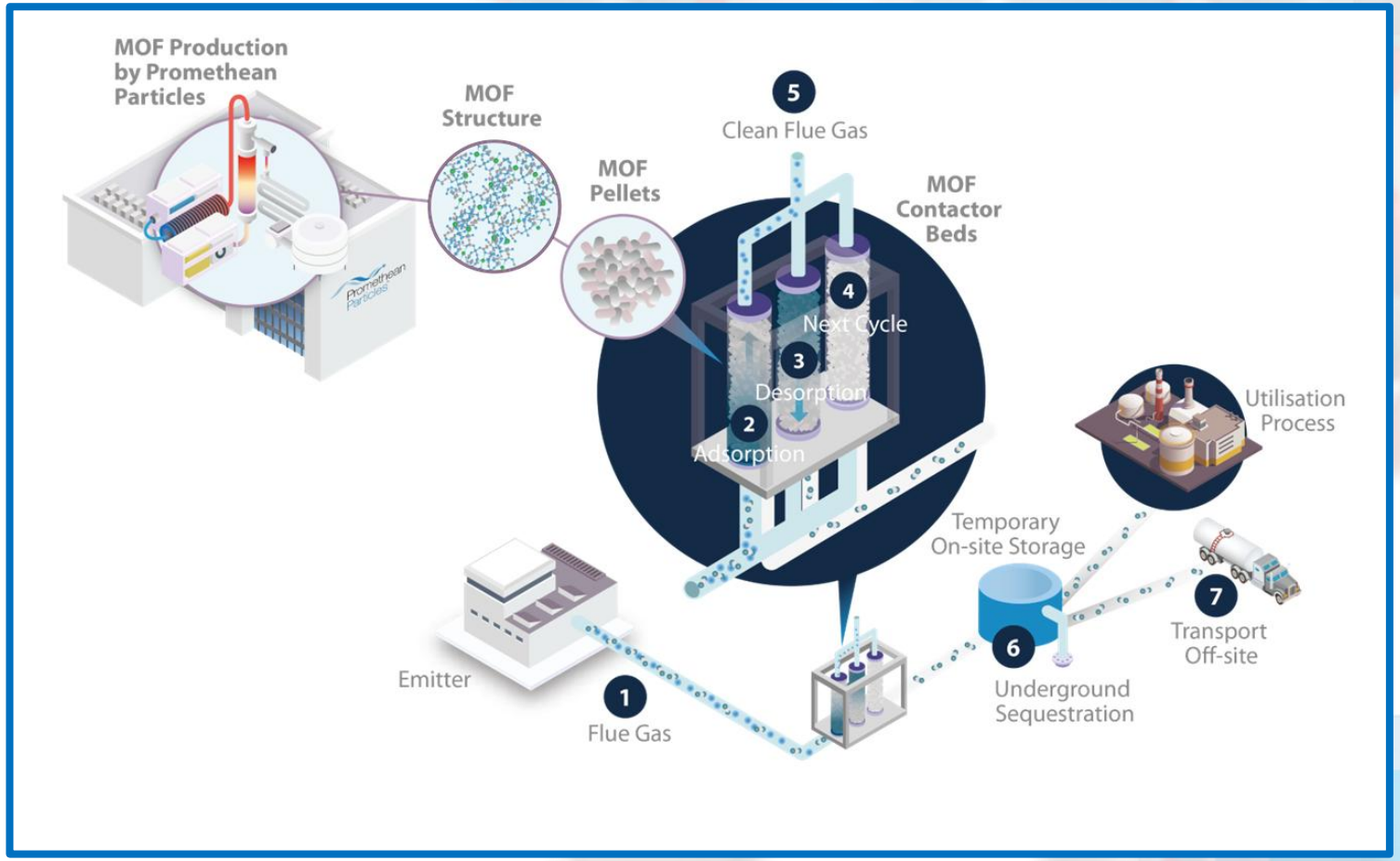
Objectives

- Analyse current **Carbon Capture technologies**, and highlight those that can offer potential improvements in effectiveness and emissions
- Use **LCA methodology** to assess the environmental impact of **metal-organic frameworks**, a promising group of solid sorbents
- Discuss the **limitations and challenges** of the analysis
- Analyse **key results obtained** and discuss how these **inform future developments** of the technology

Background

- CCS has been highlighted as a **‘priority technology’** for the UK’s energy transition
  - The benefits of the technology outweigh cost

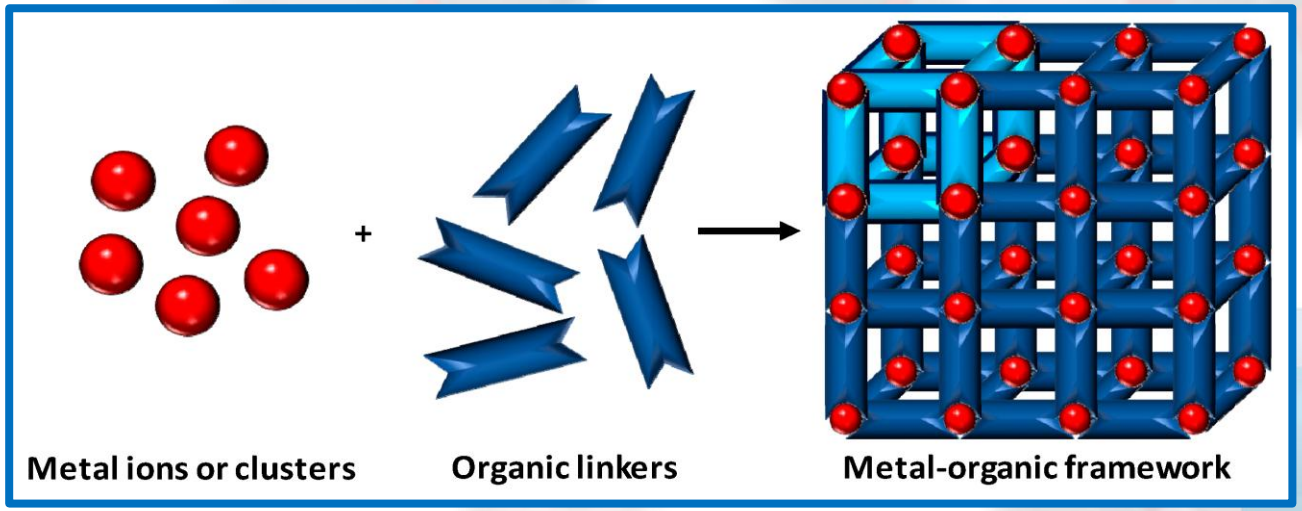
- The majority of CCS systems use **amine solvents** as their capture technology, but these have issues:
  - Solvent losses are **expensive**
  - **Corrosive** and **degrade** over time
  - **Handling and disposal** require care



https://prometheanparticles.co.uk/carbon-capture/

Metal-Organic Frameworks (MOFs)

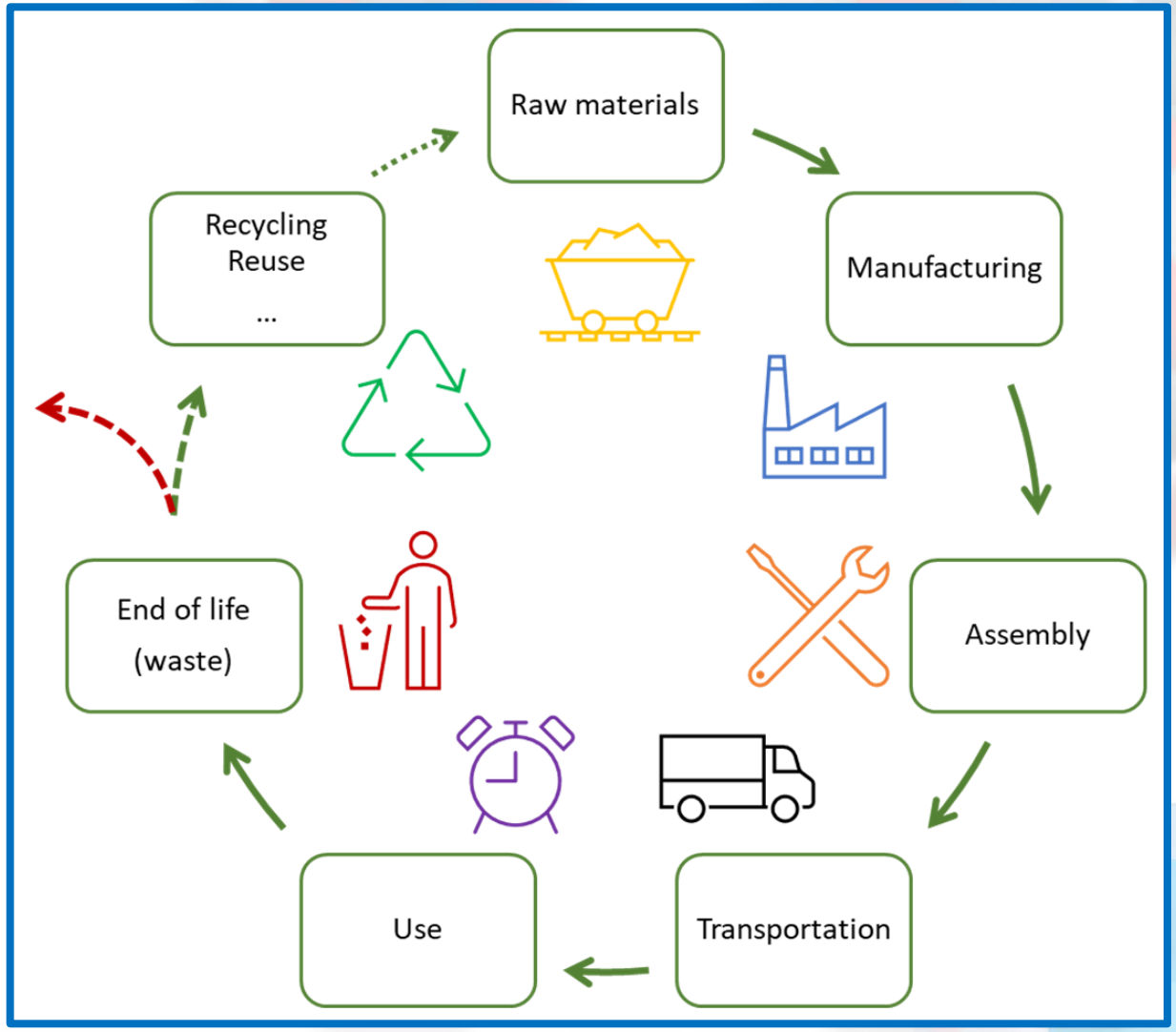
- **Solid sorbents** which 'trap' CO_2 from gas mixtures (e.g flue gas)
- **Infinite number of combinations** of metals and linkers
- May be more **environmentally friendly** and **energy efficient** than current market equivalents
- Identified as a promising technology for **Post-Combustion Carbon Capture**
- Very little research relating to the **environmental impacts** of MOFs (especially compared to amines)



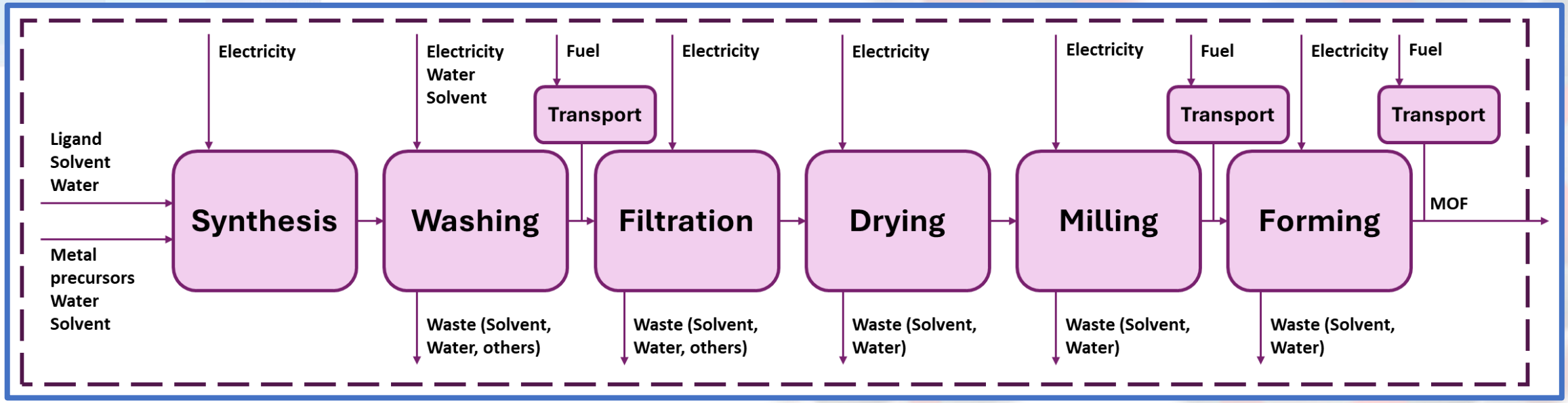
https://doi.org/10.3390/bios8040092

Life-Cycle Assessment (LCA)

- Methodology to **track a product or service** through its life cycle
- Most comprehensive method of modelling **complete cause-effect chain** of a process
- Numerous **software packages** to construct complex LCA models
  - **Extensive databases** containing information on process inputs
- Current LCAs on MOFs are limited
  - Most use **theoretical or simulation data**



Goal and Scope



- Assess the **Global Warming Potential (GWP)** of a selected MOF
- System Boundary (above) for the LCA study
- **Operational conditions** only (no setup parameters considered)
- Functional unit – **1kg of MOF** manufactured

Inventory

- **SimaPro** – LCA software used
  - Access to numerous databases that contain data on:
    - Production of **input materials** at various stages
    - **Electricity** consumption
    - Vehicle **transport** data
    - **Waste treatment** streams

- **ecoinvent** – most comprehensive database available for sourcing information
  - Many other databases pull their information from it

- Majority of quantities (input material amounts, operational times and conditions etc) come from **real data of company sponsor**

Inventory – Unavailable Materials

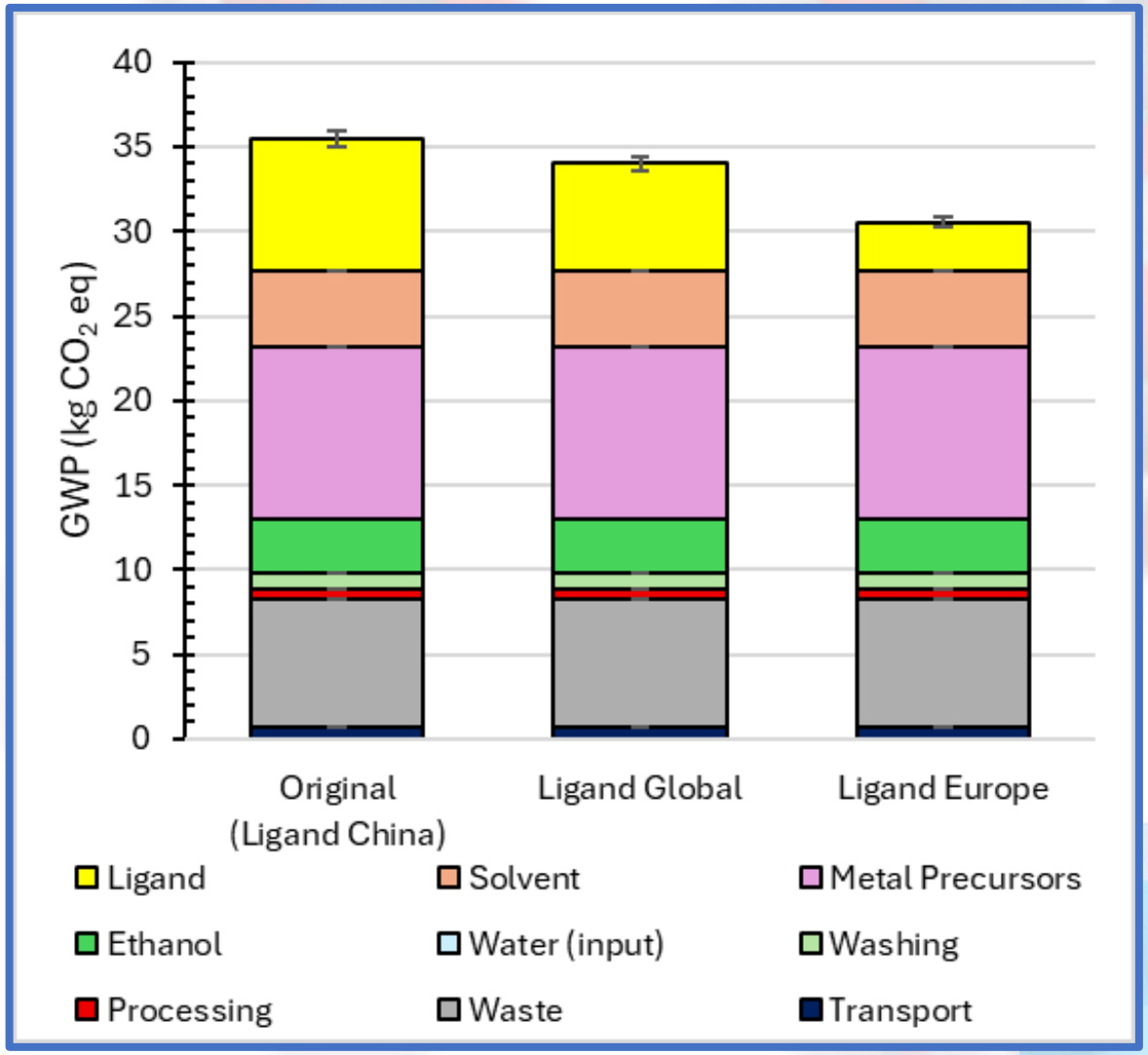
- Certain materials required have **no production data** in the available databases
  - Vital **metal precursors**

- Materials made ‘from scratch’:
  - Information on production **(stoichiometry)** gleamed from literature
  - Additional **energy requirements or waste products** determined
  - Relevant quantities found in database
  - **New ‘material’ created**

- Not as complex as database materials processes, so have higher uncertainty for validity of results
  - A **range of uncertainty** has been considered and shown in results where applicable to account for this

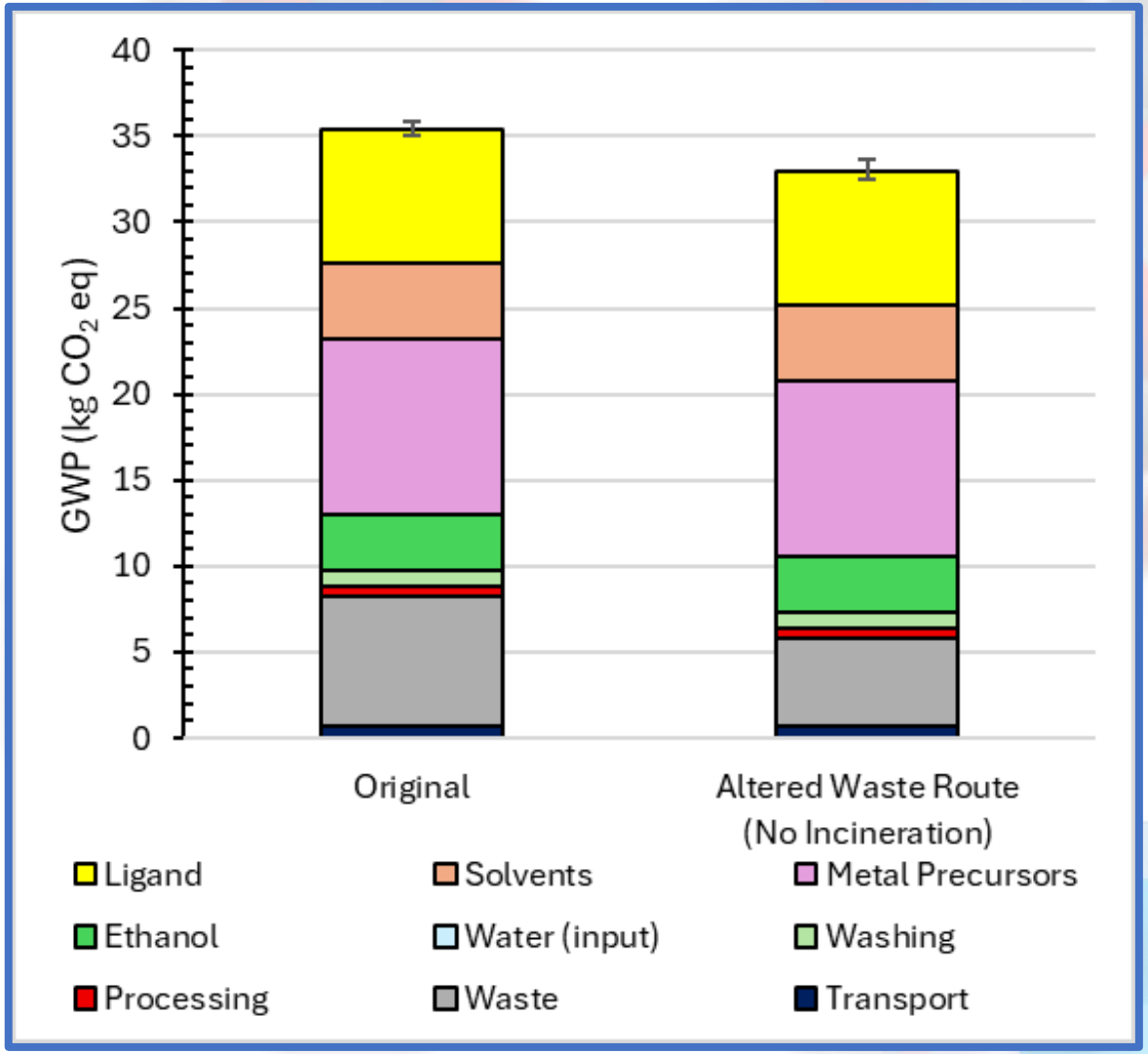
Impact Assessment – Region of Origin

- ecoinvent database contains **many variants** of most of its input processes
- Most input materials have **'Global' parameters**, which are made up of data from various countries
- Ligand used is sourced from **China**
- If the 'Global' version was used, the **emissions are lower**
  - Other sources aren't as polluting
- Sourcing this material from Europe instead would **reduce emissions considerably**, but carry different cost profiles



Impact Assessment – Waste Treatment

- Waste from most processes is taken away by **waste disposal companies**
- Waste treatment options in ecoinvent are **very limited**
  - Have had to group waste materials together and categorise them based on closest descriptor
- Waste sent away to be incinerated was instead taken **entirely to landfill**
  - **Minor improvement** to emissions
- **Spent solvent was largest waste contributor** to emissions
  - Recycling material would reduce this

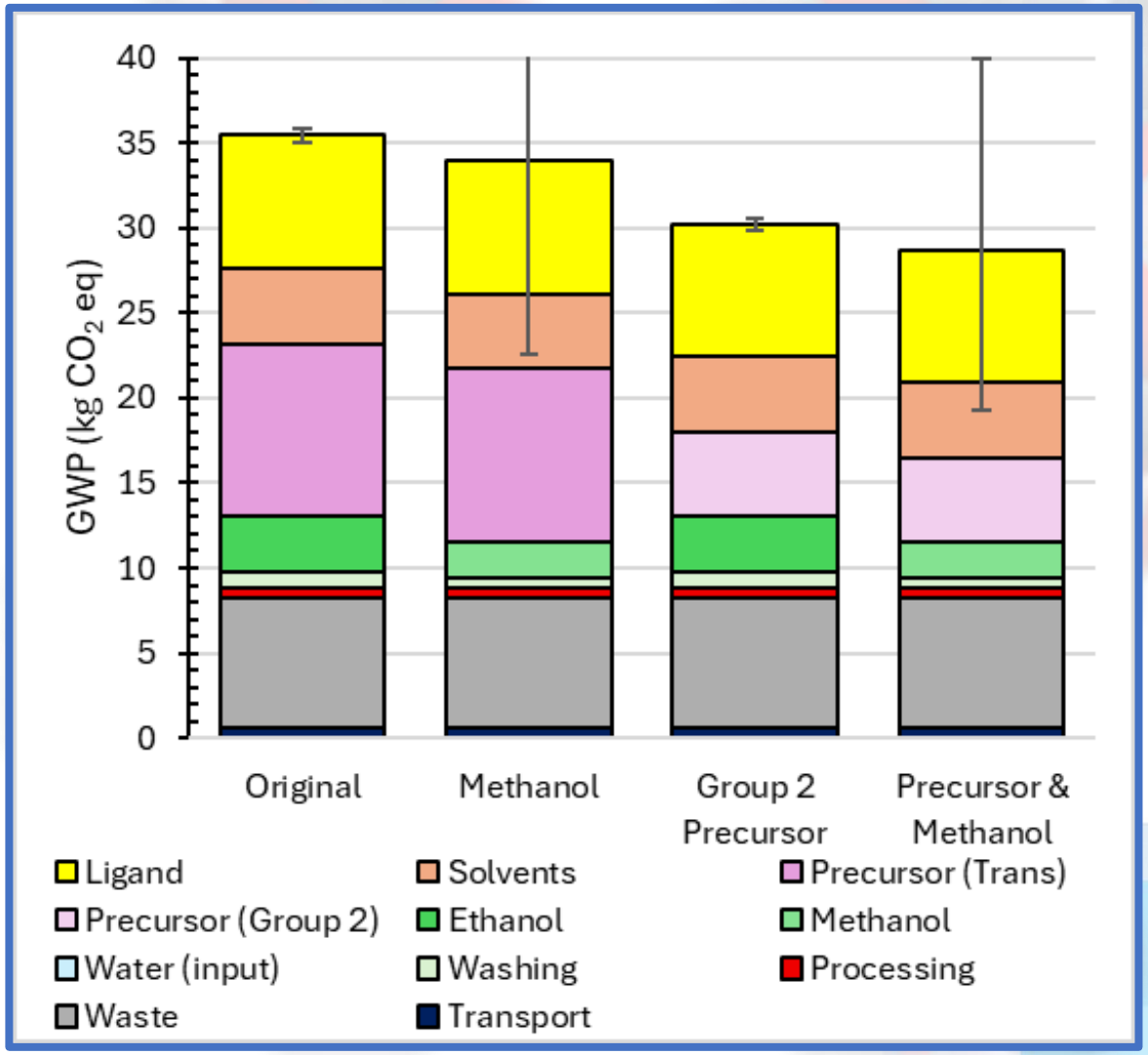


Impact Assessment – Altering Input Materials

- Input materials of the original MOF were directly **swapped with alternatives**:
  - Ethanol to methanol
  - Metal precursor – from a ‘transition’ metal to a ‘group 2’ equivalent

- **Larger uncertainties from methanol** as this is inputted twice and contributes to waste from all processes

- **Clear benefits** in reducing emissions from making these alterations
  - Methanol has different **hazard profiles** to ethanol, so requires different handling considerations to keep operators safe



Sensitivity Analysis (Input Materials)

- Used to **validate a computer model**, and show how minor changes in a variable can affect the outcomes of the factors investigated

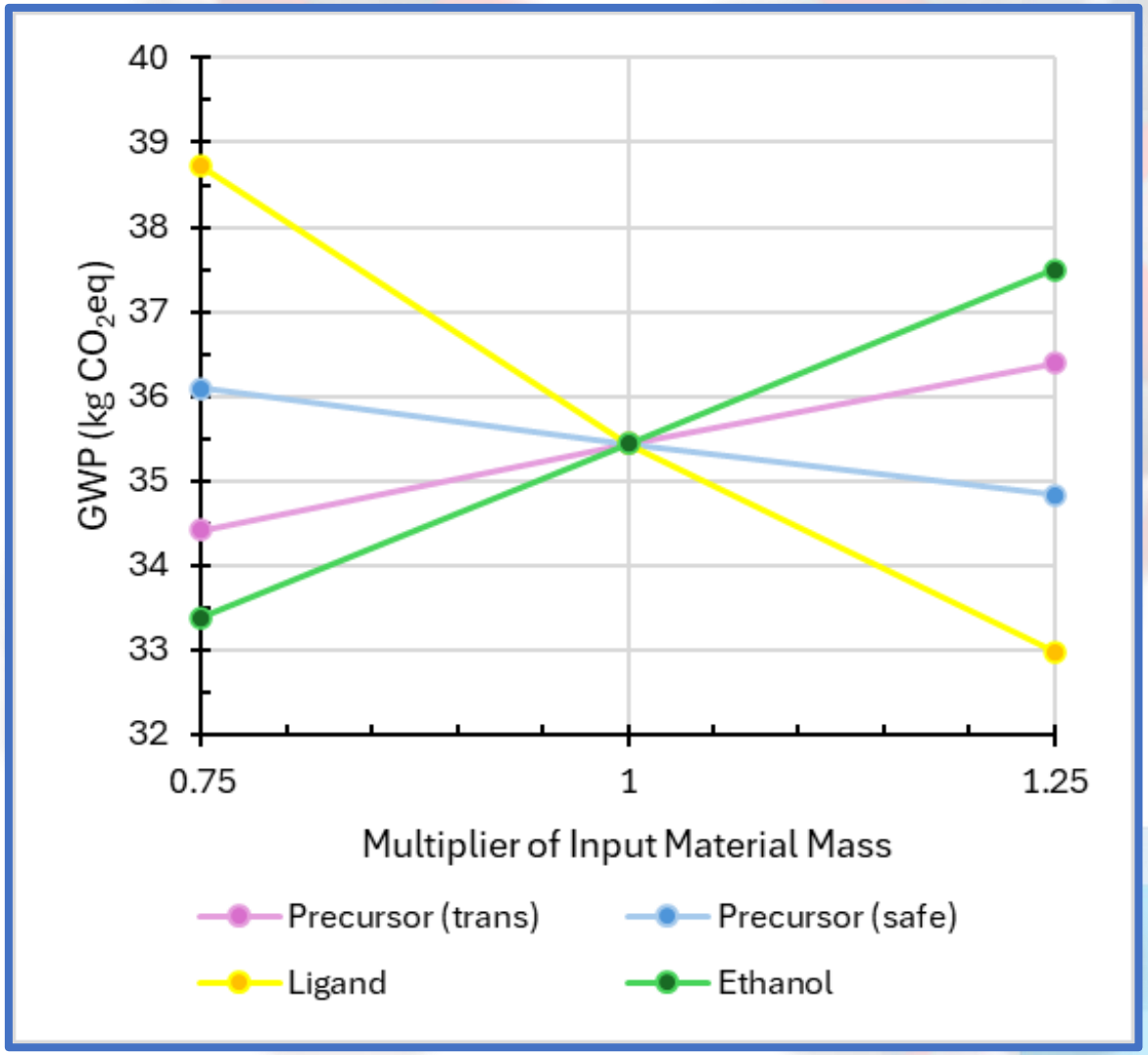
- Analysed how **changes to 'Original'** manufacture model affects results

- Quantities varied:
  - **Masses of Input Materials**
    - Ethanol and water added in Washing included
  - **Electricity Consumption** of all processes

- Values varied by **+/-25%**
  - Masses automatically vary throughout model

Sensitivity Analysis (Input Materials)

- Transition precursor and ethanol have **lower GWP** with less input mass
- Ligand and other (safer) precursor **increase GWP** with lower mass
- Reducing mass of **inputs reduces its own GWP contribution, but increases that of other inputs** (and vice versa)
  - Transition precursor has large enough decrease (or increase) to outweigh these changes
- Other inputs make **no major difference** to GWP results
  - Between **+/-0.4-0.7%**



Conclusions

- LCAs of MOFs are an **under-represented area of research** that not only provide vital information on their **environmental impacts** to assess the manufacturing process, but also offer insights and **highlight improvements** that can be made
- Swapping **metal precursors and solvents** used for synthesis show clear reductions in emissions
- Changing **region of origin** for ligands has a clear effect on results, so should be considered as a simple but important method of reducing impact
- **Recycling materials** instead of disposing will reduce waste treatment
- Further work is required **to clarify the accuracy of the study**, taking into account unknown factors such as materials not found in databases

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EP/S022996/1