PIM-MOF Composites for Use in Hybrid High Pressure Hydrogen Storage Tanks

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Introduction

- Hydrogen has been proposed as a potential long term sustainable energy storage solution, particularly in light duty vehicles.
- The current industrial state of the art in hydrogen storage for vehicles is compression [1]. However this technology presents some major issues:
  - Relies on pressures as high as 70 MPa to store enough hydrogen for a 500 km range [1].
  - Uses very expensive materials to achieve the lightness and pressure resistance required.
  - Fails to meet the U.S. DoE’s On-board Hydrogen Storage Goals [2].

One of the routes to hydrogen storage that is being pursued is storage by adsorption, which uses nanoporous materials to physically bond hydrogen, so increasing the volumetric density.

The aim of this project is to determine whether a composite material of the well known adsorbents PIM-1 and MOF-5 is feasible, and if so, if a hybrid tank featuring this material as a liner could provide a benefit over current hydrogen storage solutions.

Metal Organic Framework (MOF-5)

- MOF-5 is composed of ZnO\textsubscript{4} clusters attached by 1,4-benzenedicarboxylate linkers.
- Has isoreticular topology (alternatively known as IRMOF-1).
- Industrial interest from Ford, General Motors, BASF [4].
- Rouquerol BET surface area of 3508 ± 129 m\textsuperscript{2} g\textsuperscript{-1} (N\textsubscript{2} isotherm at 77 K).
- Highly microporous pore size distribution; Horvath-Kawazoe (HK) model gives a modal pore size of 0.9 nm.

Polymer of Intrinsic Microporosity (PIM-1)

- Bright yellow powder is soluble in polar aprotic solvents (e.g. chloroform, THF).
- Initially synthesised using the optimised method of Song et al. [5], although this resulted in a material that formed brittle, cracked films (M\textsubscript{w} = 9765 g mol\textsuperscript{-1}, PDI = 2.66).
- Synthesis using the original method of Budd et al. [6] resulted in a better quality PIM (M\textsubscript{w} = 76261 g mol\textsuperscript{-1}, PDI = 2.53).
- TGA under N\textsubscript{2} flow determines thermal stability up to ~430 °C.
- Helium pycnometry gives skeletal density of 1.24 g cm\textsuperscript{-3}.
- Rouquerol BET surface area = 621.2 ± 3.0 m\textsuperscript{2} g\textsuperscript{-1} (N\textsubscript{2} isotherm at 77 K).
- Pore size distribution reveals more than half the pore volume is microporous (HK total pore volume = 0.463 cm\textsuperscript{3} g\textsuperscript{-1}).

Future Work

- Synthesis of PIM-1/MOF-5 composite (in progress).
- Continued analysis of adsorbent properties of materials, including fitting to a model developed at the University of Bath to determine parameters such as adsorbate density and pore volume.
- Analysis of mechanical (tensile and flexural moduli), thermal (specific heat capacity, thermal conductivity) and binding properties of materials.
- Develop ‘rule of mixtures’-style correlations between composite content and properties.
- Design of hybrid hydrogen storage tank with a composite liner.

References