Optimization of greener epoxidation process catalysed by polymer-supported Mo(VI) complex *via* response surface methodology

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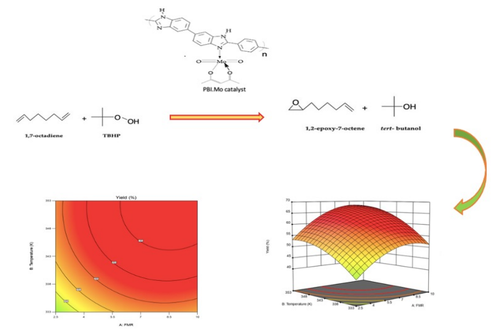
Motivation



Greener and efficient process

Reduce manufacturing costs by reducing waste products and making the process environmentally friendly.

Important raw materials

Epoxides can be transformed into plasticisers, perfumes, food additives pharmaceutical drugs etc.

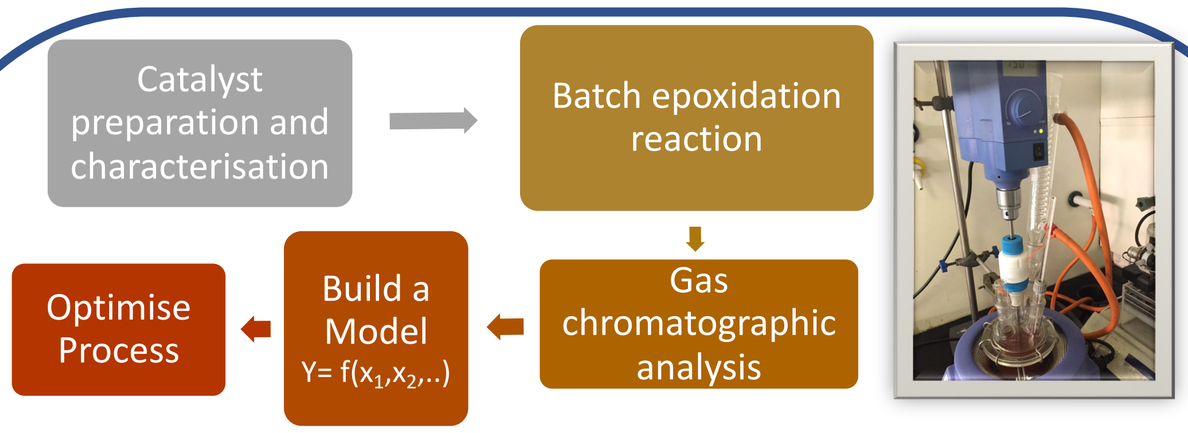
Biochemical and physiological effects

1,2-epoxy-7-octene can act as an antioxidant and found to have anti-cancer properties.

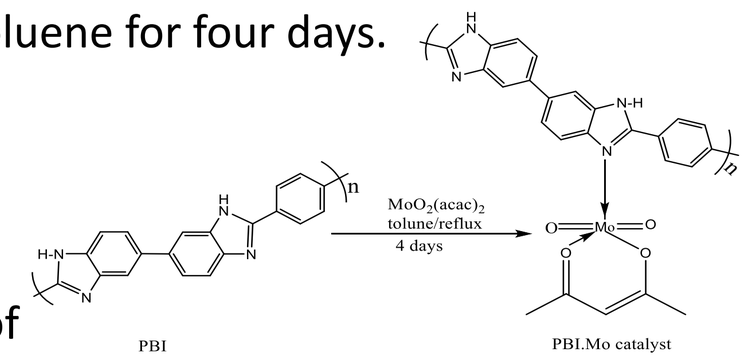
Aim

To synthesise 1,2-epoxy-7-octene using polymer-supported Mo catalyst and evaluate the catalytic efficiency in batch epoxidation reaction *via* response surface methodology.

Methodology



- PBI resin was reacted with Mo $O_2(acac)_2$ in the stoichiometric ratio of 2:1 in toluene for four days.



- Batch epoxidation of alkenes with TBHP in the presence of PBI.Mo catalyst was conducted in a 0.25 L jacketed four neck glass reactor.
- Applied design of experiments technique to optimise reaction parameters.

Results

❖ Catalyst preparation and characterisation

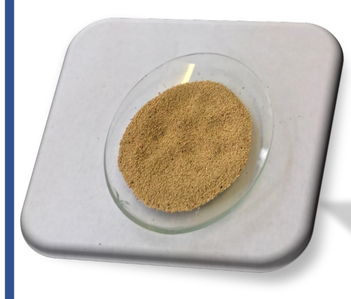
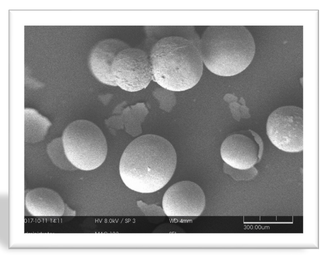
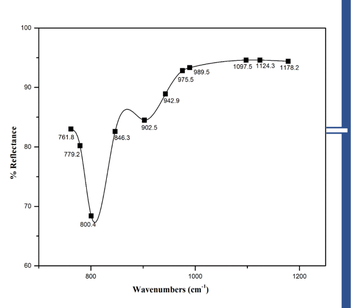


Image of PBI.Mo catalyst

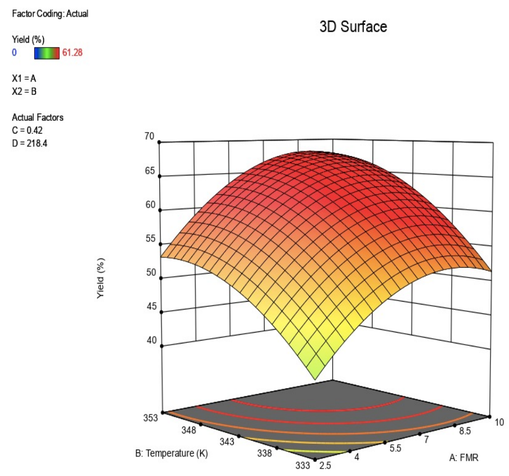


SEM image of PBI.Mo catalyst



FTIR spectra of PBI.Mo catalyst

❖ Optimisation study



3-D graph showing the effect of feed molar ratio and temperature on epoxide yield

- The numerical optimisation technique concluded that the maximum yield that can be reached is 66.22% at a feed molar ratio of 7.97:1, reaction temperature 347 K, 0.417 mol% catalyst loading, and reaction time of 218 min.

Conclusions

- PBI.Mo complex could be used as an effective catalyst for a greener and more efficient epoxidation of 1,7-octadiene with TBHP as an oxidising agent.
- Characterisation of PBI.Mo catalyst confirms the presence of Mo(VI) metal centre in the polymer resin.
- The optimisation result has been validated experimentally resulting in an epoxide yield of 64.97% with a relative error of 1.92%.

References

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