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Reaction Network Determination of Methane Pyrolysis through Data Science.

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Introduction

Hydrogen production via hydrocarbon reforming using various techniques is a research focus for many groups. Pyrolysis is one of them where hydrocarbon is decomposed with out water or oxygen into hydrogen and carbon. TCD of methane is a fully green single step technology for producing hydrogen and nano carbon.

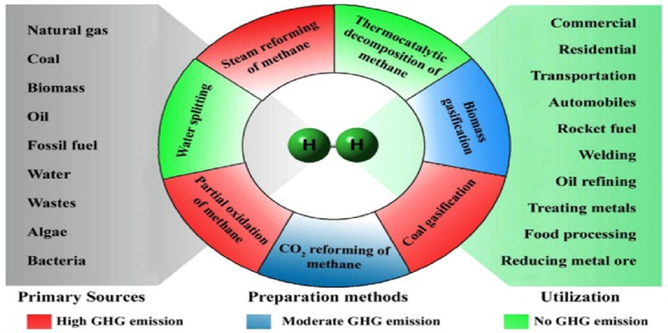


Fig. 2. Schematic representation of the sources, preparation methods and utilization of hydrogen.

Goals and Objective

*PLR Studies on Pyrolysis of Methane.

* Analysis of the collected data to understand the reaction network

* Use of appropriate machine learning tools to analyze data.

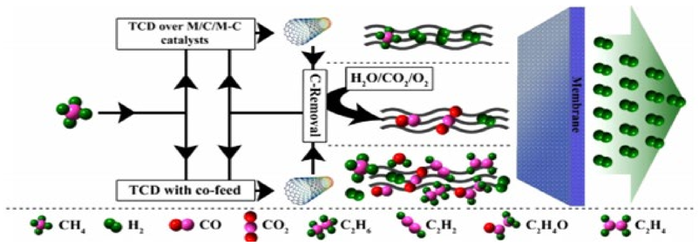
Methods/Materials

*Primary literature Review studies on 40+ relevant articles/reviews. Still ongoing. process.

*Collected data with different parameters like catalysts, temperature, deactivation, yield, flow rate etc.

*Use of software to analyze data in progress.

Results



Ref	Catalyst	Weight(g)	Flow rate	Max conversion(%)	Yield (H2 %)	Stability and acivity maintained @	
						Temp(C)	Time(h)
1	Ni	0.04	45000(1)	35	NA	650	130

CH_4--->C+ $2H_2$

A variety of metal catalysts studied.

Methane to CH_3OH/ CH_3COOH yet to be optimized.

Kinetic point of view, temperature and pressure are the determining factors for Hydrogen production (yield).

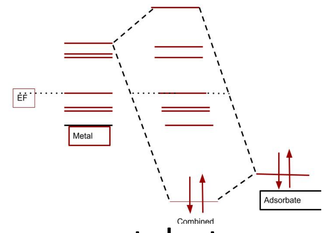
The rate determining step is the C-H bond breaking.

A wide range of activation energies are reported based on experimental conditions.

Due to high bond energy(440kJ/mol)and symmetry CH_4 is very inactive. Pyrolysis involves 5 steps (details in mechanism).

Proposed Mechanism

Binding of hydrocarbon to catalyst leaving it to adsorbent stage where transfers electron density occurs.



1. Chemisorption of methane on catalyst

2.$(CH_4)_g$ ---->$(CH_3)_a$+$(H)_a$

3.$(CH_{3-x})_a$ ---->$(CH_{2-x})_a$+$(H)_a$

4.2$(H)_a$ ---->$(H_2)_g$

5.Carbon aggregation into encapsulated carbon

Conclusion

*Pyrolysis is considered to be the most reliable and beneficial method for H2 production

*Achieves GHG free H_2 production. The byproduct C can be easily sequestered

*Further research on using the nanocarbon side product directly into technology to avoid GHG produced during purification.

* Use of appropriate machine learning tools(LR, SVR, ESSR, RFR, LASSO etc.) to analyze data and understand the reaction net work.

Acknowledgements & References

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2. 2.Holidays, J.D, Hu, J. King D.L, Wang Y. An overview of hydrogen production technologies, Catalysis Today, 2009, 139, 244-260.