Methane Pyrolysis Simulation: An Analysis of Products Produced Through Thermal Decomposition

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Introduction

Pyrolysis is an up-and-coming technology that involves the thermal decomposition of natural gas to produce fuels. This project specifically looks at methane or CH4 as the feedstock gas in this process. Ideally, methane pyrolysis gives a product of various kinds of carbon that can be used for production, hydrogen that can be used as an energy source, and there are no carbon emissions like the ones that come with the traditional burning of fossil fuels. The primary means for current hydrogen production (over 95%) is through SMR (steam methane reformation) which uses catalysts and water to get desired products, which often produce CO_2 emissions. Methane pyrolysis has an advantage here as there are no carbon emissions and the energy needed is nearly half of what is required for SMR [1].

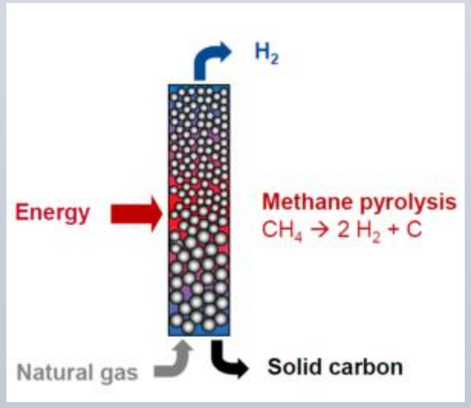
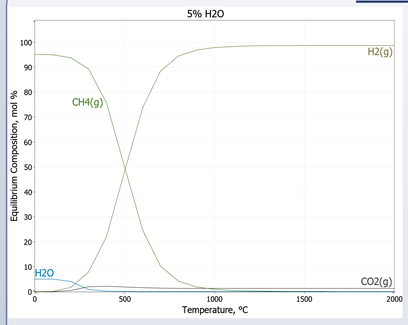


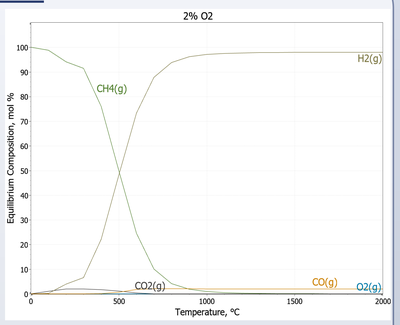
Figure 1. Image of a methane pyrolysis process

Objectives

- Use HSC Chemistry to simulate reactions and species in various percentages
- Calculate selectivity and show products produced under various conditions

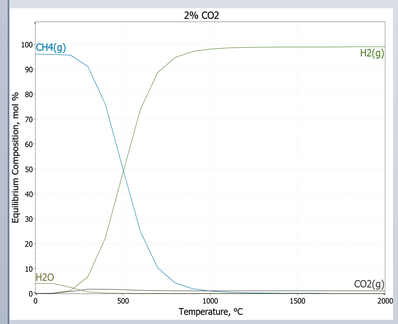
Results

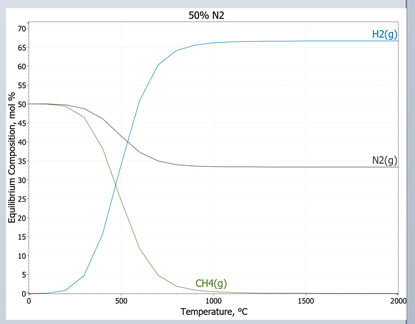




- Effect of presence of 5%, 2%, 1%, 0.1%, 0.01% H2O
- Products: H2 and CO2
- 0.01% yielded the best selectivity

- Effect of presence of 2%, 1%, 0.1%, 0.01% O2
- Products: H2, CO
- 0.01% yielded the best selectivity





- Effect of presence of 40%, 20%, 10%, 5%, 2% CO2
- Products: H2 and CO2
- 2% yielded the best selectivity

- Effect of presence of 50%, 65%, 80%, 95% N2
- Products: H2 and N2
- 50% yielded the best selectivity

Materials and Methods

Equations used:

CH4 → C + 2H2

CO2 + 4H2 → CH4 + 2H2O

CO2 + H2 → CO + H2O

CH4 + 2O2 → CO2 + 2H2O (CO may also be present)

CO2 + 2H2 → C + 2H2O (combination of equations 1&2)

Species list: C(s), CH4(g), H2(g), CO2(g), CO(g), O2(g), H2O, N2(g)

Conclusions

In conclusion, adding CO2, H2O, or O2 to our decomposition reaction gave us a composition of mostly hydrogen with CO2 or CO being the primary products at high temperatures where the reaction takes place. The reaction with no carbon dioxide emissions was the nitrogen and it has the lowest selectivity of the bunch. Compared to the original decomposition reaction, the presence of water, oxygen, or carbon dioxide significantly upgrades how much hydrogen gas is produced with the composition for the original being around 67% H2 and the new reactions being close to 100% hydrogen product. Further research into using molten metal reactors will show us how this process works in a real-life scenario and if it's feasible to offset possible emissions with what the reactor produces as well as being competitive with SMR [2]. Overall, the methane pyrolysis process can be upgraded to produce more hydrogen to use in fuel or industry with minimal undesirable species.

References

[1] *R&D Opportunities for Development of Natural Gas Conversion Technologies*. United States Department of Energy, Nov. 2017.

[2] Pérez, Brandon José Leal, et al. "Methane Pyrolysis in a Molten Gallium Bubble Column Reactor for Sustainable Hydrogen Production: Proof of Concept & Techno-Economic Assessment." International Journal of Hydrogen Energy, Pergamon, 3 Dec. 2020, www.sciencedirect.com/science/article/pii/S0360319920342816.

Acknowledgements/Contact

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