Executive Summary

In our capstone project *Pyrolysis for Making Hydrogen and Biochar from Biogas*, our goal is to develop a reaction system for methane pyrolysis, which is a chemical reaction that thermally decomposes methane (CH4) to hydrogen (H2) and solid carbon (C) with the help of catalyst. [motivation] Although hydrogen is a clean energy source, current industrial production of hydrogen leads to high CO2 emissions. Also, biogas, mainly composed of methane, is a powerful greenhouse gas that contributes to global warming. Therefore, we study pyrolysis to utilize greenhouse gasses to produce a clean energy source without carbon emissions. At the preliminary of this research project, we decided to develop a detailed design for the main reaction chamber that promotes the H2 yield with mechanical design.

This pyrolysis reactor was requested to be designed by our sponsor Praneet Chotalia, for lab scale research of the creation of hydrogen gas.

The requirements were developed after thorough research to establish what would be important for a pyrolysis reactor. The most critical requirements include first the high methane conversion rate, as we need to achieve at least a 60-70% conversion rate, the percentage of methane converted to hydrogen and solid carbon, which was requested by our sponsor, Praneet.

The concept generation process started with the entire reaction system with 12 sub-systems, which created a collection of design challenges instead of just one. Due to the time and cost limitation of this project, for the final design, we closed in on the reaction chamber where the pyrolysis reaction happens. We selected a two-stage continuous stirred-tank reactor (CSTR) as our selected concept. Two-stage means both molten and solid catalyst are used so the methane could react with the catalyst for two times; the CSTR is a type of chemical reactor that provides constant stirring, allowing the reactants to be uniformly distributed, allowing the reaction to advance at a uniform rate, and promoting conversion rate, which is required for our reactor. Thus, we find the two-stage CSTR to be the most suitable liquid/gas mixing system for our project.

Further developed after this, was a Rushton style mixer to enable this reactor to mix the catalyst effectively. To model whether this mixing of the molten catalyst would be useful, a COMSOL model was created to determine the effect this mixing would have on the conversion rate of the methane. This model predicted an increase in conversion rate of over 20%, getting us to the desired conversion rate between 60-70% in our requirements. We examined sensitivity of the model to confirm that the parameters examined behave how they were expected to.

For future work, the kinetic equations modeling the behavior of the conversion rate relating to the molten catalyst should be edited through careful research. Additionally, to fully verify the results of our design, a physical prototype must be developed. While our simulated model suggests there would be an increase in conversion from mixing, there cannot be certainty of this until it is properly validated. Our research focused on continuous verification, so our design still lacks in areas where validation is necessary.

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Pyrolysis for Making Hydrogen and Biochar from Biogas

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Revised Abstract

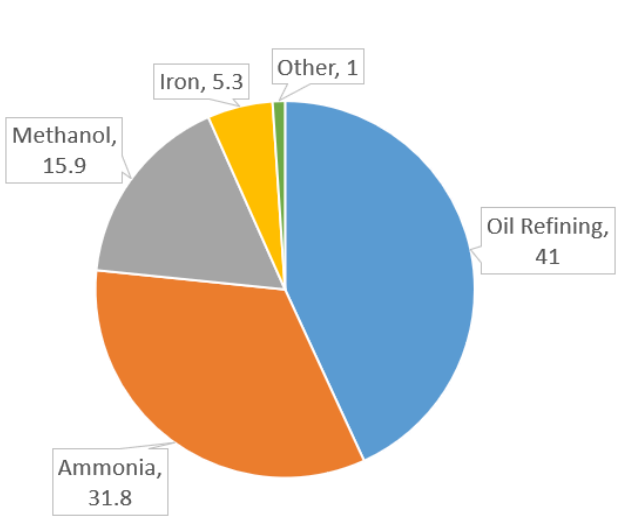
In order to develop greener methods of producing power, the aim of this project is to create a methane pyrolysis reactor design to produce Turquoise Hydrogen with sustainably sourced biogas. Methane pyrolysis avoids the pitfalls of other hydrogen generation methods by avoiding CO2 emissions during the reaction process, while also yielding solid carbon which, depending on the quality of carbon produced, can be a valuable resource. To produce a valuable reactor, considerations must be made for increasing yield, increasing catalyst lifetime, and safe storage of hydrogen.

Project Introduction, Background, and Information Sources

Introduction and Background

This methane pyrolysis project aims to design a reactor that makes advancements in our ability to convert biogas into usable hydrogen, that is safe and maximizes the yield of both hydrogen and carbon. The sponsors of this project are the University of Michigan and Praneet Chotalia (graduate student at the University). This project exists in response to the growing demand on hydrogen and the common goal of zero net emission of greenhouse gasses.

Hydrogen is an important ingredient for industries. In 2022, a total of 95 million tons of hydrogen was produced in the world, where 41 Mt of hydrogen was used for oil refining, 31.8 Mt was used for ammonia production, 15.9 Mt was used for methanol production, and 5.3 Mt was used for direct reduced iron (*Figure. 1*). The production of 95 Mt of hydrogen in 2022 was dominated by fossil fuels. 62% of it was produced from natural gas without carbon capture (which produces 10~13 kg of CO2 per kg of H2), 21% was produced from coal (which produces 22~26 kg of CO2 per kg of H2), 16% was produced as a byproduct from petroleum or chemical industries (*Figure. 2*). For comparison, natural gas with carbon capture will only produce 1.5~6.2 kg CO2 per kg of H2. [1]



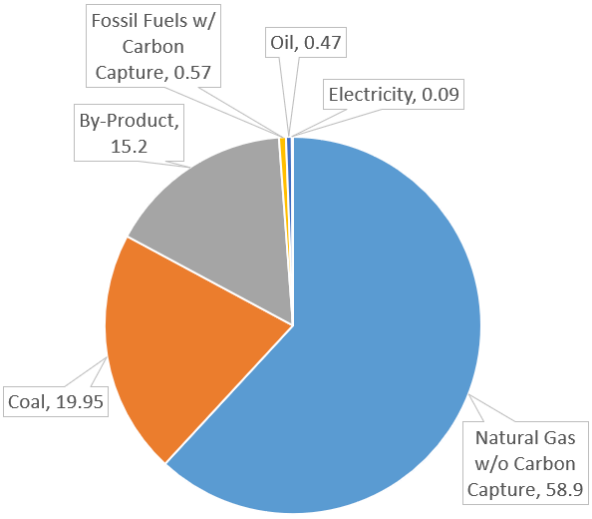


Figure 1 (left): Hydrogen Usage in 2022 (Units: Mt) [1]
Figure 2 (right): Hydrogen Production by Methods in 2022 (Units: Mt) [1]

Hydrogen is sometimes considered as a clean energy form because its combustion produces nothing other than water. However, the problem lies in the production process. As mentioned above, most of the hydrogen is produced from natural gas (methane). The 2 most common methods for that are partial oxidation and steam methane reforming:

Partial Oxidation of Methane Reaction

$$CH_4 + \tfrac{1}{2}\, O_2 \rightarrow CO + 2H_2$$

Steam-Methane Reforming Reaction

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Both methods will also produce carbon monoxide which will eventually become carbon dioxide. This overlooked carbon emission makes hydrogen less "clean" than how it seems. In Figure 3, which compares several hydrogen production technologies, Methane Pyrolysis has the smallest carbon footprint, Steam Methane Reforming has a footprint that is twice as large.

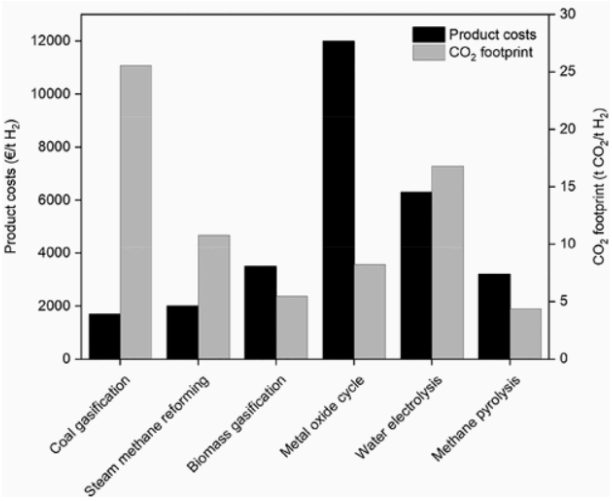


Figure 3: The Carbon Footprint of Hydrogen Producing Technologies vs Product costs[2]

Carbon emission, or greenhouse gas emission, has brought up environmental concerns. By 2022, greenhouse gas emissions have already led to 1.1 C global temperature increase, compared to pre-industrial levels. The act of net zero emission by 2050, which involves more than 130 countries covering over 88% of global greenhouse gas emissions, is to keep this temperature increase below 1.5 C. Considering the possible application of hydrogen to replace fossil fuels in end uses such as heavy industry, long-haul transportation, and seasonal energy storage, the global hydrogen demand is predicted by the *Hydrogen Council and McKinsey & Company* to be 660 Mt in 2050 when zero net emission is to be achieved. Hydrogen will have the potential to contribute to 10% of that goal. [3]

Pyrolysis as a process, has existed since ancient times, with people in ancient egypt using a primitive form of pyrolysis to produce materials for burial. [4] The process specifically heats up a material until it is above the temperature for decomposition. This breaks down the material into its parts. Through the years as humanity has desired to break down components into more distilled products, designs for reactors to optimize the process have grown more complex. Methane pyrolysis as a process has been conceptualized since the 1960s, but only within the last 20 years has research focused on it as a source of relatively green or Turquoise Hydrogen. [5] When carbon dioxide is produced in the process, hydrogen production is referred to as Blue or Gray hydrogen.[6]

In order to decarbonize the hydrogen industry and further decrease greenhouse gas emission, methane pyrolysis can be used as an alternative for the aforementioned 2 methods of producing hydrogen. The

process is straightforward: at high temperatures (typically 1100~1200 C), methane decomposes into hydrogen and solid carbon:

$$CH_4 \rightarrow C + 2H_2$$

Depending on different reaction conditions, the solid carbon can have different forms such as carbon black, carbon fiber, carbon nanotube, etc. They all are useful in other industries while not being converted into carbon dioxide. To actually aid decarbonization, we want to look into this process as being used for future renewably produced biogas, which does contain other adulterants within it, which is not shown with the more easily digestible chemical formula. Adulterants common in biogas are carbon dioxide, water vapor, siloxanes, hydrogen sulfide, and volatile organic compounds (VOCs). The carbon and hydrogen produced in our decomposition of the methane can bond with these adulterants and produce harmful chemicals such as carbon disulfide, and work against the aim of our project and produce more carbon dioxide. There is currently not much literature on a mixture of adulterants and methane, so our focus is going to be on improving the existing technology for methane pyrolysis.

The ultimate goal of our sponsors is to design and build a complete lab-scale reactor which runs on biogas containing methane, carbon dioxide, and some impurities. This will take years to complete. Currently at the initial stage of the project, we are assuming the biogas is filtered and the reactor will be fed with pure methane.

Benchmarks

Methane pyrolysis is a relatively new technology in trying to broaden the availability of hydrogen. There are a few commercial players within the field of hydrogen pyrolysis. Monolith Materials, Hazer Group, Aker Solutions, and BASF are the major commercial players for more large-scale production of hydrogen in this manner. Currently, the field is largely the focus of academic research versus commercial, there is a massive amount of variety within the academic space on how these reactors are being built driving progress [5]. Therefore, our benchmarking data largely comes from research papers on lab-scale experiments. Since our objective is also to design a lab-scale reactor, we can directly reference these benchmarks when designing our own.

To break down the base process of a methane pyrolysis reactor, we need to look at how the methane is being processed on a practical level within a generic reactor. First for the reactor, the methane is preheated to be able to undergo the process of the actual reactor, if it is not preheated it may not be able to get up to temperature for the decomposition process to occur within the chamber. [7] This initial heating is the pre-treatment of the methane before it enters the chamber. Then, methane is pumped into the chamber for the reaction. There is a source of heat applied to the chamber where the reaction is taking place, as the methane must be heated to an appropriate temperature to undergo decomposition into its components, hydrogen and carbon. This heat can be applied within the chamber, or around the reactor. A few standard methods of heating are plasma pyrolysis, microwave pyrolysis, and electric heating. Plasma pyrolysis simply is a method of using a plasma torch or plasma pulse from the center of the reactor to heat the methane. Using the plasma pulse method has the benefit of heating the methane itself, without putting the entire apparatus at a high temperature. Plasma torches still produce a higher temperature [8]. Microwave pyrolysis uses the relatively simple technology of microwaves to impart heat into the system. This is not a microwave as thought of for cooking purposes, but a device that can produce lab use microwaves to heat the chamber in a controlled way where precise temperature measurements can be made. Electric heating

can use the principles of resistance or inductance to produce a heat on the gas.[7] This chamber being heated is pressurized, but at a very low pressure. In Figure 4, the highest methane conversion rate, the percentage of methane converted to hydrogen and carbon, is reached at lower temperatures. This reduces the amount of energy used in the form of heat to create this hydrogen gas.

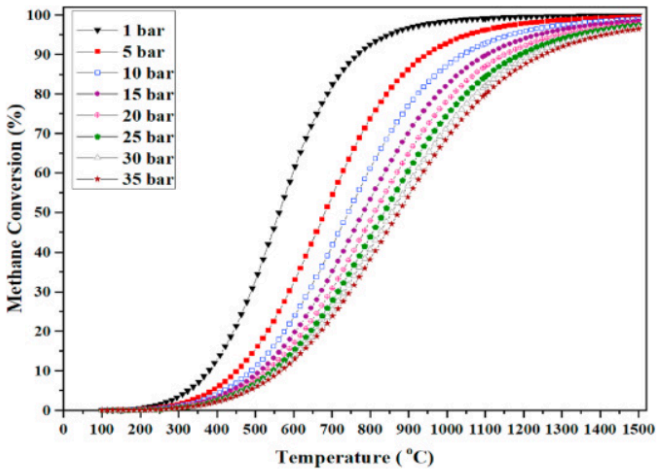


Figure 4: Methane Pyrolysis at 1-35 bar, Methane Conversion Percentage vs Temperature [9]

To get the pyrolysis reaction to occur at a lower temperature, catalysts are used, from Figure 6 depicting the operating temperature ranges of three different types of catalysts and non-catalytic pyrolysis, pyrolysis that does not use a catalyst. This figure shows that reaction temperatures in reactors with catalysts are much lower showing the range of the non-catalytic section of the graph.They also allow researchers to increase the yield of the hydrogen from the reaction depending on the catalyst being used as depicted in Figure 8. These catalysts exist in a variety of forms as shown in Figure 7. They are held in place with membranes within the chamber where the methane undergoes the reaction process as shown in Figure 5. These membranes are made from certain types of non-reactive metals or ceramics that methane is able to diffuse through, these membranes are commonly fused to the sides of the chamber through welding. Not all reactors use catalysts, as the main requirement for decomposition is that the methane is hot enough to reach the point at which it separates into its components of carbon and hydrogen. [7]

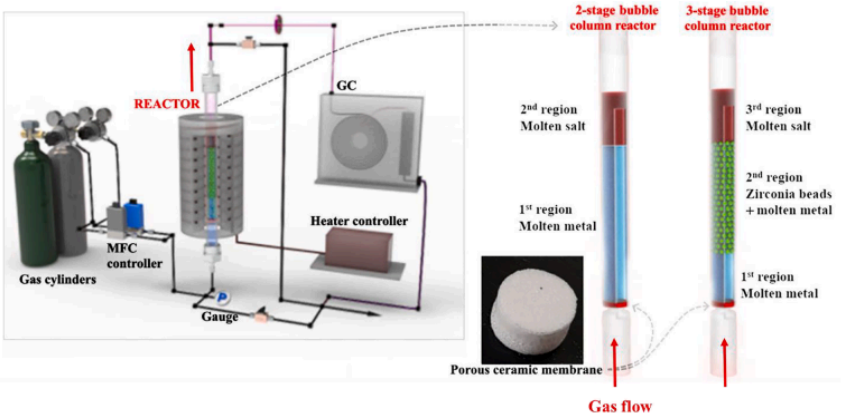
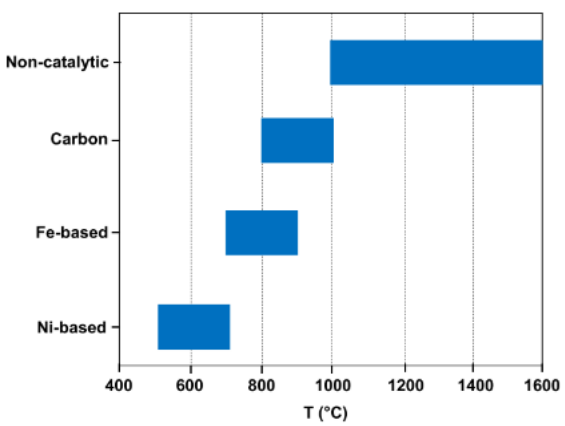
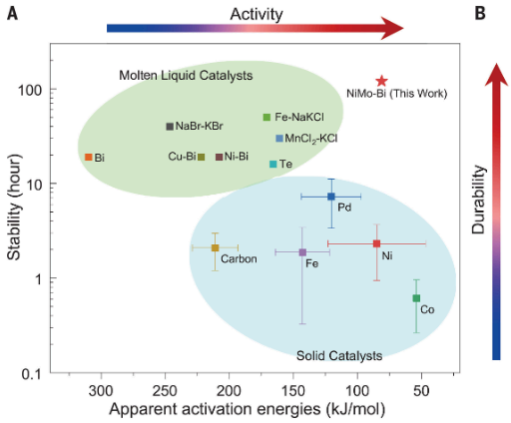


Figure 5: 2 and 3 Phase Catalytic Reactor [10]

Another consideration is the lifetime of the catalyst within the reactor, a key part of the reaction process is the production of solid carbon, while this carbon is desirable, the way carbon can build up on the catalysts, liquid or solid, can affect operability of the reactor over time. This reduces the efficiency of the reactor, by reducing the catalytic properties in the liquid catalyst, and causing coking in the solid catalysts. This coking, the carbon buildup, in the solid catalysts causes the chamber to get blocked up, and reduces its effectiveness and makes it less reactive. From Figure 7, we can see from the stability metric, which refers to the time that the catalyst can last before needing to be renewed in some regard, that liquid catalysts have longer lifetimes, but solid catalysts have advantages that can make them more effective for other reasons, like higher activation energies leading to lower operating temperatures as shown in the Figure 8 Venn Diagram. Solid catalysts can have a larger yield of hydrogen as referenced in Figure 8.





Figures 6 (left) and 7 (right): Performance of Different Catalyst Types [11]

Depending on the usage of catalysts, we may want to regenerate the catalysts used in the reaction process. This means a mechanical or chemical process that removes the buildup of solid carbon in the liquid or solid catalyst. To also prevent carbon buildup, moving mechanisms that stir liquid or solid catalysts can be used to prevent clogging and increase surface contact with the methane, an example of a diagram of such a mechanism is in Figure 9. Carbon also builds up on the walls but has a minimal impact on the rate of decomposition even after the reactor has been running for more than 15 days. [12]

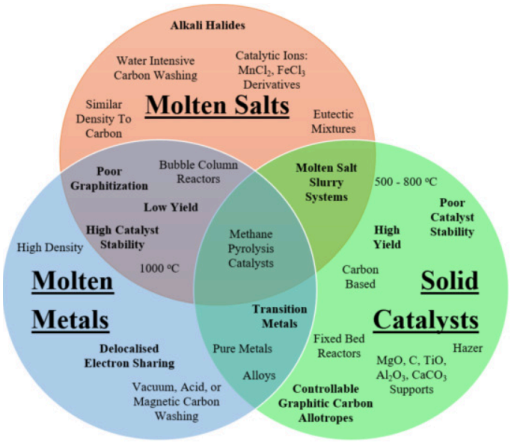


Figure 8: Venn Diagram of the Traits of Different Types of Catalysts [13]

These are more commonly used with liquid catalysts as it is not as effective to stir the solid catalysts. Solid catalysts are more commonly just removed from the chamber and the carbon is removed externally. Another way to prevent carbon build up is with a moving carbon bed. These are very useful but a significantly more complicated and expensive method of carbon removal, that is not generally used when keeping the carbon is a goal. [7] Moving carbon bed describes a system, where carbon is used as a medium moving around the tank, the gas is sent through and heated up. The methane separates into hydrogen and carbon collects on the other moving carbon within the tank, where it can be fed back into the tank and reused.

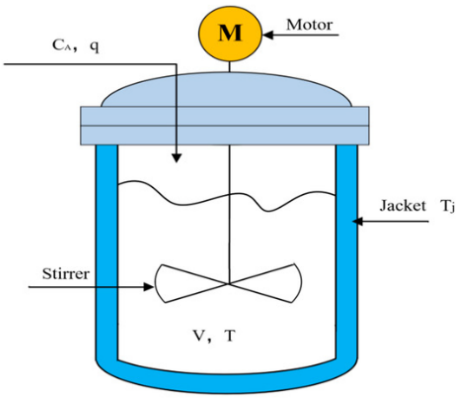


Figure 9: Diagram of a Continuous Stirred Tank Reactor (CSTR) [14]

As the methane moves through the catalysts, it decomposes into its parts, the solid carbon and the hydrogen gas. There is however going to be some leftover undecomposed Methane gas, which needs to be filtered out after the process to have pure hydrogen gas. Various methods exist to separate the gasses including pressure swing adsorption, where under high pressure certain gasses are stuck to solid surfaces, and membranes often a high temperature metal which are able to only let through hydrogen gas molecules, because they are very small while methane is a much larger molecule, these are the most common methods of separating the gasses.

The hydrogen gas after that needs to be stored, in Figure 10 you can see one way to do it is use a small metal pressure vessel. In this case the pressure vessel is directly off of the reactor.

Reactor chambers are commonly constructed with strong heat resistant materials, in Figure 10, the reactor is constructed with a quartz glass interior chamber, and the outer chamber is stainless steel. This reactor is heated by being put in a lab furnace. The top of this reactor is bolted on to ensure no gas escapes. [15] This reactor is fed through a small valve on the bottom of the tank. The reactor in Figure 5 uses the same materials.

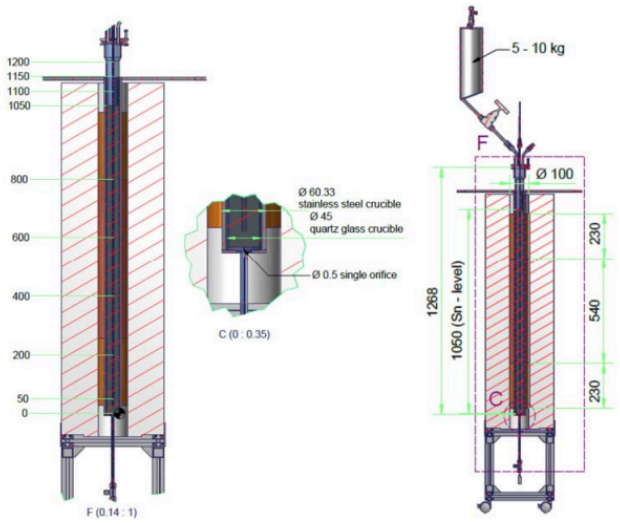


Figure 10: Experimental Liquid Metal Bubble Column Reactor Design [15]

Figure 11 gives us a good sense of the size and scope of the lab scale models our team is trying to replicate. To be close to lab size the length of the reactor is under 1 m, with most of the reactors in this chart under 0.5 m. The nozzles for inputting gas into the chamber are built to be between 0.2 mm and 2 mm or use a membrane with multiple small holes. To define some terms within the chart, and for the rest of the paper they list the feed rate, the amount of gas entering the reactor. The chart also covers residence time, the time the gas stays in contact with the catalysts. Operation time is how long it can operate unassisted. The carbon morphology is the shape and type of carbon collected. [6]

Molten Medium	Ga	Sn	5% Ni/Sn	KCl	NaBr:KBr	Co-Mn (2:1)	Ni/Bi = 27/73, NaBr	Ni/Bi = 27/73, ZrO_2, NaBr
Temperature (°C)	1119	1000	1050	1000	1000	850–1000	985	985
Feed Rate, Composition	450 mL/min, 50% CH_4/Ar	25–250 mL/min, 100% CH_4	70 mL/min, 35% CH_4/N_2	20 mL/min, 50% CH_4/Ar	15 mL/min, 100% CH_4	45 mL/min, 33% CH_4/Ar	9 mL/min, 67% CH_4/Ar	9 mL/min, 67% CH_4/Ar
Residence Time (s)	0.5	n.a.	n.a.	0.3	0.69–0.76	n.a.	n.a.	n.a.
Operation Time (h)	n.a.	n.a.	5, steady state	40, stable conv.	24	24, stable conv.	50, stable conv.	50, stable conv.
Max. CH_4 Conversion (%)	91	n.a.	19	1.8	5.85	10.52	32	38
Carbon morphology	carbon black	soot	graphite	amorphous	graphite + amorphous	graphite + amorphous	70 wt% graphite	74 wt% graphite
Reactor Material	Quartz	n.a.	Alumina	Quartz	Quartz	Quartz	Quartz	Quartz
Reactor Diameter (mm)	36	35	30	15	16	16	8	8
Reactor Length (mm)	n.a.	100	450	250	250	250	650	650
Reactor Filled Height (mm)	50	23	100	75	190	190	65	86
Bubble Generator Diameter	0.2 mm porous distributor	0.5 mm nozzle	n.a.	2 mm orifice	2 mm orifice	2 mm orifice	porous membrane	porous membrane

Figure 11: Different Pyrolysis Reactors and their Construction [6]

One associated challenge with pyrolysis is the cost, in Figure 12 there is an Investment column. This column represents the euros spent per kg/h hydrogen produced. The important rows on this column are the molten metal rows showing that this process is fairly expensive. Each of the molten metal pyrolysis rows is over 20,000 euros per kg/h.

Source	Reactor concept	Catalyst	Heat supply	Nominal H_2 capacity [kg/day]	Carbon yield [kg C/kg H_2]	Electricity consumption [kWh/kg H_2]	Methane consumption [MJ/kg H_2]	H_2 purification or use case	Investment [€/(kg/h H_2)]	Cost elements in Investment	Annual O&M cost [% of Investment]
Plasma processes											
[19] [a]	TP	No	TP	88,668	3.0	12.2	222.1	n/a	25,336	n/a	1.0%
[16]	TP	No	TP	1,914	3.1	16.1	304.8	n/a	[a]151,914	n/a	n/a
[22]	TP	No	TP	4,000	3.0	14.3	223.5	PSA	35,470	E, C, I	18.6%
[21]	TP	No	TP	18,263	3.0	17.8	223.5	PSA	[a]106,354	n/a	3.9%
[20]	TP	No	TP	13,683	2.8	11.7	222.1	n/a	[a]111,568	n/a	5.0%
[23]	TP	No	TP	402,901	3.0	[a]11.1	242.3	n/a	3,331	n/a	2.0%
Molten metal systems											
[18]	MM	No	EA	547,945	3.0	14.3	222.1	PSA	26,487	E, F	5.0%
	MM	Future	EA	547,945	3.0	[a]6.5	222.1		23,974		
	MM	catalytic	CH_4	547,945	3.0	0.0	252.6		23,233		
	MM	molten metal	H_2	547,945	3.7	0.0	274.3		24,386		
[17]	MM	Ni-Bi	CH_4	273,973	3.0	−0.5	272.7	PSA	30,634	E, I, M	2.0%
Gas reactor systems											
[26]	BR	No	EH	27,397	3.0	7.2	222.1	n/a	[a]32,850	n/a	n/a
[24] [b]	FBR	Nickel	CH_4	253,950	3.0	2.3	332.5	PSA	13,798	E, I, P, C	4.0%
	FBR	Carbon					294.7		13,892		
	FBR	No					294.7		13,892		
[9]	GR	No	CH_4	26,344	3.0	0.0	306.3	Product gas for	11,268	E, I, P	2.0%
	GR	No	EH	22,698	3.0	17.7	224.4	electricity	8,506		2.0%
	FBR	Nickel	Carbon	26,002	1.7	1.2	221.4	production	25,604		2.0%
	HER	No	EH	19,358	3.0	19.8	228.8		12,463		2.0%
[10]	HER	No	CH_4	2,158	3.5	0.0	266.8	Membrane	35,962	E,C	2.0%
	HER + G	No	CH_4	2,158	0.5	0.3	155.6		26,263		2.0%

Figure 12: Economic Factors associated with Methane Pyrolysis [2]

Although we are making our design from zero, besides referring to the benchmarks, there are various standards for us to follow. Safety is always the most important, especially when our project involves high temperature, high pressure, and highly inflammable gasses. There are safety standards on the operation of lab equipment, the configuration of the lab, and fire prevention. The catalysts contain various chemicals so there will also be standards on the manipulation of them. We will follow these standards to ensure safety. Other standards include standards on pressure vessel design and standards on storage or transportation of the hydrogen or methane.

Design Process

Our team decided to follow the ME Capstone Design Process Framework shown in Figure 13 below. We have considered following a number of different design processes including activity vs. stage based processes, solution vs. problem oriented processes, and abstract vs. procedural vs. analytical processes.

In our initial step of literature search, we followed a combination of abstract approach and procedural approach. In the beginning, since it was our first time working on the topic of pyrolysis, we had zero understanding of it. The best approach for us to learn about the topic would be the abstract approach where the subject is described at a high level of abstraction while specific details are not provided. We first read literatures of general overview of the methane pyrolysis process as well as the alternative steam

methane reforming process. After having a general understanding about the topic, we were ready for the next step of the procedural approach. The procedural approach is more specific and more relevant to practical situations. In this step we read literature of specific methane pyrolysis methods that are currently used by different labs and companies around the world to gain a baseline idea for our project as well as possible areas for improvements.

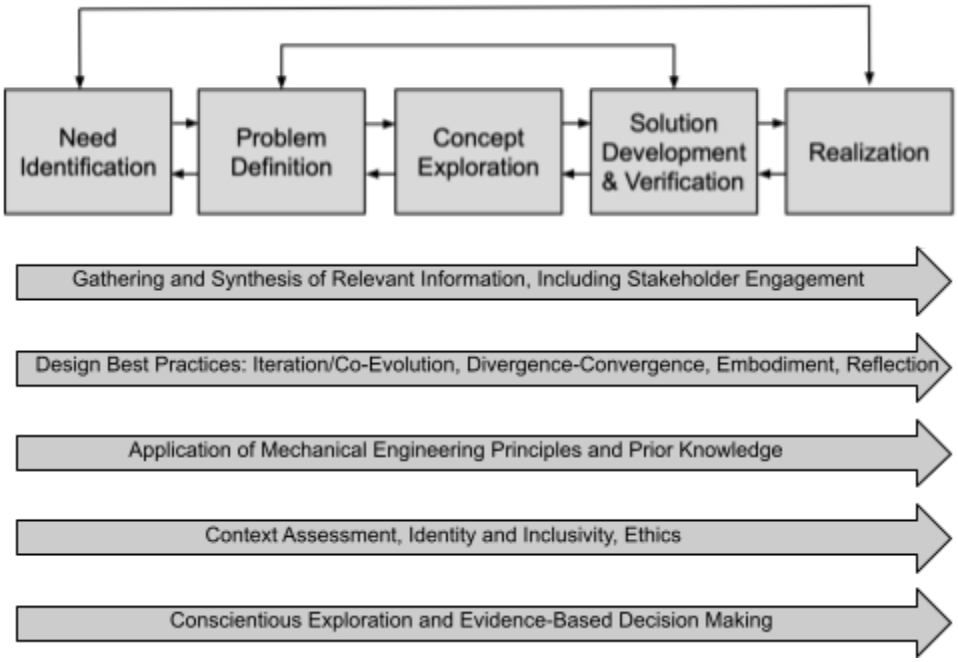


Figure 13: ME Capstone Design Process Framework

Many of the models presented in Wynn and Clarkson's *Models of Designing* [16] were considered in our selection of a design process.

First, we considered the advantages and disadvantages of stage-based and activity-based models. Stage-based models have a linear structure where different stages of the process are connected in a chronological order. The activity-based models have a cyclic structure where rework can occur at different places. Because of these fundamental differences, the advantage of stage-based models over activity-based models is that it will have a better-defined timeline for when each part will be completed. And the advantage of activity-based models over stage-based models is that we will be able to update the previous outcomes if we have new findings or problems later. For the scope of our project, which we are gradually getting familiar with and will take years to complete, we decided that the problem-based models are more applicable in our case because we will continuously update our knowledge and understanding about the topic and make improvements throughout the process, and the quality of work is more important than following a strict timeline.

We also considered if a problem-oriented approach or a solution-oriented approach was more effective for our project. In a problem-oriented approach, the emphasis is on the problem itself. First, a thorough analysis of the problem is conducted and then a range of potential solutions are generated. In a Solution-oriented approach, the focus is on an initial solution proposal. As the requirements and specifications are being explored, this initial solution will be continuously analyzed and modified to meet all the requirements. The advantage of problem-oriented approaches is that it allows for a thorough exploration of the solution space and provides the possibility for innovation. The advantage of solution-oriented approaches is that it presents a rough solution at an early stage and leaves more time for improvements. For our project, we chose to follow a problem-oriented approach because methane pyrolysis is a relatively new technology and it needs innovation by nature, as well as our thorough understanding of the topic. If we use a solution-oriented approach, it will be difficult for us to propose an initial solution since we have no experience with pyrolysis reactors.

We considered following a variety of different design process models including Beitz and Paul's Steps of the Planning and Design Process [17], French's the Design Process [18], and Pugh's Original vs Adaptive Design Process [19]. Ultimately, we found that the ME Capstone Design Process Framework was most aligned with our goals and most efficiently allows us to design our project successfully. We are using the same concept of the design process that was initially given to the class, as the design framework allows for a lot of playing around with concepts, all of the steps in the process are interlinked and we can restart any process over again. The format of this design process is extremely compatible with the structure of designing for problems in ME450, this is partially due to the nature of the design reports asking about aspects of each section in the given design process. This design process is a problem oriented process in which a lot of consideration is given to the ultimate goals of fixing the problem, which is how we want our design process to be implemented.

Design Context

We divided our main stakeholders into three categories: primary, secondary, and tertiary. The primary stakeholders are people who directly impact (or are impacted) by our project. These include:

The University of Michigan and Praneet. They sponsor this project and provide necessary resources for us. In return, we are transferring the intellectual properties created in this project to the University. Also, after successfully building the reactor, the researchers of the University will be able to use it to do experiments. Their expectations are to first have a working model or design and then the University will consider to actually build it.

Natural Gas or Biogas Suppliers. They supply the key ingredient that we feed into the reactor. They can be commercial natural gas or biogas sellers. If our project is successful, in the future they will experience increased demand for their gasses. They can also be the other research groups in the University that produce biogas, since the reactor is only lab-scaled. Their expectation for the current project is that we buy gasses from them. However, in the long term, they might see potential conflicts. With the development of our project (and methane pyrolysis technologies) it will become commercialized and the numbers of hydrogen producers (by using methane pyrolysis) will increase. Hydrogen and natural gas are

substitute products in some areas such as household heating or electricity generation. Therefore, the natural gas suppliers would experience a decreased demand from those end users. However, the hydrogen producers will also buy the natural gas from natural gas suppliers. Natural gas suppliers will need to figure out whether the net change in demand will increase or decrease.

Catalyst Suppliers. They supply the catalysts (molten metal and solid metal) of the reactor. The catalysts stay inside the reactor and will directly affect the performance of the reactor. The catalysts are different kinds of metal so the catalyst suppliers will be metal producers. For the current stage, they are not expecting much from us except the one-time purchase of catalysts. In the long term, our project will bring down the price of hydrogen which is an ingredient for metal refining. Therefore, the metal producers will benefit from this project.

The secondary stakeholders are groups which do not experience the problem and are not directly impacted by the problem or solution, including:

Traditional Hydrogen Producers. This includes steam methane reforming companies, coal gasification companies, electrolysis companies, and others. More than 95% of all hydrogen is produced by these companies and they are actually part of the problem context. These processes do not have a step of carbon capture, which results in excessive carbon emission. Methane pyrolysis is a direct competing method and can reduce the carbon emission significantly. Therefore, the traditional hydrogen producing companies might experience losses in their market share with lowered hydrogen prices. They might also be required by governments to reduce their carbon emissions which will increase their costs of operation. For instance, the average cost of production for gray hydrogen (produced from natural gas) is $2.13/kg while the cost for blue hydrogen (produced from natural gas with carbon capture) is $3.10/kg. [20]

Hydrogen Consumers (Oil Producers, Ammonia or Fertilizer Producers, etc.) As mentioned, oil refining (41Mt) and ammonia (31.8Mt) are the 2 biggest parts of global hydrogen consumption. With the success of this project, there will be an alternative source of hydrogen and increased supply, resulting in lowered hydrogen prices.

Hydrogen Vehicle Companies and Users. Similar to the other hydrogen consumers, hydrogen vehicle companies or users will benefit from the lowered hydrogen price. Generally, hydrogen vehicle is more expensive than gasoline vehicles and the advantages of hydrogen vehicle are better fuel economy and no carbon emission. Currently, the Toyota Mirai (a hydrogen fuel cell electric vehicle) has a starting MSRP of $50190 whereas the Camry starts only at $26420. [21] The MPGe(gasoline equivalent) of the Mirai is between 65 and 74, or 1.5 kg H2 per 100 miles. [22] The average cost of hydrogen for vehicles is between $13 and $16. [23] The cost for driving a hydrogen vehicle will be $21.75 per 100 miles. In comparison, the Camry has MPG between 25 and 32, which is 3.55 gallons per 100 miles. [24] The national average price for gasoline is $3.346/gal as of Mar 3, 2024 [25] and that results in a cost of $11.88 per 100 miles to drive the gasoline Camry. Based on these numbers, we can say that hydrogen vehicles are cheaper to drive only in certain areas where the gas prices are significantly higher than hydrogen. If the supply of hydrogen increases and the price lowers, then people will be more willing to buy hydrogen vehicles and the hydrogen vehicle manufacturers will sell more cars.

Our tertiary stakeholders are outside of the immediate problem context but have the potential to influence it:

Traditional (Gasoline) and Electric Vehicle Manufacturers. As of Feb 27, 2024, there are only over 18000 hydrogen vehicles in the US, because of the high cost. [26] However, if the price of hydrogen is lowered, hydrogen vehicles will be an effective competitor to gasoline vehicles and electric vehicles. In addition, If the sales of gasoline vehicles decreased, then gasoline producers will also experience a decrease in their sales.

Power Generation Companies. In 2023, 60% of electricity in the US was generated using fossil fuels (43.1% natural gas, 16.2% coal, and 0.7% others) and natural gas took the biggest portion [27]. Hydrogen is not directly used for power generation but can be a substitute for natural gas, especially if people decide to reduce the carbon emission and after the hydrogen price is lowered. Existing natural gas power plants can be modified to run on hydrogen and some already have the ability to run on hydrogen. For example, a Siemens SCC5-4000F1S power plant can switch between 100% natural gas and 100% hydrogen operation. With an efficiency of 59.4%, the hydrogen operation will save 335 g CO_2 per kWh electricity. [28] Although transforming a conventional power plant costs money, the reduced CO_2 emission will save money on CO_2 taxation.

Tire Producers. Methane pyrolysis also produces various forms of carbon as a by-product, including carbon black, carbon fiber, and carbon nanotube. These are important ingredients for tire production. With the development of methane pyrolysis, the supply of the carbon will rise and the price will decrease, which will benefit the tire producers.

Industries that Need Carbon Nanotubes. Carbon nanotube has its unique material properties (high elastic modulus, yield strength, electrical and thermal conductivity, and compatibility with biomolecules). These properties make CNT important for many industries including biomedical technologies, composite materials, microelectronics, solar cells, etc. Similarly, the development of methane pyrolysis will benefit all these industries by lowering their cost for CNT.

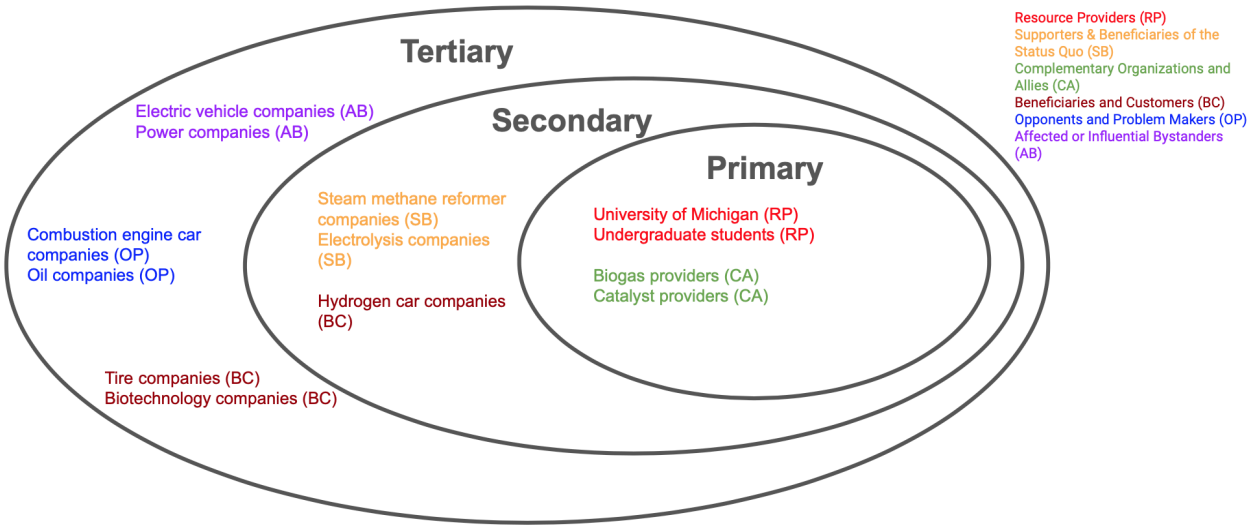


Figure 14: Stakeholder Map

One of our motivations is to slow global warming and produce less CO2 to reduce the amount of greenhouse gasses in the atmosphere. This project supports moving away from fossil fuels in the long run, as the process of biogas pyrolysis creates a possible green energy source in the form of hydrogen gas. Preventing further global warming will reduce already prevalent natural disasters, such as wildfires, tropical storms and hurricanes, as well as harsher snowstorms. Overall reduction in natural disasters is a humanitarian societal aim, as people are able to more easily stay out of poverty, less people will lose their homes to flooding, and other financial or physical harms.

There have been pushes by the Biden administration to fund more environmentally conscious products so there could be some financial motivation. Our sponsor may be motivated more broadly by a desire for education on the process of pyrolysis and how it could be innovated upon. Environmental impact is likely a significant consideration. However, it seems like the larger concern for the sponsor is pursuing knowledge in the field of hydrogen production. For our team, the environmental and educational aspects of the project play a large role in what we end up designing for this project. The project is supposed to pursue sustainability while being used in an educational context. In theory, making a process more sustainable should make a greater positive impact, by reducing emissions. Using the project for educational aims should also increase the positive social impact of the creation, by making greater progress in green energy.

We are using other people's intellectual property to come up with our own ideas from viewing patents and unique reactors outlined in research papers. They provide not exactly an outline but general inspiration and specific rules to follow when designing a reactor that we can develop from reading their work. This means the intellectual property we are concerned with is copyright for the contents of the research papers that we have been reading, and design patents over the mechanical ideas that we may be creating or using for our project. The university will own the intellectual property, and we may be partial inventors after the project but not the owners of the intellectual property, so we would not control the rights to any produced intellectual property, as we are working under the university to develop a reactor for their use.

The point of our project is to reduce carbon emission in the process of creating hydrogen out of methane. The manufacture of the reactor will produce greenhouse gasses and pollutants as the transport and manufacture within creating metal shapes have a lot of steps to get to a final destination. The disposal would be semi-sustainable since the reactor will be made of a lot of recyclable or reusable metal materials. However, the recycling or reusing processes may use a good amount of power which, with our current electrical grid, will produce greenhouse gasses.

The operation of the product in early stages for this project will likely not be very sustainable. The power consumption of the reactor will be very high as we are heating materials to very high temperatures. If a laboratory furnace is used it can pull in the range of 2kW to 12kW [29]. Other methods may be less power intensive such as cold plasma reactors which can use 5 to 72W on a lab scale [8], but produce a much lower yield from the methane. Ideally, the project would be running on renewable power sources to heat the reactor, which would dramatically reduce the environmental impact the reactor would have. Furthermore, as we keep improving the design, we will try to reduce the heat loss from the reactor and recover more waste heat to improve the energy efficiency.

Possible ethical concerns arise about this project. One of them is the conflict minerals. Tungsten, because of its mechanical properties such as high melting point, can be used on high temperature reactors like ours. Since the reactor will contain both molten and solid catalysts, we might use tungsten to hold the solid catalyst in place to separate from the molten catalyst. However, tungsten from Rwanda (the 5th largest Tungsten producing country) can be a conflict mineral. [30] In 2006 the government announced privatization of the mining sector [31]. As a result, a great portion of the mining sector is informal and small-scale, meaning it could be difficult to regulate, dangerous or environmentally destructive, use child labor, violate human rights, and help fund war and armed conflicts. And there is no guarantee that the tungsten we use is conflict-free. Therefore, we might need to find alternative materials for our design.

Our personal ethics are more similar to the university than to a future employer or client. They have their codes of ethics but their goal is more focused on making profit rather than to reduce environmental or social impacts. Some of them may have some more significant ethical boundaries that we may align with, but they in general form ethical principles around business practices rather than doing ethical good.

Visible power is in who we choose to talk to regarding the project. The amount of power we hold over end users is a bit harder to define relative to us. We have hidden power over what ideas we choose to explore as a team and which ones we might ignore. We have similar power with our sponsor where we can take their advice but we have the power to disregard suggestions. We have scheduled weekly meetings with our primary sponsor Praneet to discuss our progress and ask his requirements.

We are all from different backgrounds and to make sure we are inclusive in our search for information and ideas. We will make sure we keep in mind our own biases and differences in upbringing and education that may lead us to choose one possibility over another in our search for solutions.

Further Exploration on Social Impacts of the Project

Our project is at the very beginning stage which is to design a lab-scale reactor. Eventually, our sponsor will scale it up to pilot-scale and commercial-scale plants. At that time, despite the benefits of producing hydrogen and carbon with lowered carbon emission, the project will also have implications at a society level.

The Olive Creek 2 is a completely commercialized methane pyrolysis facility planned by Monolith. It is planned to be built in Lancaster Nebraska and is a 12-time-upscope of the Olive Creek 1 which is also a commercial scale facility but mainly used for testing purposes. The Department of Energy has composed an environmental assessment for the OC2 facility to evaluate its possible impacts [32]. Because of the similarity between our project and Olive Creek, we can refer to this environmental assessment to estimate the social and environmental impacts of our project. Some of the key areas analyzed in the assessment include:

Air quality and GHG analysis. The construction process of the facility will generate fugitive dust emissions and air emissions caused by the construction equipment and vehicles. Actions such as watering and other dust suppression methods will be taken to minimize the impacts. According to the DOE, the

effects of emissions will be “temporary and minimal”. The operation of the facility (production of hydrogen and carbon) will generate hazardous air pollutants and greenhouse gasses. The emission of these pollutants is regulated and the OC2 has received permit from the local health department, with allowed amounts listed in Appendix E *Table 1*. Again, the OC2 is considered a “minor source” and its “impact to air quality is not anticipated to be significant”.

A life cycle analysis of the gas emissions is also performed on the OC2 facility. The analysis is based on the production of 198416 tons of carbon black and 319333 tons of ammonia per year. The results are compared to the emission from usual methods of producing the same amounts. The results show that the OC2 facility will produce 38000 tons of CO2 equivalent per year whereas usual production methods produce 823000 tons of CO2 equivalent per year, with a reduction of 80%. Detail shown in Appendix E *Table 2*.

Biological resources, including vegetation and wildlife/birds. The proposed expansion of OC2 is 37 acres but the construction process requires an additional approximate 38 acres. The land will be temporarily impacted and will return to agricultural use after the construction is finished. According to the Nebraska Department of Agriculture, the construction activities may increase the proliferation of noxious and invasive weeds. To control these weeds, the disturbed land will be revegetated. To protect the wetland area, aquatic safe herbicides will be used to treat these noxious and invasive species.

Public and occupational health and safety. This section mainly concerns emergency medical services for the facility because the operation involves risks. Specifically, the facility is placed 25 miles from an emergency medical service and 0.5 mile from a fire department. This makes us think about our project. If eventually we are choosing places to build a facility like OC2, it is important to choose places where emergency services are available. Further analysis on the chemical hazard indicates that it is not anticipated to be significant, and that the carbon back dust, although combustible and explosive at high concentration, requires higher minimum energy to ignite and has lower risk of explosion. In addition, it does not cause respiratory or dermal irritation.

Socioeconomics. Analysis predicts that the construction of the OC2 will need 800 temporary high-skilled workers over 24~30 months and 60 permanent workers. This will create job opportunities for the local people as well as people from other places. In the first quarter of 2021, it was estimated that the business activity had an economic impact of $54.6 million, including $25.9 million annual labor income spread over 247 jobs. When the construction is completed, there will be a statewide annual economic impact of $338.9 million, including $88.4 million in labor income spread over 848 jobs. This will benefit both the state of Nebraska and the local businesses.

Soils and Prime Farmlands. Lancaster county has more than 420000 acres of farmland and the OC2 will use 75 acres (37 acres permanent use for the facility and 38 acres temporary use for the construction process which will be restored). The reduction is less than 0.01% and is negligible. This will be another important thing for our stakeholder to consider when they are scaling up.

Waste Management. The report estimates the wastes produced during the construction process from 2021 to 2024 and the annual operational wastes shown in Appendix E, *Tables 1* and *2*. A great number of

wastes will be recycled or processed by certified waste facilities, and the impacts of waste management are not anticipated to be significant.

User Requirements and Engineering Specifications

Considering the many factors that go into a methane pyrolysis reactor, we built our requirements and specifications around those parameters. We built our requirements around 4 subcategories: 1) Storage safety of methane and hydrogen; 2) The scale of the reactor; 3) Mixing requirements; 4) Conditions of pyrolysis reaction; 5) Efficiency of pyrolysis reaction. To determine the priority of these requirements, we utilized the MoSCoW method for the categories of stakeholder significance, practicality, cost-effectiveness, and temporal factors. The MoSCoW analysis is shown below in *Table 3*.

Table 1: MoSCoW Analysis of Requirements and Specifications

	Stakeholder	Practicality	Cost-effectiveness	Temporal factors
Storage Safety of Methane and Hydrogen	Must Have	Must Have	Should Have	Should Have
The Scale of the Reactor	Must Have	Should Have	Should Have	Should Have
Mixing Requirements	Must Have	Should Have	Should Have	Should Have
Conditions of Pyrolysis Reaction	Must Have	Must Have	Should Have	Should Have
Efficiency of Pyrolysis Reaction	Could Have	Could Have	Should Have	Could Have

With the stakeholder significance and practicality as the most important factors, we have the storage safety as the highest priority followed by conditions of pyrolysis reaction, the scale of the reactor, efficiency of pyrolysis reaction.

The first and most important factor we took into account for our project is the safety and storage of the reaction. As responsible and ethical engineers, our first priority is always to make sure the people that will be operating the reactor can do so safely and without risk of injury. Our beginning and end products, methane and hydrogen, are both inflammable gasses and they will be stored near a high temperature and pressure reactor as detailed below. Thus, it is our utmost priority to make sure that our reactor is safe to use. To determine these specifications, we primarily used standards outlined in the 2020 Hydrogen Storage DOE and FMVSS 304 for hydrogen storage and methane storage respectively. For hydrogen storage, as specified in the 202 Hydrogen Storage DOE, must be kept under 25°C at 20 MPa [33]. For methane storage, as specified in FMVSS 304, must be kept at around 26 MPa and under 30°C [34].

Next, our second most important specification we identified are our pyrolysis reaction condition specifications. Since there aren't any standards that specifically revolve around the temperature and

pressure of a pyrolysis reaction, given that it's a newer technology, we decided to base our specifications on research articles on pyrolysis reactors that have already been built as well as catalyst conditions. We learned that methane pyrolysis is most efficient at high temperatures and low pressures so we built our requirements for the temperature and pressure of the molten catalyst to be at 400°C to 500°C and 400 kPa to 500kPa [9].

Our third most important specifications we identified are for the reactor gas mixing system. For our reaction chamber, we are setting a residence time of 1 hour for the reaction to reach completion. Although this may be an overestimate of how long it takes for the reaction to complete, we are setting this as a placeholder and will be optimized through experimentation later on. Next, we set the methane inlet specification for 1 liter within the residence time. This is because with the reactor size being limited to 2-3 liters, we felt that 1 liter was a reasonable estimate for how much methane can be reacted while still having good surface contact and conversion rate with the catalyst within the reactor. We also wanted to maximize surface contact between the catalyst and the methane gas so we set bubble size and density specifications for the methane gas. We set the bubble size to be 3.0 mm and the density to be 0.2534 kg/m^2 in order to maximize contact with the molten catalyst [35]. Finally, the flow rate of the methane gas was calculated to be 1.2 kg/hr given our hydrogen production rate specification specified by our sponsor.

Our fourth most important specification we identified are the specifications around the scale of the reactor. It is important for us to determine the scale of the reactor because a reactor can scale anywhere from a laboratory scale to a commercial scale, which would greatly impact the amount of work expected of our team. The size of the reactor chamber specification was defined for us by our sponsor to fit reasonably in a lab (potentially at the University of Michigan). The high hydrogen production rate specification was also defined for us by our sponsor as a goal for us to reach with our design.

Finally, for our least important specification, we identified it as efficiency of the pyrolysis reaction. Firstly, these are all of our goals we have set for ourselves to enable the most efficient reaction for our system. For our methane pretreatment requirement, we require the gas to be heated up to 350 °C to 400 °C before entering the chamber because this is where 1% of the decomposition occurs for the methane [36]. Next for our conversion rate specification, we desire a 60-70% conversion rate of the methane to hydrogen and carbon as specified by our sponsor, Praneet. Since the conversion rate of the reaction isn't at 100%, we want to maximize output per methane input so we will feed all of the unreacted methane back into the reaction chamber. Due to the solid carbon buildup around the solid catalysts, this would cause the reaction to slow down over time. As explained in the background section, catalyst regeneration is the act of removing solid carbon from the catalyst. For catalyst regeneration, we desire an efficient reaction with low down time, so we will aim for a catalyst regeneration time of under 4 hours. Finally, we desire a low carbon buildup deposition rate, so the reactor will be able to run for 20 hours unassisted. We want to ensure that the reactor is able to run self-sustained for at least 20 hours without a need for catalyst regeneration of the solid catalyst for better efficiency of the process.

These requirements and specifications are shown below in *Table 4*.

Table 2: Requirements & Specifications

	Requirements	Specifications	Justifications
1	Methane Storage	Cylinder storage temperature <30 °C at pressure = 26 MPa	Store methane away from any heat source, safety requirement based on safety data sheet
	Hydrogen Storage	Cylinder storage temperature =25 °C at pressure = 20 MPa.	Store hydrogen away from any heat source, safety requirement based on safety data sheet
2	Heat Resistant Reactor	Withstand T = 700 °C while P = 500 kPa	The wall of the reactor should withstand the reaction temperature and pressure.
	Pyrolysis Temperature	Molten catalyst temperature keep at 400°C to 500°C	Temperature source for methane pyrolysis process should have constant heating across the reactor.
	Pyrolysis Pressure	Molten catalyst pressure keep at 400 kPa to 500kPa	Pressure of methane pyrolysis process is driven by kinetics of reaction should happen in a safe condition.
3	Residence Time	The reaction time should be under 1 hour	Give the methane and the catalysts ample time to react. Specified by our sponsor, and will be optimized later on.
	Methane Inlet	1 liter of methane will be inputted into the reactor for the specified residence time	Provide sufficient volume of methane for catalyst present
	Bubble Size	The bubble size of the methane inlet gas should be 3.0 mm	A smaller bubble size results in better contact between the gas and the catalyst for better reaction
	Density	The density of the methane inlet gas should be 0.2534 kg/m^3	Density of the methane gas in a high temperature chamber
	Flow Rate	The flow rate of the methane gas inlet is 1.2 kg/hr	Based upon our desired 0.3 kg/hr of hydrogen production, we require this mass flow rate of methane gas
	Mixing Conversion Rate	60%-70% conversion rate	After mixing, the catalyst should accelerate the pyrolysis reaction process, specified by the sponsor.
4	Impeller Viscosity	Flat-blade turbine impeller viscosity should be between 1 to 10^4 centipoise	Viscosity range for which the impeller is the most effective at mixing
	Motor Torque	Motor torque needs to be	Required torque for the motor to spin the

		between 0.818 to 4.09 Nm	impeller
5	Sized for Laboratory Scale	Reaction chamber <200 mm Diameter, <500 mm Length, 2-3L Volume	Laboratory scale reactor, specified by sponsor
	High Hydrogen Production Rate	0.21 kg/hr of Hydrogen	Should produce hydrogen at a steady rate, specified by sponsor
6	Methane Pretreatment	Gas heated to 350 °C to 400 °C	Methane should be preheated before entering the reaction chamber till 1% of the decomposition state for faster reaction, specified by sponsor.
	Reuse of excess reactant	100% of excess CH4 go back to methane storage cylinder	Reuse excess reactant for higher yield ratio, specified by sponsor.
	Catalyst Regeneration	Time for catalyst regeneration should be under 4 hours	Regenerating catalyst is a batch mode process so the time for catalyst regeneration should be as short as possible, specified by sponsor.
	Low Carbon Deposition Rate	The reactor should be able to run unassisted for 20 hours without the need of catalyst regeneration	Carbon deposits should be limited to allow longer operation time to ensure efficiency.

In the following section, we summarize which requirements are of most importance, which must be met, and which are our goals and wishes.

1) Storage safety of methane and hydrogen are safety standards based on safety data sheets. These two extremely inflammable gasses should be stored in designated gas cylinders away from the reaction chamber. These safety codes must be met. For safe operation of our system, we will follow some of the existing safety codes related to our system. These include NFPA 2: Hydrogen Technologies Code, NFPA 45: Standard on oFire Protection for Laboratories Using Chemicals, and NFPA 59A: Standard for the Production, Storage and Handling of LNG.

2) Conditions required for pyrolysis reactions to happen are very important requirements. The reaction chamber should be constantly heated and all reactants should be kept under high temperature environments. Otherwise, the methane would not decompose. These requirements must be met.

3) Conditions for the reactor chamber mixing system. The methane gas inlet conditions should be set to maximize its contact with the catalyst to maximize the conversion rate and optimize the mixing process of the reactor.

4) The scale of the reactor defines the size of our reaction chamber, which is specified by our sponsor. Our sponsor would like to use our design for his lab experiment. These requirements must be met.

5) Efficiency of pyrolysis reaction should be high as specified by our sponsor. To ensure the high conversion rate of CH4, our sponsor wants us to pretreat methane and reuse the unreacted CH4. Also, to minimize the interruption of production flow, our sponsor wants us to limit the carbon deposition rate and regenerate catalyst within the shortest time. These requirements are not mandatory, but we would put most of our efforts in achieving these goals.

In order to verify and validate these requirements and specifications, a variety of different methods could be used. The main source of verifications for our project is making sure that we meet specific temperature and pressure thresholds. We will verify these measurements using different instruments. In particular, we will be using pressure gauges and thermocouples at various points in the reactor to measure the pressure and temperature respectively. In addition, we also have requirements for production rate of hydrogen and the conversion rate of the methane. We will use a flow meter to measure the flow of hydrogen out of the reactor to make sure that it meets our requirements. In order to measure the bubble size, we can use an image analysis or optical probe technique. In order to make sure it meets the conversion rate requirement, we will measure how much hydrogen is produced and through stoichiometry we can calculate how much of the methane was converted and as a result get the conversion rate. Our final requirements detail the time it takes for catalyst regeneration and carbon deposition rate. We can verify these requirements by observing the carbon buildup around the catalyst over time and making sure that the carbon buildup meets the required time limit and we are able to complete the catalyst regeneration without selecting the concept in the time frame allotted.

Concept Generation

The team started the concept generation process by using a combination of concept generation techniques in the initial stages of concept generation that largely utilized morphological matrices and design heuristics. Initial ideation was started by just timed brainstorming, where we got out as many ideas onto the page as possible in a limited amount of time. This produced a large variety of ideas with a combination of realistic and less realistic ideas. One concept that came out of this section of the brainstorming as can be referenced in Appendix D: Brainstorming, team members already knew that considerations had to be made for heating. This concept was to wrap a heating element around the reactor chamber, using design heuristic 11, allow users to reorient, and allow the heating element to be adjustable. The thought was that we could have the heating element be removable. Another not realistic concept was just heating the canister on open combustion flame. It would not likely we would use this but it was in our brainstorming.

After this each team member produced their own flow charts to decompose the pyrolysis reactor into its most basic sub functions. We broke it down by thinking of the inputs into the system and outputs, and what has to happen to get the inputs to become the outputs. These created flow charts are found in Appendix D: Functional Decomposition, each of these flow charts followed the same rough ideas for the sub functions. These flow charts were then combined and discussed with our sponsor, to determine the most important sub function considerations. The subfunctions we ended up determining were Methane Storage, Methane Pre-Treatment, Reactor Shell, A method of holding the catalysts in place, Reactor Heating, Gas Flow, Methane Inlet, Liquid/Gas Mixing, Continuous Collection of Carbon, Batch

Collection of Carbon, Flushing, Catalyst Regeneration, Hydrogen Filtration, and Hydrogen Storage. Methane needs to be stored before entering the reactor. Before getting into the reactor chamber, the methane also needs to be heated so it can get up to temperature to properly decompose. [7] We need to make considerations on the walls of the chamber so it can withstand the proper temperatures. There are also considerations to separate the catalysts from each other and hold them in place within the reactor chamber. The reactor must be heated to create the pyrolysis process. The gas must have a pump of some kind regulating the flow of gas between the supply tank and reactor chamber and the reactor chamber and hydrogen storage tank. [7] The methane inlet is a necessary consideration because the size of the flow in the tank can promote contact between catalyst and methane increasing yield of hydrogen. Mixing within the tank is important to promote the contact of the methane and keep the carbon from settling within the tank and blocking the flow of methane. Both batch and continuous collection of carbon is important because for a liquid and solid catalyst, there are different methods of collection, with the solid catalyst needing batch collection. To clean out the reactor a gas needs to be flushed through it to clear it out for further experimentation. [7] We want to be able to continually use the same catalyst and not spend more money purchasing catalysts, and be able to extract the carbon deposited on the catalyst. The hydrogen produced by this process then needs to be stored after being separated from remaining methane. Before creating a final morphological chart, each team member created their own morphological chart with as many ideas they could come up with for each process for the previously mentioned sub functions. From this one idea that was thought of was graphene mesh to filter out the hydrogen. This idea is a little more grounded than the previous ideas but may not be super accessible.

Using these sub functions, we created the final morphological chart and applied several of our previously brainstormed ideas along with coming up with a few new ideas. The team evaluated and reflected on the previous ideas before adding them to the chart. This chart was discussed with our sponsor to see if there were any possible additions to the chart. This chart is in Appendix D: Final Morphological Chart, this chart expanded the options for more quality ideas. For the gas flow sub function, we came up with a variety of specific types of pumps that could be used, the list including a lobe pump, radial flow pump, scroll gear pump. Each of these ideas was significantly more directly applicable to the project, than the initial brainstorming sessions. Each of these pumps is a specific method of pumping the gas from one section into another. As we developed ideas further we got to a point where they were more realistic and viable. This brought the team to a point where there were many options for the broad aspects of the project.

Concept Selection

In order to select our final design, we considered doing a weighted pugh chart or a concept evaluation matrix. However, with our system having over 10 subsystems, many with very different functions, we decided it was best to use a concept evaluation matrix as it would give us a better overview of all the factors that we are considering without restricting our choices with arbitrary weights. Almost all of the categories selected are essential functions of each subcategory, and being unable to meet them would be unacceptable for our design. We analyzed all of our different subsystem options by color with green indicating it does work, yellow indicating it may work, orange indicating it may not work, and red

indicating it does not work for each different requirement. We found it to be the most reasonable and logical to use a concept evaluation matrix in evaluating all of our subsystem options.

Through using the concept evaluation matrix, we were able to select concepts for each of our subsystems. The subsystems are separated into two categories: pre-reactor heating and post-reactor heating. A summary of all of the selected concepts for each subsystem is shown below in *Table 5 (pre-reactor heating)* and *Table 6 (post-reactor heating)*. A flow chart of all of the subsystems and how they are interconnected is shown below in *Figure 15.*

Table 3. Pre-reactor Heating Methane Pyrolysis Subsystem Selection

Concept	Selection
Methane Supply/Storage	Compressed Natural Gas
Pretreatment	Inductive Heating (electric)
Gas Feeding/Inlet	Multi Point Feed Inlet
Methane & Molten Catalyst Mixing	Continuous Stirred Tank Reactor (CSTR)
Reactor Shell Material	Quartz
Reactor Heating	Inductive Heating (electric)
Carbon Removal (Molten Catalyst)	Pneumatic Overflow Weir
Carbon Removal (Solid Catalyst)	Ultrasonicator

Table 4: Post-reactor Heating Methane Pyrolysis Subsystem Selection

Concept	Selection
Gas Separation	Metallic Membrane
Overall Flow Control	Diaphragm Pump
Flushing	Nitrogen Batch Mode Flushing
Hydrogen Storage	Compressed Gas

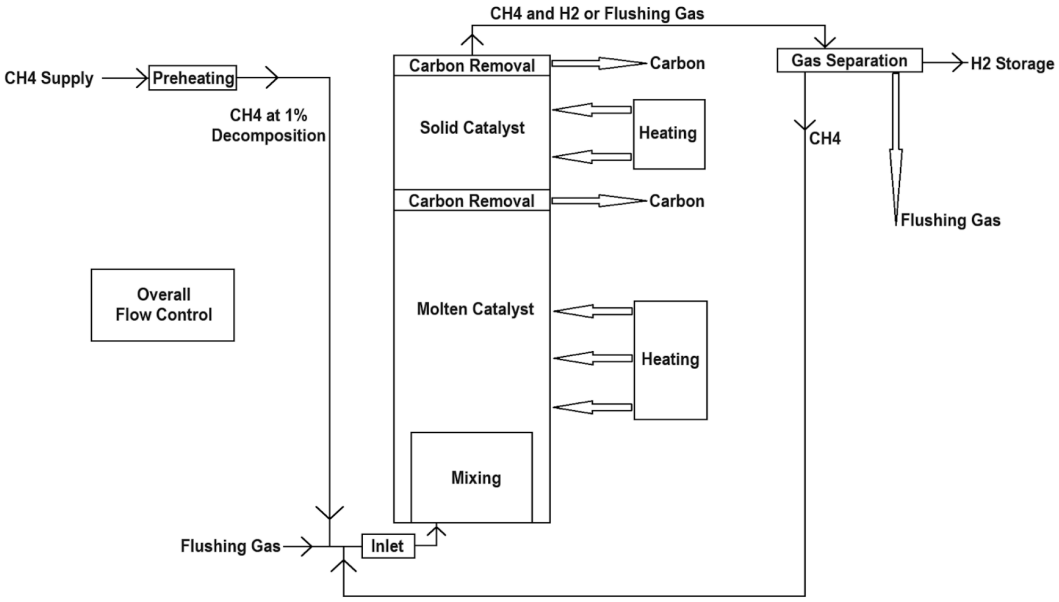


Figure 15. Flow Chart of Methane Pyrolysis System

Due to having many subsystems, we will present decision matrices that focus on the five most important subsystems in our reactor design. The subsystems we're choosing to focus on are: the reactor shell, the reactor heating, the liquid/gas mixing, carbon removal & catalyst regeneration, and hydrogen filtration. The rest of the decision matrices can be viewed in *Appendix B*.

The first subsystem is the reactor shell. Since the reactor shell will constantly be subjected to a temperature of up to 600°C, the reactor shell material needs to be heat resistant and be able to sustain that temperature. The material also needs to be heat resistant to limit heat loss to the environment and keep the reactor at the desired temperature. Additionally, the material needs to not degrade easily and not react with the methane and hydrogen gas within the reactor as well as the catalyst. Finally, since the reactor shell will have a somewhat complex geometry, we need to make sure that it is machinable and able to be customized. The requirements are listed below in *Table 7* as well as our analysis of the different materials considered for it.

Table 5. Reactor Shell Material Concept Evaluation Matrix

		Do not work	May not work	May work	Do work
Option No.		Heat Resistant: Continuous service temperature >600° C	Machinable: Allows Customization	Thermal Insulation: Low heat loss	No Degradation under CH4/H2 Environment	No Reaction with Catalysts
1	Ceramics					
2	Stainless Steel					
3	Ni-based (GH747)					
4	Quartz					
5	Plastic					
6	Alumina					

Based upon our analysis, we found quartz to be the most suitable material for the reactor shell. Many of the materials that were considered are not heat resistant and would possibly lose a lot of heat during the reaction and may not be able to sustain the required temperature over time. Furthermore, this would lead to a lot of energy waste and not make our process less efficient. Each of our requirements are crucial for the shell material, so we decided upon using quartz. Quartz is also a material that is commonly used in the pyrolysis reactors in a lab setting for the reactor shell, so it has been proven to be reliable and doesn't react with any of the content inside the reactor, making it an ideal material [6].

Our second subsystem is the reactor heating system. The most important requirement is the temperature. With the reactor being subjected to a temperature of up to 600°C, we set a requirement for the reactor to be able to reach 700°C to give the requirement a safety factor and ensure it's able to perform the task. Additionally, we want to make sure that the heat source has a high heat transfer rate and low heat loss to the environment. Finally, we want the heat source to be energy efficient to make our system sustainable and environmentally friendly. The requirements are listed below in *Table 8* as well as our analysis of the different heat sources considered for it.

Table 6. Reactor Heating Concept Evaluation Matrix

		Do not work	May not work	May work	Do work
Option No.		Able to reach 700 °C	Heat Transfer Rate	Heat Loss	Energy Efficiency
1	Furnace				
3	Microwave Radiation				
4	Solar Heating				
5	Infrared Heating				
6	Electricity (Resistance)				
7	Electricity (Inductance)				
9	Heat Pump				

We chose to use electric inductance heating as our heat source for the reactor. Inductance heating is reliable and has the lowest heat loss in comparison to the other methods. With the energy being transferred directly to the parts being heated, this heating method is a very effective method of heating. Furthermore, it also results in significant power savings helping us make the system more sustainable.

Our third subsystem is the carbon removal and catalyst regeneration process. For this process, we require that the process is fast, falling within our requirement of under 4 hours. We also want to make sure that the process also doesn't damage the catalyst in the process and is able to remove all of the carbon in the process. Finally, we want the process to be carbon neutral, so no carbon dioxide emission can occur during the process. The requirements are listed below in *Table 9* as well as our analysis of the different heat sources considered for it.

Table 7. Catalyst Regeneration Concept Evaluation Matrix

		Do not work	May not work	May work	Do work
Option No.		Fast Operation	No Damage or Contamination on Catalyst	No Remaining Carbon	No CO2 produced
1	Boiling in water				
2	Ultrasonicator				
3	Chemical treatment (H2O2)				

Based upon the analysis above, we selected ultrasonicator as our catalyst regeneration method. This would occur with the solid catalyst after it has been given requisite time to cool down to a safe handling temperature. The ultrasonication process would happen in a fume hood after the solid catalyst has been removed from the reactor manually. After the system has been flushed the only remaining product on the solid catalysts is the solid carbon. The ultrasonicator method is the most reliable method because there is significant scientific backing behind this method and the catalysts were able to regain its full activity without damage to it [37]. Furthermore, there is no carbon dioxide emission from this process as well.

Our fourth subsystem is the hydrogen filtration. For this subsystem, we need to make sure that it is capable of separating the hydrogen and the methane in the system while filtering out the impurities within the system. Since all the gas leaving the reactor will be at high temperature, the filtration system will be susceptible to high temperature. Therefore, it must be heat resistant as well. Similarly to the other subsystems, the hydrogen filtration system should be energy efficient and have low energy consumption. The requirements are listed below in *Table 10* as well as our analysis of the different heat sources considered for it.

Table 8. Hydrogen Filtration Concept Evaluation Matrix

	Do not work	May not work	May work	Do work

	Option No.	Separation Rate	Hydrogen Purity	Low Energy Consumption	Heat Resistant: can withstand up to 600° C
1	Polymeric Hollow Fiber Membrane				
2	Metallic Membrane				
3	Hydraulic Filters				
4	Distillation (Different Boiling Point)				
5	Pressure Swing Adsorption				

Based on the analysis above, we decided to use a metallic membrane for our hydrogen filtration system. A membrane system is the most commonly used method for hydrogen filtration in pyrolysis systems because it is the simplest and cheapest method for hydrogen filtration. Furthermore, it has no energy consumption, making the process very environmentally friendly. Between the two membrane options, metallic membranes are able to sustain high temperatures while polymeric hollow fiber membranes may melt from the high temperature [38]. Thus, we selected the metallic membrane as the best option for hydrogen filtration

Finally, for our last subsystem, we have the liquid/gas mixing system. For this subsystem, we need it to be able to distribute the methane gas uniformly within the molten catalyst. In addition, we need it to be able to operate continuously. The requirements are listed below in *Table 11* as well as our analysis of the different heat sources considered for it.

Table 9. Liquid/Gas Mixing Concept Evaluation Matrix

	Do not work	May not work	May work	Do work

	Option No.	Promote the uniform distribution of CH4 in molten catalyst	Works Continuously
1	Continuous Stirred-Tank Reactor		
2	Plate Column Reactor		
3	Rotating Drum Reactor		

The continuous stirred-tank reactor (CSTR) was selected as the best liquid/gas mixing system. A CSTR is a type of chemical reactor that provides constant stirring, allowing the reactants to be uniformly

distributed and allow the reaction to advance at a uniform rate. This allows us to easily control the temperature, pressure, and concentration of the reactor by adjusting the flow rates of the reactants and products [39]. For our purposes, the CSTR is able to uniformly distribute the methane gas in the molten catalyst and also operates continuously. The CSTR is also usually used for reactions that require high conversion rates, which is required for our reactor. Thus, we find the CSTR to be the most suitable liquid/gas mixing system for our project.

Due to time constraints, we have decided to make the CSTR reactor design the main focus of our project since there is the most uncertainty in the area and where we can add the most value. We want to focus on the mixing system because we can make the biggest impact by slowing down the carbon buildup. The carbon buildup within the solid catalyst is a problem many pyrolysis companies are currently facing and with our novel idea, we can help solve this issue. The reactor will consist of 7 parts: gas inlet, molten catalyst mixing, low solid catalyst carbon deposition, solid catalyst regeneration, hydrogen filtration, heating system, carbon collection, and the reactor material. These subsystems are labeled in *Figure 16* below along with a diagram of our reactor design.

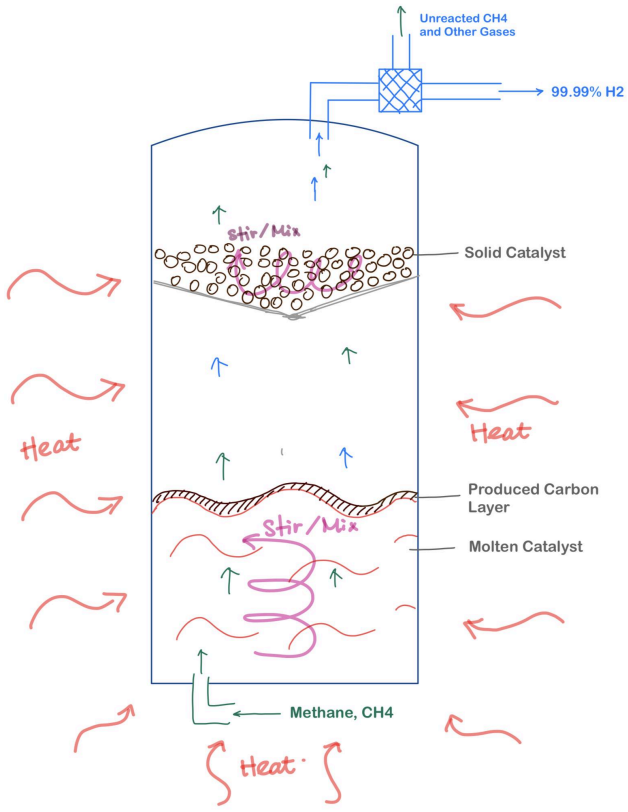


Figure 16. CSTR Reactor Design Subsystems

As already discussed above, the shell of the reactor will be made of quartz, the heating system will be an electrical inductance heating system, the catalyst regeneration method will be ultrasonicator, and hydrogen filtration will be done with a metallic membrane. The rest of the subsystems are summarized above in *Table 5 & 6*. To give an overview of the process within the reactor and how the systems interact

with each other, the gas inlet will feed the methane gas in at a rate of 1.2 kg/hr through a multi point feed. The methane gas will then be subjected to the molten catalyst where a stirring mechanism will mix the methane gas and molten catalyst for better conversion rate of the reaction. The carbon produced from the reaction will float to the top of the molten catalyst where it will be collected through the pneumatic overflow weir method. The unreacted methane will continue to flow to the solid catalyst where it will finish the reaction. The residence time for the reaction will be 1 hour, the chamber is left alone to give time for the gasses to fully flow through the solid and liquid catalysts and flow into the outlet tube. Going through the outlet tube, the hydrogen and methane gas will be separated by a metallic membrane. When carbon buildup on the solid catalyst starts to significantly affect the solid catalyst reaction, we will conduct an ultrasonicator on it to remove the carbon buildup and regenerate the solid catalyst. A detailed flow chart with all of the subsystems is presented below in *Appendix C*.

The reactor mixing system is the design we will focus on for our alpha design. We will discuss this design in more detail in the next section.

Alpha Design

Due to the time limitation of this semester-long project, we put most of our focus on developing a solution for the main reaction chamber. Combining all selected concepts on subsystems in the previous sections, we came up with a flow chart of the entire system *(Figure 15)* and a detailed sketch of the main reactor *(Figure 17)*.

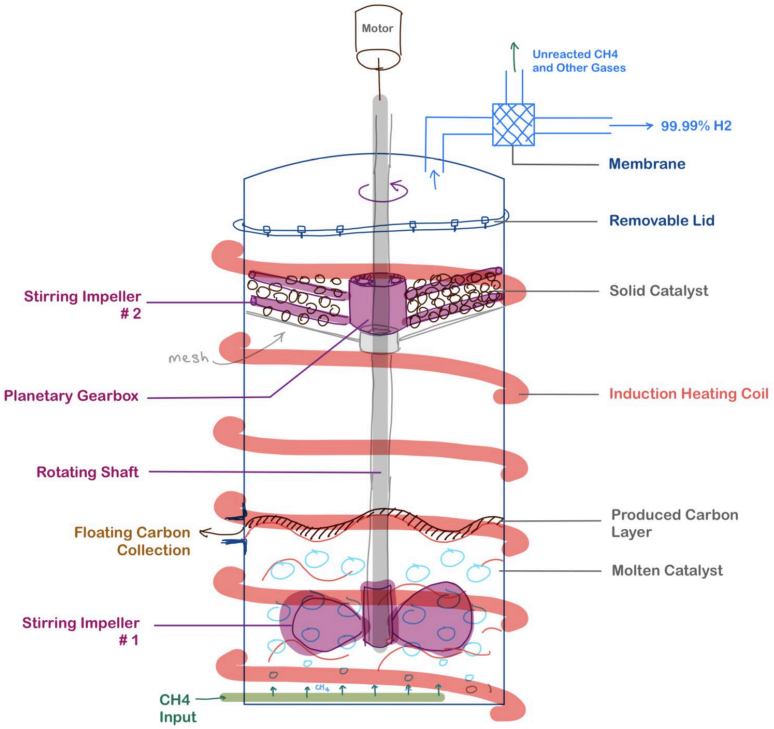


Figure 17. Detailed sketch of the main reactor

This design of the main reactor is adapted from a CSTR reactor. Its key components are shell, gas nozzle, 2 sets of stirring impellers with transmission system, and induction heating system.

The inner volume of the reaction chamber is 3 Liters, and the outer diameter is 200 mm with a height of 500 mm. Dimension requirements are decided by our stakeholder Praneet.
The reactor is heated by induction coils surrounding a stainless steel outer shell. The inner layer of the reactor shell is quartz, decided through previous concept selection. To accommodate the differential thermal expansion between stainless steel and quarts, we may consider putting fillers between the outer and inner shells.

The size and number of holes on the gas feed inlet will be decided based on the required gas flow rate. Further analysis on outlet pressure is also required to determine what type of pump should be used.

The mixing mechanism is composed of two sets of impeller blades for molten and solid catalysts and one rotating shaft at center. The first set of stirring impellers are for better gas-liquid mixture in molten catalyst. We will conduct COMSOL simulation and theoretical calculations to solve the best shape, dimension, angle, and number for impeller blades, based on factors such as molten catalyst viscosity, density, targeted methane bubble size, and bubble density. The second set of stirring impellers are designed to slow down the carbon deposition rate. The stirring process leads to collisions between the carbon-covered solid pellets, causing the removal of the covering carbon layer and slowing down the carbon build-up process on catalyst pellets. The number, shape, size, and gap of stirring rods would be determined based on dimension and geometry of the catalyst pellets selected by our sponsor.
We need to further review research literature and establish our own fluid dynamics model to figure out the best rotation speed for stirring. As the optimal stirring speed must be differ for the molten and solid catalyst, we would use a set of planetary gearboxes for speed adjustment.

The transmission is driven by a motor at top of the system. The selection of the motor will be determined based on the speed and torque required based on our fluid dynamics model. The rotating shaft will be composed of high temperature non-conductive material, further analysis is required for final selection of material.

Induction is used to heat the reactor and provide energy for the pyrolysis process. Our immediate next step is to build a heat transfer model for our system, in order to determine the amount of energy required for maintaining required reactor temperature.

No special H_2 gathering device is required for gathering produced H_2. Because H_2 is significantly lighter than any other gas involved in this system (CH_4 and N_2), it naturally flows to the top of the reactor and will be pushed out by pressure. Therefore, we only need to use a metallic membrane to filter H_2 out from other gasses.

The top part of this reactor is removable, so we could open the reactor to collect carbon and regenerate solid catalyst pellets. As our sponsor proposed, this part is mounted to the reactor by bolts and nuts. Further pressure analysis on internal stress and strain is required to decide the number and size of bolts.

This alpha design is at a very preliminary state compared to what we targeted as a final solution. Extensive theoretical analysis, calculations, modeling, and simulation need to be conducted to justify the choice of geometries, dimensions, and materials to develop this design.

Engineering Analysis

In order to perform our engineering analysis, we had to reevaluate our requirements and specifications to determine what was currently a priority and where we add the most value with our current timeline and skill sets. With our initial specifications, we prioritized the storage safety of methane and hydrogen, the conditions of the pyrolysis reaction, and the mixing requirements as our top 3 most important requirements and specifications. However, after further consideration and discussion with our sponsor and as a team, we decided to focus on the pyrolysis reaction and the mixing requirements for our verification and validation process.

The main reason we are not prioritizing the methane and hydrogen storage and safety requirements is that it is not within our scope given the limited time and resources available to us. The safety precautions of the pyrolysis reactor design and all the components associated with it is always our top priority so that we can ensure the safety of anyone that operates the device. However, we are not able to conduct a thorough analysis of all our requirements and specifications, so given this constraint we have decided to focus our efforts on the pyrolysis conditions and mixing requirements.

We believe that as an engineering team, we can add the most value with these requirements. It is important to note that we will not conduct any validation for our engineering analysis, and focus solely on the verification of our requirements. As we are in the beginning stages of our design process of the reactor, we will focus on the verification process to ensure that our requirements and specifications are reasonable before moving onto the validation phase and building prototypes of the reactor and testing experimentally.

Firstly, we need to verify our mixing requirements. The mixing is the most novel aspect of our design as most methane pyrolysis reactors do not have a mixing system implemented within the reactor to increase the yield of the reaction. Thus, we believe that it is important that we verify that the mixing is practical in an engineering context within the reactor. We will verify various aspects of our mixing requirements such as the flow rate into the mixing chamber. We will also verify the torque and different types of impellers we can use. We will also analyze how the bubble size affects the residence time and yield as well as how much the mixing will improve the conversion rate. We will conduct this analysis through a combination of research, calculations, and simulations detailed in the sections below. The specifics of our verifications are documented in *Table 10.*

Next, the conditions of pyrolysis reaction are the second most important requirements for us to verify. The reactor that we are using will be subjected to a significant temperature and pressure, which will cause various stresses on the reactor shell. Thus, we must design accordingly with these conditions in mind and make sure that it will not fracture, yield, or burst from the stresses and forces it will feel. Below, we will detail different calculations done to confirm the validity of the material and design parameters that were

chosen. We will also further verify our requirements that we set to make sure that our reactor can be safely operated given the requirements we set.

One of the most important specifications is that the reactor should be able to withstand the temperature and pressure during the reaction. This is safety related and has priority over anything else. The analysis will involve the shape and dimension of the reactor, the material properties (quartz), the pressure and temperature of the reactor. Since the shape of the reactor will be cylindrical, there will be two types of stress acting on it: axial stress and circumferential stress, shown in Figure 18. And the stresses are calculated by Equation 1 and 2

$$\sigma_{axial} = \frac{Pr}{2t} \quad [1]$$

$$\sigma_{circ} = \frac{Pr}{t} \quad [2]$$

where P is the pressure inside the reactor, r is the mean radius of the cylinder, and t is the wall thickness of the reactor.

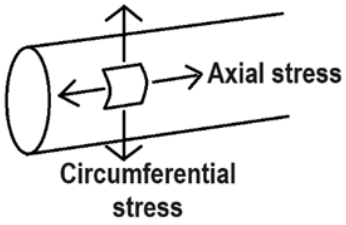


Figure 18. Cylindrical Pressure Vessel Stresses

After comparing the stresses and the strength (yield strength) of the chosen material, we will know if the design will fail or not. This can also be done by computer simulation (finite element analysis) which can evaluate parts of the reactor that are of irregular shapes, which is hard to calculate by hand. However, the most effective way to test is experiment, because theoretical analysis might be inaccurate especially when the material properties might change at high temperature and material fatigue might occur when we frequently turn the reactor on and off. To conduct the experiment, we will need to build the reactor prototype, pressurize it to the specified pressure and heat it to the specified temperature. To simulate steady state operation, we will maintain the temperature and pressure for an extended period of time. To include the effect of material fatigue, we will vary the temperature and pressure from room temperature and pressure to the working temperature and pressure to simulate the turning on and off of the reactor. To include safety factors, we will test it with higher temperature and pressure.

One of the key parameters is that the reactor should process 1 L of methane at 500 kPa per hour. We need to check if our selected compressors can provide the flow rate at the required pressure. Both theoretical analysis and experiments are essential for this. We anticipate having at least 2 air compressors in the system. One to pressurize the feed gas and one to compress the produced hydrogen for storage. To determine if the chosen compressor is sufficient, we will first obtain the power and maximum pressure

ratings of the compressor. And then compare the ratings to the required numbers. The required power for the compression process can be calculated as follows:

First, calculate the mass corresponding to that volume of methane using the methane molecular weight and the ideal gas law:

$$PV = nRT \quad [3]$$

where P = 500 kPa, V = 1 L, T = 500 C, and R = 8.314 J/mol*K. The number of mols is calculated to be $7.78*10^{-5}$. With a molar mass of 16.04 g, the mass of the methane will be $1.245*10^{-3}$ g. Assuming a 100% conversion rate, and using conservation of mass ($CH_4 \rightarrow C + 2H_2$), we can calculate the hydrogen production rate is $3.135*10^{-7}$ kg per hour. After that, we can calculate the work needed to compress the hydrogen from 500kPa to 20MPa which is the specified pressure for storing it using Equation 4:

$$W = P_1 V_1 ln(\frac{P_1}{P_2}) \quad [4]$$

where P_1 and V_1 are the pressure and volume before compression, and P_2 is the pressure after compression. W is calculated to be 92 J and the minimum continuous power is 0.026 W.

Experiments will be more effective than theoretical analysis because the ratings might be inaccurate and it is difficult to include factors like flow resistance or friction and other kinds of energy loss in the flow system. To conduct the experiment, we need to have the fully assembled prototype of the flow system (heating is not necessary). We will feed methane into the system at the desired flow rate and measure the pressure at different stages in the system to determine if the numbers satisfy our specifications.

Another thing to consider is the heating power of the heaters, including both preheating and main reactor heating. Sufficient heating power is needed in order to heat the gas and the reactor to desired temperatures to have a high conversion rate of methane. To analyze the heating process, we examine the gas at 3 different stages in the reactor, as shown in Figure 19.

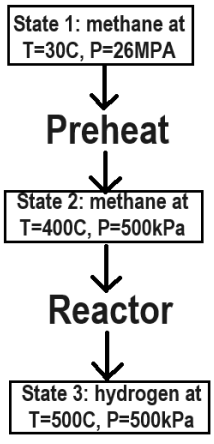


Figure 19. Different States of Gasses

To calculate the required power for preheating, we compare the states of the gas before and after preheating, and the required power can be calculated by Equation 5:

$$P = C\, m\, \Delta T \quad [5]$$

where C is the specific heat of methane, m is mass flow rate of methane, and ΔT is the temperature difference before and after heating. With these specified parameters, the power needed is calculated to be 0.005 W.

To calculate the heating power needed for the reactor, we compare the state of the gas when it just enters the reactor against the state when the gas leaves the reactor. One thing to notice is that the pyrolysis process is endothermic so it cannot be calculated directly from the same equation used for preheating. The enthalpy change for the reaction (75.4 kJ per mol of methane) should also be included. And the required power is calculated to be 0.003 W. In this case, it is more easily analyzed theoretically than experimentally. However, it becomes a little more complex when we consider the heat loss from all the parts of the system (reactor or pipes), and of different forms (conduction, convection, and radiation). In addition, since we are using inductive heating, there will be additional energy losses associated with that energy transfer. These factors are possible to be included into theoretical analysis but will increase the difficulty of it. Computer simulations will be very helpful in assessing the heat losses and inductive heating efficiency. The total required heating power will be the sum of the power for reaction and the heat losses. The advantage of computer simulation over theoretical analysis is that simulation may provide a clear view of the temperature distribution over the system which can give us insights on how to improve the design to reduce heat loss (for example, places to put thermal insulation). It will then save the operational power consumption.

Note that all the calculations are performed with 1 hour residence time (which is just the upper bound so the actual residence time will be much shorter) and that is the reason why the calculated power values are small.

We have decided to incorporate stirring mechanisms into the reactor to help with mixing the gas and molten catalyst and to clean the solid catalyst. Therefore, we need to analyze the power needed to drive the stirrers. The analysis can be conducted either through fluid simulation or experiments. To conduct fluid simulation, we will need completed reactor CAD design, catalyst properties such as the viscosity and density, as well as the stirrer geometry. One way to estimate the power is to set a speed for the stirrer, and obtain the resulting resistance force on it from the simulation. The power can be calculated with Equation 6:

$$P = \tau\, \omega \quad [6]$$

where τ is the resistance torque acting on the stirrer and ω is the angular speed of the stirrer.

This can also be analyzed experimentally which is more accurate but also involves more challenges. To experimentally test it, we need the fully assembled reactor prototype with heating and catalysts in it, as well as the stirring mechanism. We will choose a motor with a sufficiently high power rating to stir the catalysts and adjust the power so that the stirring speed matches the specification.

The effectiveness of mixing can be specified by the gas bubble size, and residence time. These 2 factors are essential for the high conversion rate of the reaction. Since the reaction mainly takes place at the interface between the gas bubble and the molten metal catalyst, we desire a high surface area to volume ratio of the bubbles, as shown in Equation 7:

$$\frac{A}{V} = \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = 3/r \qquad [7]$$

where r is the radius of the bubble. From this equation we decide that we want the bubble size to be as small as possible to have a better conversion rate. Residence time is another factor that governs the conversion rate. The longer the gas is in contact with the catalyst, the higher the conversion rate. The bubble size and residence time are impossible to analyze theoretically and will need the help from computer simulations. We will test various stirrer geometry and stirring speeds and choose the best design.

The stirrer and shaft design will require special attention because molten metal is usually much more viscous and denser than water, which means the stirrer and shaft will experience greater stress. While the shaft will be uniform and can be analyzed theoretically (torsional shear stress is calculated by Equation 8, and it is compared to the shaft material yield shear stress), the strength of the stirrer (which will be non uniform) will rely on computer simulations.

$$\tau = \frac{T r}{J} \qquad [8]$$

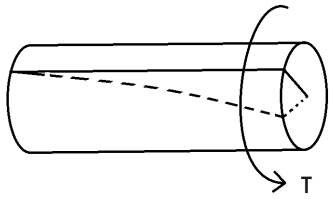


Figure 20. Torsional Deformation of Shaft

Torque Calculation

To calculate the power required to mix the liquid catalyst within the reactor, a mix of fluid dynamic equations as well as knowledge of motor efficiency must be used. From a source on motor mixing efficiency, it is likely with the gaseous liquid, there could be an efficiency loss of nearly 80%, so to calculate a max motor power this must be accounted for in calculations. Full mixing calculations can be found in Appendix G. First, the most important step is determining the Reynolds number applicable for the speed you are mixing the liquid at, shown in Equation 9:

$$Re_i = \frac{N_i D_i^2 \rho}{\mu} \qquad [9]$$

With N_i representing the speed in RPMs, the molten metal is being mixed at, D_i being the diameter of the mixing blade shown in Figure 21, a diagram to show different features of a similar reactor that includes baffles, ρ being the density of the liquid being mixed, and μ being the viscosity of the liquid, in this case these equations specifically are indicating the mixing capacity of the Rushton mixing blade style which we have chosen for our final design. The Reynolds number helps us to determine the type of flow we are seeing within the reactor. With liquid mixing, a Reynolds number above 10^4 displays turbulent behavior in the liquid.

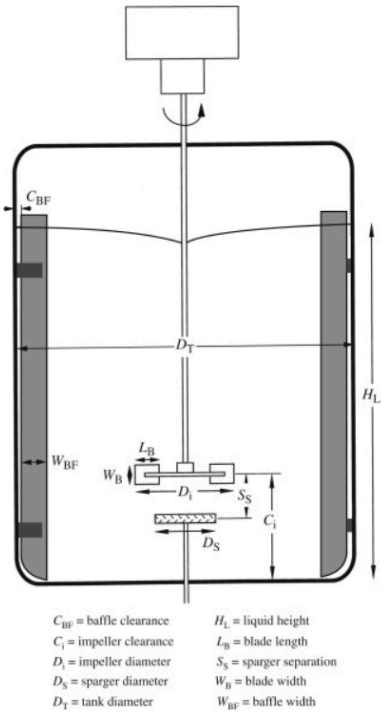


Figure 21. Stirred Tank with Rushton Turbine, including baffles [40]

While under it is laminar flow, with different amounts of vortexing, disturbance in the smooth laminar flow. Next, there are two equations to calculate the torque required to overcome the force of the liquid at rest, one for when the liquid is turbulent and one for when the flow is more laminar. Equation 10, to calculate power when the flow is completely laminar and Equation 11, when the flow is turbulent.

$$P = k_1 \mu N_i^2 D_i^3 \quad [10]$$

$$P = N_P \rho N_i^3 D_i^5 \quad [11]$$

N_P and k_1 are factors used to implement the effect of different types of flow on the mixing power. These equations are both used when the construction of the tank is standard [41]. When the vessel is non-standard to calculate power Equation 12 must be used, to properly account for geometry.

$$P = \phi(\rho N_i^3 D_i^5)(N_i^2 D_i/g)^{[(\alpha - log_{10}Re_i)/\square]} \quad [12]$$

ϕ is a factor calculated from the geometry of the tank. α and $\square$ are the ratios between different aspects of the tank, height of the liquid versus diameter of the tank and height of the liquid versus the height of the gas inlet, g is gravitational acceleration. From there P, provides you with the minimum amount of power required to operate the machine, assuming only liquid resistance. To account for efficiency loss it is then necessary to divide the resulting power by 0.2. Actual torque can be calculated from Equation 13 where M is torque. Using the previous two values we can come up with a range of torques that can give us an estimate to determine a usable motor.

$$P = 2\pi N_i M \quad [13]$$

Yield Stress Analysis

The yield stress of a material can be calculated to determine the yielding of the material due to the pressure and temperature of the pressure vessel. However, since the material we are choosing to build the reactor out of is quartz, a brittle material, it typically would not exhibit yielding like a ductile material such as stainless steel or aluminum would exhibit. Brittle materials tend to fracture instead of deform plastically and generally do not have a reported yield strength, so we will focus on the fracture stress analysis instead for this report [42].

Fracture Stress Analysis

To perform the fracture stress analysis of the cylindrical pressure vessel, we will need to determine if the stress intensity on the pressure vessel is greater than fracture strength/ tensile strength of the material. The stress intensity can be calculated with the hoop stress equation above in Equation 1 and 2. The fracture strength of quartz is 48 MPa [43].

For our analysis, we will assume that no outside torque will be applied to the pressure vessel. We will assume that the mixing mechanism will be built outside of the pressure vessel and will apply the torque to a shaft through the reactor but not to the reactor material itself. We will also be using the assumption detailed in our flow chart in Appendix C, that our maximum pressure achieved is 500 kPa. Finally, we will be considering a thickness of 5 mm and outer radius of 100 mm as an initial calculation.

Leak Before Break Analysis

The leak before break analysis is performed to determine the fracture mechanics that a crack would grow through the wall. In order to perform this analysis on the cylinder pressure vessel, we will need the fracture toughness of the material we are using, quartz. The fracture toughness of quartz is about 1.74 MPa$\sqrt{}$m [44].

In order to determine the fracture stress and how a crack will affect the pressure vessel, we will use the stress intensity factor equation for cylindrical pressure vessels. The stress intensity factor of a cylindrical pressure vessel can be calculated using Equation 14 below.

$$K_I = \sigma_{axial}\sqrt{\pi a} \quad [14]$$

where K_I is the Mode I stress intensity factor, σ_{axial} is the axial stress, and a can be calculated as 2 times the thickness.

For this analysis, we will assume a circumferential crack with a length of 3a and a depth of 0.5a. This is shown below in the visual in Figure 22.

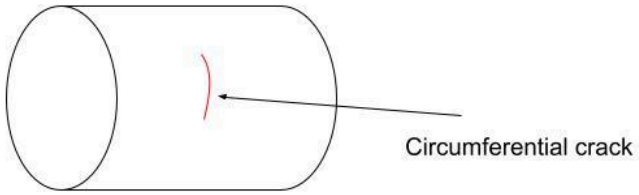


Figure 22. Cylindrical Pressure Vessel Crack

There are some specifications that are difficult to analyze theoretically or experimentally. One of them is that the reactor should have a high conversion rate and reuse excess reactants. The actual conversion rate of the reaction is hard to analyze theoretically and is best to be tested experimentally. This will be a challenge because it needs the fully assembled working prototype, which is still far from our current stage in the design processes. We can try to look into computer simulations to see if they are capable of solving the conversion rate for our system.

Another specification says the reactor should run at least 20 hours without needing to regenerate the catalysts. It is difficult to model the carbon deposition in the solid catalyst and the effectiveness of the solid catalyst stirring mechanism so this can only be tested experimentally. And that also requires the fully assembled working prototype which we currently do not have.

Final Design

Based on the engineering analysis, we developed our alpha design into a final design. Due to the time limitation of this semester-long project, we put most of our focus on creating a solution for the main reactor.

In the alpha design, we detailed 5 subsystems including reactor vessel, heat source, methane inlet, mixing mechanism, and hydrogen collection. Our sponsor has decided to use an induction furnace as the heat source, which ensures uniform heating of the entire reaction chamber. We moved our focus away from the hydrogen collection system because it is beyond the main reaction. Therefore, when building our final design, we focused on three subsystems strongly correlated with the main pyrolysis reaction–reactor shell, methane inlet, and mixing mechanism. A detailed design solution This is shown below in Figure 23.

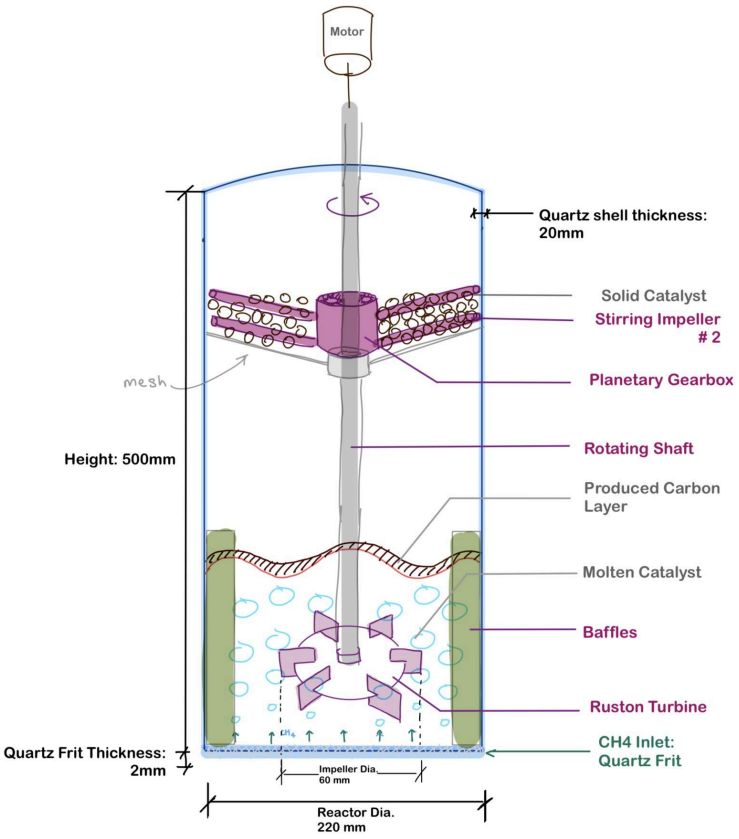


Figure 23. Detailed Sketch of the Main Reactor

The reaction chamber is a two-stage, CSTR reactor. The material we are choosing to build the reactor out of is quartz. The inner volume of the reaction chamber is 3 Liters with an outer diameter of 220mm, and a height of 500mm. Dimension requirements are decided by our stakeholder Praneet. The thickness of the quartz shell is set at 20mm, established through leak before break analysis with a safety factor of 4. This ensures structural integrity and safety throughout operation.

In the alpha design, a dual-layered construction was proposed, featuring a stainless steel outer shell and a quartz inner shell. This configuration was intended to accommodate the use of an induction coil as the heat source, necessitating an electrically-conductive outer shell for heat generation. However, with the adoption of an induction furnace as the new heat source, the requirement for an electrically-conductive outer shell is obviated. Consequently, the final design simplifies to a single-layered construction, utilizing quartz as the sole material for the reactor vessel's shell.

Methane gas is going to be fed into the reactor with quartz frit. We chose quartz frit over sparger for better manufacturability. By utilizing quartz frit as the material for the gas inlet, it allows for seamless integration with the reactor shell, which is also made of quartz. This ensures that both components can be joined together effectively, forming a unified structure. According to the literature reviewed, the research team utilized a quartz fist with a thickness of 2mm, which produced densely packed microbubbles of

methane. The size of these bubbles ranged from 10 to 15 micrometers [45]. This design is able to withstand our target mass flow rate of 1.2kg/hr.

To ensure optimal mixing of methane and molten catalyst, impellers and baffles were employed to generate radial flow with high shear levels, facilitating uniform distribution throughout the reactor vessel. Emphasizing our sponsor's objective of achieving a high conversion rate of methane while minimizing waste, particular attention was devoted to subsystems enhancing the methane-catalyst reaction.

Key strategies focused on prolonging methane bubble residence time and maximizing the total surface area available for reaction. This approach not only extends the duration of methane bubbles within the reactor but also augments the overall surface area for interaction, thereby fostering enhanced reaction efficiency. In the verification section, COMSOL simulations were employed to substantiate the efficacy of these strategies in improving the conversion rate.

The selected impeller design features a Rushton turbine—a flat horizontal disk equipped with vertically-mounted blades. The presence of baffles could also increase the shear levels in the flow[41]. This design promotes radial flow with high shear levels, ensuring uniform mixing of methane and molten catalyst throughout the reactor vessel, as shown in Figure 24. Following the principle guiding radial flow impeller design, the turbine diameter is set at one-third of the vessel diameter, measuring 60 mm in this instance. This ensures optimal mixing performance while maintaining compatibility with the reactor vessel's dimensions. The baffle size still needs to be determined by further testing as we have not decided a baffle size.

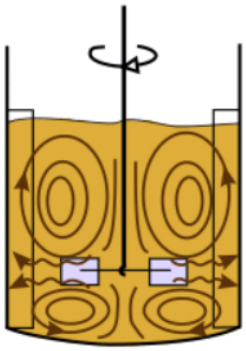


Figure 24: Radial Flow with High Shear Levels Created by Rushton Turbine and Baffles

While significant progress has been made in finalizing key components, certain subsystems, such as the solid catalyst stirring mechanism and transmission system, remain under ongoing development and optimization.

The second set of stirring impellers are designed to slow down the carbon deposition rate. The stirring process leads to collisions between the carbon-covered solid pellets, causing the removal of the covering carbon layer and slowing down the carbon build-up process on catalyst pellets. The number, shape, size, and gap of stirring rods would be determined based on dimension and geometry of the catalyst pellets selected by our sponsor.

The transmission is driven by a motor at top of the system. The selection of the motor will be determined based on cost and the speed and torque requirements. The rotating shaft will be composed of stainless steel. As the optimal stirring speed is different for the molten and solid catalyst, we would use a set of planetary gearboxes for speed adjustment.

Verification and Validation Plans

We have previously verified in the requirements section of this report through largely research from a wealth of literature specifically on methane pyrolysis, our technical specifications. To verify that our specific final design meets the specifications that we have set out, we have outlined in *Table 10* the processes that we will go through to ensure our design is meeting those requirements. Some methods are easily completed at this juncture, however some shown in the chart as not tested, are unable to be evaluated until further research into reaction kinetics has been completed to make the simulation of our reactor chamber more accurate. Reaction kinetics being the method by which COMSOL is able to simulate the ability of the catalyst to help along decomposition of the methane.

Table 10. Verification Table

Requirement	Engineering Spec	Verification Method	Priority	Status
Heat Resistant Reactor	Withstand T=700C while P=500kPa	Stress analysis on the reactor shell	Critical	Pass
Pyrolysis Temperature	Reaction Temperature T=500C	Calculation of minimum required heating power to sustain the chemical reaction and maintain reactor temperature, including heat losses	Critical	Pass
Methane Flow Rate	1.2kg/hr	The analysis of other functions is based on this flow rate. Experimentally, we will set this flow rate and check if other subsystems match their specifications	Medium	Pass
High Methane Conversion Rate	60%~70%	Will be tested through creating a Comsol model, which with the heating and fluid modeling capabilities can reflect a modeled conversion percentage to meet our desired methane conversion rate. Will further test mixing to see if mixing improves the modeled conversion percentage and reaches the desired methane conversion rate.	High	Pass
Impeller	1 to 10^4	Discuss the mixer types in regards to	High	Pass

Viscosity Range	centipoise	viscosity and fluid dynamic capabilities. Prove that the Rushton Mixer can mix our molten catalyst at the optimal range and meets our mixing requirements		
Motor Torque	0.818 to 4.09 Nm	Perform calculations on the motor torque needed to move the molten catalyst at the necessary RPM and compare it to existing motors in the market to make sure it meets standard practice and are available	High	Pass
Bubble Size	Methane inlet bubble diameter <3mm	Through simulation and directly observe the bubbles with a working prototype	Medium	Not tested
Sized for Laboratory	Reactor diameter <200mm, length <500mm, volume 2~3L	Check prototype dimensions against this specification	Medium	Not tested
Hydrogen Production Rate	0.21kg/hr	This is directly related to methane flow rate and conversion rate. It will pass if methane flow rate and conversion rate both pass. (see below)	High	Not tested

Fracture Stress Analysis

Using the equations in the section above, the stress intensity using the hoop stress was calculated to be 9.5 MPa shown in Appendix F below. The fracture strength/ tensile strength of quartz is 48 MPa. Thus, we can calculate a safety factor of 5.05. Based on these calculations, we can confidently conclude that the quartz material will not fracture from the pressure inside the pressure vessel.

Leak Before Break Analysis

Using the equations in the section above, we calculate the stress intensity factor to be 842 kPa shown in Appendix F below. The fracture toughness of quartz is 1.74 MPa$\sqrt{m}$. This will give us a safety factor of 2.07 for the leak before break condition. Thus, the pressure of the pressure vessel is not a concern for our current design.

Influence of Methane Bubble Size on Residence Time

The molten catalyst speeds up the pyrolysis reaction which only takes place at the interface between the methane gas and the molten catalyst (at the bubble surface). As previously shown, we want the bubble size to be small so that it has a high surface area/volume ratio for higher methane conversion rate.

In addition, since the conversion takes time, we also want the bubbles to stay in the molten catalyst for a longer time (lower rising velocity). To achieve this, we first studied previous research articles about

another gas (Argon) and other molten metals (Tin, Lead, Copper) [46]. As shown in Figure 25, the rising velocity decreases as the bubble radius decreases, in an approximately linear relationship.

We then ran COMSOL simulations to check if this relationship still holds for our system (Methane and molten catalyst). For the simulations we set the height of the molten catalyst to 150 mm. The physical properties (density, surface tension, and viscosity) were assigned for the 2 kinds of fluids. For the gas we assumed it was pure methane and no hydrogen was produced when the bubbles rose. For the molten catalyst we assumed it was pure bismuth because the actual composition of the catalyst was over 95% bismuth and 5% nickel and molybdenum. 4 different sizes of bubbles were tested, 10mm, 5mm, 2.5mm, and 1mm. The simulation used the "level set" method to solve for the gas-liquid interface.

Using the results produced by COMSOL, we measured the rise time (as shown in Figure 28) for each bubble and calculated the average rising velocity. COMSOL generated a series of graphs with 0.1 second time step for each simulation with different bubble size. The graphs shown are the half cross sections of the reaction chamber, so that the left sides of the rectangles are the centerlines of the reactor and the right sides are the walls of the reactor. The blue sections are the molten catalyst and the red sections are the methane gas. The bubbles started rising from the bottom at t=0 and we counted the time when they left the molten catalyst section. The average rising velocity was calculated by dividing 150mm with each rising time. The results are shown in Figure 26 and 27, and they match the experimental data where smaller bubbles have longer residence time and slower rising velocity. Therefore, we can conclude that smaller bubble sizes will benefit our reactor.

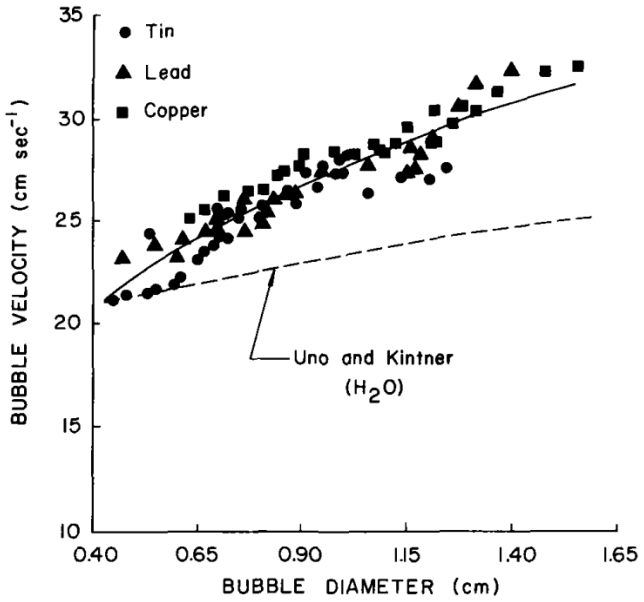


Figure 25. Experiment data of Argon bubble velocity vs. bubble size through different molten metals [46]

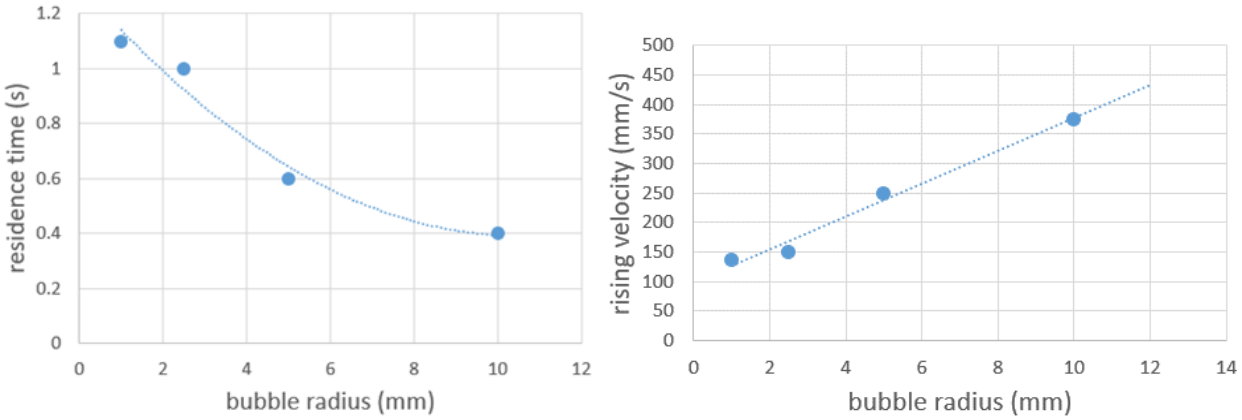


Figure 26 (left) and 27 (right). Simulation results of methane bubble rise time and velocity vs bubble size through molten Bismuth

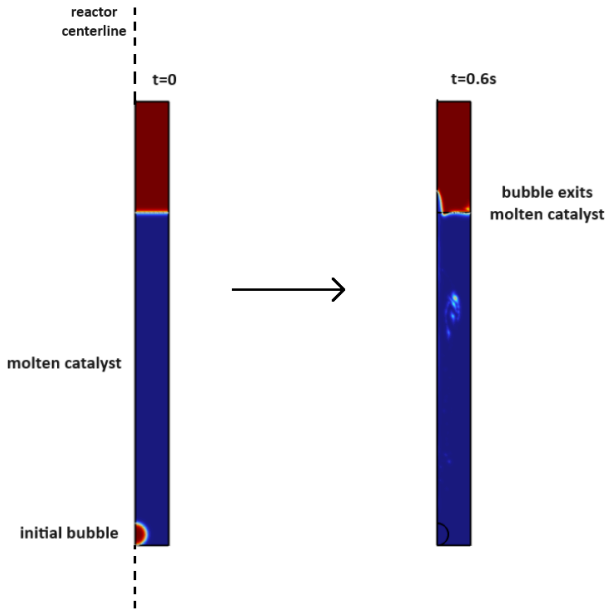


Figure 28. Measuring residence time of methane bubbles.

Heating Power

For the lab-scale reactor we have decided to use an induction furnace instead of open induction coils. This simplifies the analysis for heat loss and heating power. Considering a control volume containing the whole furnace at steady state, the heat loss from the reactor will be equal to the heat loss from the furnace walls to the ambient. The minimum heating power required will be the enthalpy change for the chemical reaction plus the total heat loss from the furnace walls.

$$Q_{req} = Q_{rxn} + Q_{loss} \quad [15]$$

Where Q_{rxn} includes both the enthalpy change of the pyrolysis reaction at constant temperature and the energy needed for the change in temperature. This can be calculated directly. For 1.2 kg of methane and 1 hour reaction time, Q_{rxn} is calculated to be 9951 kJ/hr, or 2764 W.

Q_{loss} will be complex to analyze or simulate. Instead, we refer to a research article that has a thorough analysis of the heat loss from a lab furnace [47]. The research tested a furnace with 6 different types of materials (Figure 29) and 4 different heating modes (Figure 30). We refer to this research because the temperature range and variation have similarities to our system (since we will turn the reactor off to replace the catalyst or collect carbon). As shown in Figure 31, the best of the 6 walls (wall 6) showed an average heat loss as low as ~100 MJ/m^2 over 8 days of operation for all 4 heating modes, which is approximately 145 W/m^2. Given the dimensions of our reactor, we will not need the furnace to be larger than 0.4m*0.4m*1m. The total surface area will be smaller than 1.92 m^2. Therefore, if we build our furnace with the same materials as wall 6, the heat loss from the furnace will be < 279 W. And the total required heating power for the reactor (furnace) Q_{req} will be 3043 W.

No	The chamber wall structure	Wall parameter		Maximum application temperature
		Material	Thickness, mm	°C
1.	wall 1	mineral fiber	300	1430
2.	wall 2	mineral fiber chamotte brick	300 270	1430 1370
3.	wall 3	chamotte brick	1070	1370
4.	wall 4	chamotte brick chamotte brick L10	630 460	1370 1300
5.	wall 5	chamotte brick mineral fiber	115 300	1370 1430
6.	wall 6	mineral fiber mineral fiber WDS	300 150	1430 950

Figure 29. Different Wall Materials

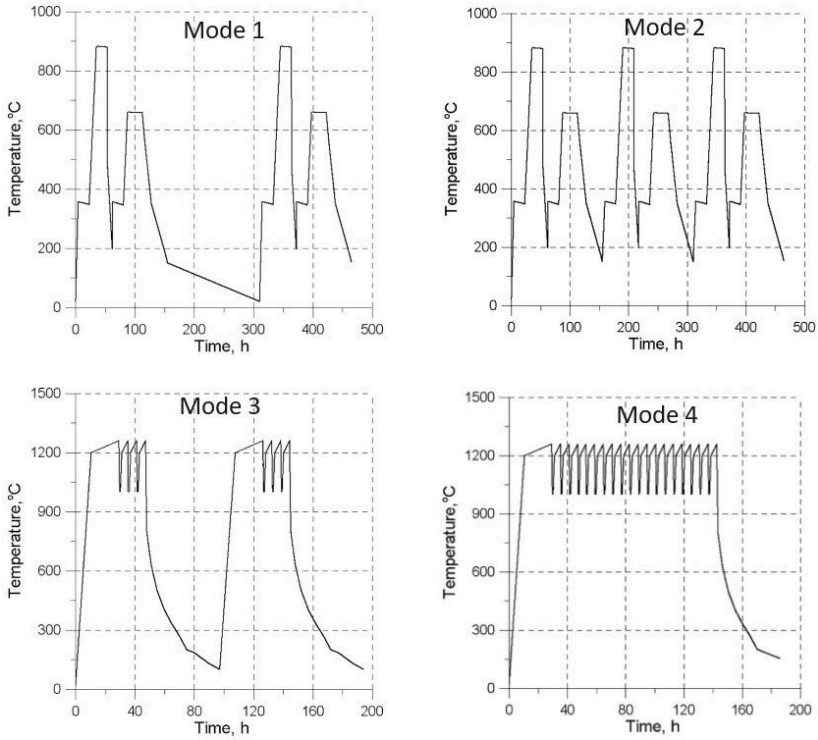


Figure 30. Heating modes used in research [47]

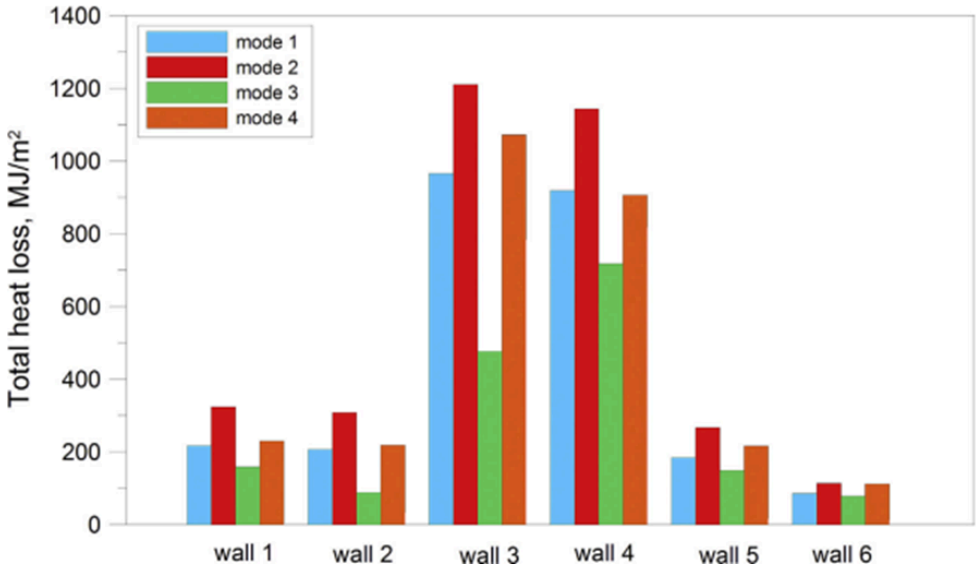


Figure 31. Heat losses of different types of furnace walls during different heating modes [47]

Effectiveness of Molten Catalyst and Methane Mixing

The mixing feature is one of the key parts to higher methane conversion rate. We want the impeller to either break the bubbles into smaller ones or to create turbulence to allow the bubbles to have longer residence time, or both. Directly simulating the interactions between the impeller, the gas, and the molten

catalyst using the particle tracing function in COMSOL will be complicated and extremely time-consuming. Instead, we looked at the overall methane conversion rate as an indicator for the effectiveness of mixing.

With the help of Praneet, we ran 2 sets of simulation. Since we were unable to find the exact equation and parameters which govern the reaction kinetics with our chosen catalyst, we used arbitrary numbers based on existing research about methane pyrolysis with other catalysts. [48, 49, 50] The purpose of running the simulations is not to determine the exact methane conversion rate. Rather, we just wanted to show that adding the impeller actually improves it.

In the first simulation the molten catalyst is at rest, whereas in the 2nd simulation we manually defined the velocity field in the molten catalyst. All other parameters were kept the same. The simulation results are shown in Figure 32 and 33. In Figure 32 the color indicates the mole fraction of methane where red is methane and blue is hydrogen. Methane enters the reactor from the bottom and has a mole fraction of 99%. After going through the 1st reactor, the gas mixture contains around 55% methane (44% conversion rate). After going through the 2nd reactor, the gas mixture contains only 28% methane (71% conversion rate). As shown in Figure 33, the difference in conversion rate between the 2 reactors is over 20% when the gas leaves the molten catalyst. This proves that the mixing feature actually improves the methane conversion rate. After we have done further research and found the specific reaction kinetics for our catalysts, we will be able to modify these simulations and get more accurate numbers of methane conversion rates.

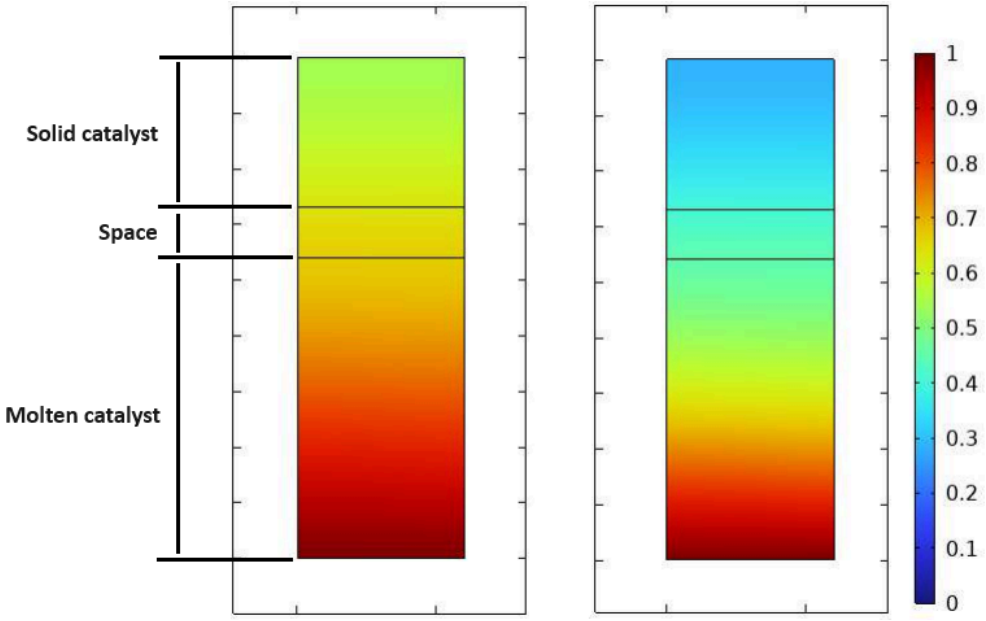


Figure 32. Half cross section views of the reactor showing concentration of methane across the reactors. Left without mixing, right with mixing. Color indicates methane mole fraction. Methane enters the reactor from the bottom with an initial mole fraction of 99%.

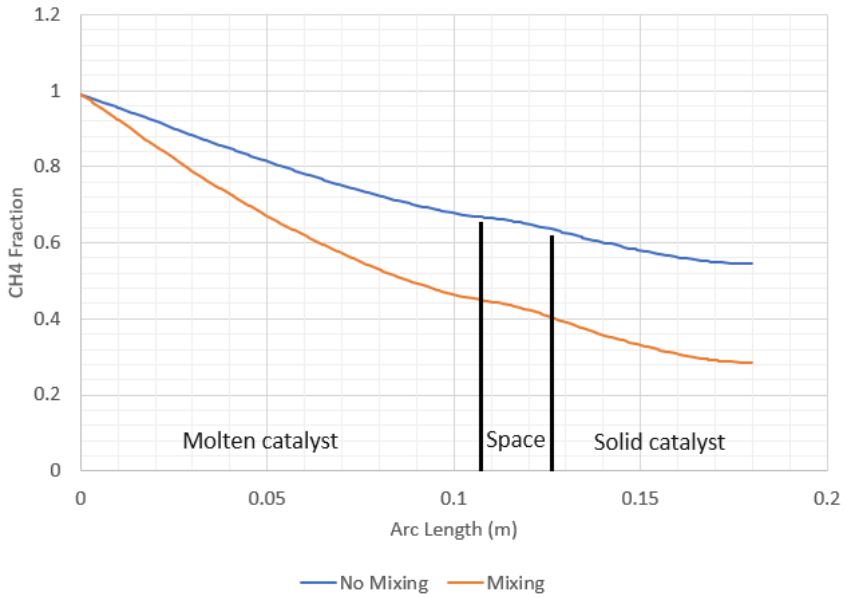


Figure 33. Comparison of mole fraction of methane across reactors with and without mixing, arc length indicates the distance from the bottom of the reactor. Methane enters the reactor from arc length = 0 and with an initial mole fraction of 99%.

Sensitivity Analysis

After performing our mixing analysis, we focused on improving the accuracy and efficiency of our model by finding the ideal conditions for the reaction. First, we needed to perform a sensitivity analysis on the main parameters of the model: methane flow rate, temperature, and pressure. Using the parameter values set in our final design, we performed a 10% perturbation to determine the sensitivity of each of these parameters. This meaning, the values were varied by 10% to determine the effect they had on the conversion rate. The results are shown in Figure 34 below.

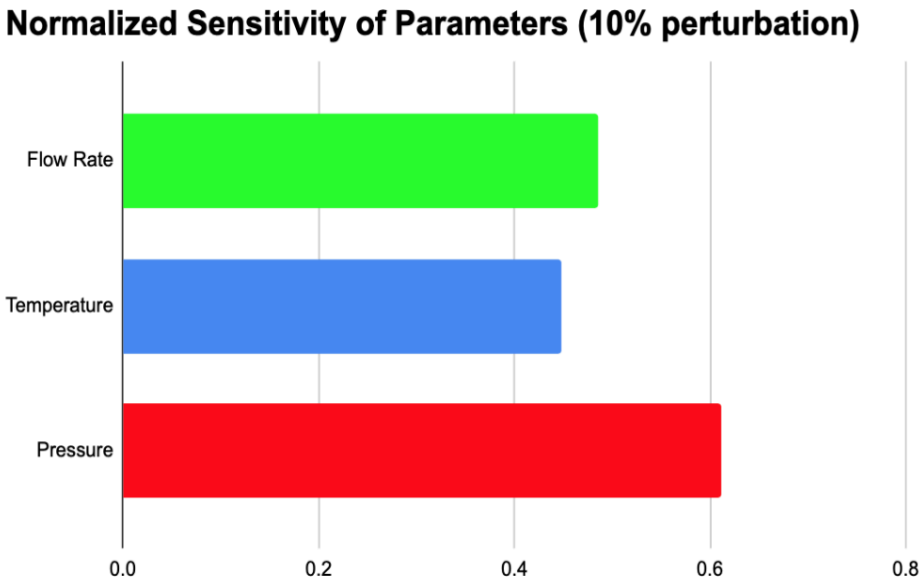


Figure 34. Sensitivity Analysis of Parameters in COMSOL Model

Based on the sensitivity analysis, we determined that pressure was the most sensitive parameter followed by methane flow rate and temperature. This is what we would expect to see from our research. The methane flow rate and pressure were inversely proportional to the conversion rate while the temperature was proportional with the conversion rate. From further analysis, we were able to determine the required parameter values in order to attain the required conversion rate. The required parameters are shown below in Table 11 below.

Table 11. Comsol Parameters to Meet Conversion Rate Requirement

Comsol Parameter	**Value**
Methane Flow Rate	< 0.0006 m/s
Pressure	> 773 K
Temperature	< 100 kPa

Verification of Rushton Mixer Type

To determine the effectiveness of different types of mixers we analyzed different types of mixing blades to see if it fits our criteria for the mixer in our liquid catalyst. These criteria include whether it can effectively mix the viscosity seen by our molten catalyst, how feasible it is to manufacture with our chosen material, how expensive it would be to purchase for a real life design, and how often it is commonly used in gas/liquid mixing. This was put into a chart to determine how each design performs, revisiting idea generation and evaluation. The main way this shape is validated is through research input into this chart, we are able to determine through various sources whether the rushton type mixer aligns for our needs.

The dynamic viscosity for our mixture of molten metals is assumed to be 2.71 centipoise which is slightly larger than the viscosity of water, reference, the mixture is a majority molten bismuth at roughly 500 degrees celsius. From Figure 35 we can see there are a range of viscosities that make sense for each type of mixing methods. The Rushton type mixer falls into the category of Flat-Blade turbine on this chart, often referred to as a 6 blade flat turbine. From this chart we can see that just over one centipoise puts it well within the viscosity ranges associated with propellers and flat blade turbines. If we were to use a type of mixer that has a range well above our viscosity, the mixer would spin around in the mixture without actually mixing anything.

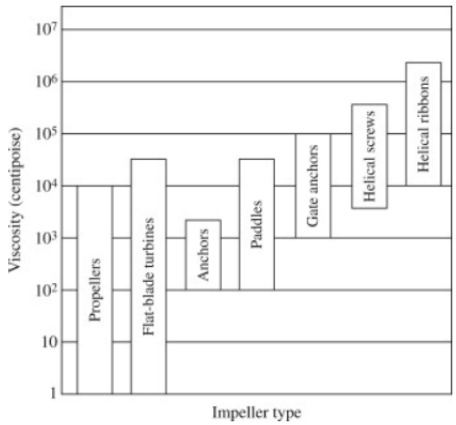


Figure 35. Types of Impellers and their ranges of viscosities over which they are effective [41]

From there we can more in detail think about the purposes of various types of propellers and flat blade turbines, in terms of how much turbulence and laminar flow action they produce as shown in Figure 36 below. With Rushton turbines, a good amount of turbulence and flow is provided, this chart also showing Hydrofoil Impellers and Pitched Blade Turbines to be comparable. We desire, for mixing, something closer to the Rushton turbine's ratio of turbulence and laminar flow for mixing our liquid catalyst. We want some turbulence as we would like the gas to have greater residence time within the molten catalyst and return greater hydrogen conversion, but we also would like the carbon to flow upwards through the molten catalyst, without being continually forced around the liquid and into the walls.

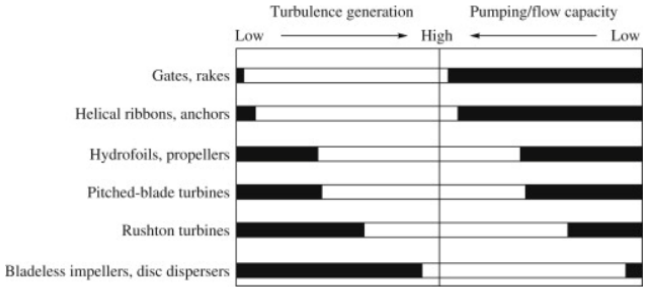


Figure 36. Proportion of Turbulent to Laminar flow by different types of propellers and flat bladed turbines [40]

Hydrofoils, Rushton Turbine, and Pitched Blade turbines are all additionally used in lab settings for mixing. Rushton Turbines are fairly easy to buy for a lab setting, they are fairly machinable so if we desire to make them out of a material other than stainless steel, we are able to do that. Since both pitched blade turbines and hydrofoils have twisted blades they would be more difficult to easily machine with other materials. From *Table 12*, summarizing the previous statements, looking at 3 styles of impeller from the 2 categories provided in Figure 33, with green meaning it works, yellow meaning it is potentially passable and red meaning not very effective, we can see that the Rushton Turbine is the clear winner.

Table 12. Table Summarizing the Effectiveness of Potential Mixers

Mixer	Within the Appropriate Viscosity Range	Has the Right Mix of Turbulent and Laminar Flow	Commonly Used in Lab Settings	Easy to Manufacture
Hydrofoil				
Rushton Turbine				
Pitched Blade Turbine				

Verification of the Motor Torque

From our provided equations 9, 11, and 13 in the Engineering Analysis Section, the calculated motor torque that needs to be produced is from 0.818 Nm to 4.09 Nm as shown in Appendix G. When researching motors, a motor can be found that meets the specifications that we expect for our design and using a standard market motor is reasonable and keeps a prototype without our group in the future more reasonable. Looking at the specifications from motor websites such as ORBEX group, a continuous stall torque above the range we desire is easy to find. [51]

Hydrogen Production Rate

The hydrogen production rate is specified to 0.21kg/hr. This can be verified after verifying the methane flow rate (1.2kg/hr) and the methane conversion rate (70%). According to the pyrolysis reaction formula ($CH_4 \rightarrow C + 2H_2$) and the molar mass of methane (16) and hydrogen gas (2), 1.2kg methane will produce 0.3kg hydrogen if with 100% conversion rate. With a 70% conversion rate, 0.21kg hydrogen will be produced. Therefore, if the methane flow rate and methane conversion rate each pass their specifications, it implies that the hydrogen production will match its specification.

Discussion

Problem Definition

The breadth of our research started out very wide, this meant that there were a lot of papers that covered some aspect of methane pyrolysis. This was good for our design process at first to get a broad sense of the process of pyrolysis, however it was difficult to quickly narrow down the process to focus. To better define a problem for our team to solve, it would have been better to develop a way to narrow down the section we were focusing on. A morphological chart to simply weigh the benefits of focusing on certain areas of a reactor for researching our project focus.

The research used by our team ranged over a lot of different periods of pyrolysis research, so it is possible inaccuracies have been corrected by later papers that were not included in our research. With more time our team would be able to more thoroughly vet the information used in construction of our model and make sure that all information used is up to date. A methodical consideration would be done of each of our sources to make sure the information is still relevant.

If we had time and more resources, our team could see if we can connect with other universities that have a lab scale model and see if we could ask them specific questions, consult more professionals with chemical engineering backgrounds. Our methods were very literature focused, because initially it was very important for us to catch up on the basics of what is happening with the process, which can be more easily gleaned from literature, as it is more directly accessible. But, if we were able to talk to more experts who use these types of technologies, we would have been able to ask more specific questions about construction of the vessels for pyrolysis, as well as the ways other pyrolysis reactors regulate the pressure in the vessel, how much of these reactors can be designed with off the shelf parts. Or at least how they specifically did it. Some of these questions can be examined by looking at research papers, but they do not always give a detailed breakdown of their actual methods of building the reactor.

Talking to chemical or materials engineers could have given us a better understanding of how specific materials interact with the gasses and catalysts within the vessel. There are several good questions that could still be asked, learning more about containment of reactants when combined with heating, outside of just references within literature.

Design Critiques

Our design for the reactor focuses on a theoretical modeling of the system and how much gas may get produced if mixing is added, specifically focusing on the usage of a rushton mixer to move molten metal in the tank.

The model focusing on the mixing aspect is a strength for our design, as we have used a design that is novel within the industry of methane pyrolysis. These mixers are commonly used in other types of reactors, but within lab scale reactors, this design style is uncommon, in our research we could find no other reactors within methane pyrolysis using a mixer on the lab scale. Lab scale reactors are often small enough that a mixer would have to be developed on a very small scale. Since our reactor was requested by our sponsor to be designed a bit larger than many lab scale reactors, a typical lab mixer could be bought, instead of specialty manufactured for this purpose.

Another strength of our design is the rough accuracy of our COMSOL model of the system where the output is the conversion rate of the methane to hydrogen. The sensitivity analysis done in the verification and validation plan section of the report, falls within what would be expected for this type of model. So it indicates that the conversion rates derived from the COMSOL model can be used to say that our suggestion for a mixer is usable.

Where our design falls short is that our scope did not narrow fast enough to develop more of a design to validate. If we had been able to complete our problem definition a bit earlier, the group may have been able to first, focus on just one section of the device, then focus on one component of it. We did do this in some ways, but it took the whole semester to get there and do the verification on that section. If we had been able to get the scope of our design narrowed down more quickly, we could have developed a small physical component to just test the specific motors we might have used, and the mixing ability of our mechanism using a liquid to mimic the viscosity of the molten metal. This would be advisable to

Another area where our design needs to be improved is in the kinetics of the model. While the COMSOL model can roughly tell us that the mixing improves the process, we could not say exactly the performance of different catalysts that might be used in a different future design. Future work to be done on this includes editing of our COMSOL models within the behavior of the methane when it interacts with the catalyst. This can be done by going through reaction rate equations to determine rates of reaction for various catalysts. Within the time allotted for our project this semester, this was not possible to get done. This would be advisable to complete for future work.

Assumptions and Risks

Challenges we encountered through the design process include the large number of components that go into the pyrolysis reactor and the fact that a lot of design changes in the literature rely on chemical engineering principles. Some of these components were considered in our analysis. Our analysis relied on a few assumptions which we did our best to make sure did not affect our final products.

Torque Analysis. For calculation assumptions within the calculation of torque, there were a few assumptions made. One calculation made is that the vessel we are using is a standard vessel, what this means is that the dimensions may be different from what is commonly used in mixed tanks. If it is non-standard, equation 12 shows the necessary calculations that need to be made for power. This could throw off the numbers used for the torque completely. This could potentially make our estimation that a standard motor would work invalid, as the operating torque range could be incorrect. This would not cause any risk to our end user but may affect a conversion rate.

Fracture Stress Analysis. Although there is relatively little risk with this analysis and the fracture stress calculated is well below the fracture strength, we are still making the assumption that the mixer motor will not exert any outside torque onto the pressure vessel itself. However, the shaft may interact with the pressure vessel unintentionally or the vibration from the motor may cause some torque onto the pressure vessel. However, since we are well below the fracture strength, it is not a great concern but still something that should be considered. There is a very small chance there could be a risk to the user, since the vessel will be contained within the furnace.

Leak Before Break Analysis. Relatively few assumptions were made for this analysis as it simulates a normal crack for a leak before break problem. However, one thing that could cause some concern is the safety factor of 2.07. Generally, a safety factor of 4 is desired but a given analysis to make the reactor as safe as possible given that it is subjected to relatively high temperatures. This can be mitigated by increasing the thickness of the pressure vessel or decreasing the outer radius of the pressure vessel which will lower the stress intensity factor calculated and by proxy increasing the safety factor to our desired value. In general, a safety factor of 4 is desired so if we increase the thickness to 20 mm, we will achieve a safety factor of 4.13. These design parameters will be optimized moving forward given all of our other analysis to give us the best design for our reactor. There is a very small chance there could be a risk to the user, since the vessel will be contained within the furnace.

Bubble Size. The simulation setting contains only 1 bubble in a column of molten metal. In the real reactor, there will be many bubbles existing in the molten metal. These bubbles might interact with each other and affect their motion, or they might combine with each other to form larger bubbles which are undesirable. This might cause the actual rising velocity and residence time to be different than that of the

simulation. To address this problem, we could add complexities into the simulation to study the interactions between the bubbles. Also, the impeller will break large bubbles so we do not expect this to be a critical issue. We can proceed with our work and see the actual effects on a working prototype.

Heating Power. We might not be able to find a furnace that exactly fits our desired dimensions, materials, and heating power. If we cannot find it, we can either customize it or choose from what is available. The heat losses and power requirement will be easy to calculate. One potential problem is that in the research we are referring to, the thickness of the insulation material is 450 mm which means although the size of our reactor can be small satisfying engineering specifications, the furnace can be big. Therefore, to make sure it still satisfies the requirement "sized for laboratory scale" we might need to specify the dimensions of the furnace instead of just the reactor chamber. Another concern of the heating power is, if the heating power of the furnace is not great enough to heat the molten catalyst effectively this will impact the conversion rate. To negate harm to the user, a safety plan should be established by the lab of the user of the lab furnace.

Lessons Learned

We learned various lessons throughout the course of the semester. One of the major issues we faced as a team was the large scope of our project and how to properly navigate the problem effectively. With all of the different and unique subsystems in a pyrolysis system, our team had difficulty dividing up the tasks needed for each subsystem. Followed by the necessity of our team to do a lot of front loaded research of our problem, our progress in the beginning was slow. Throughout the entire semester, our team constantly went back to the problem analysis stage to reevaluate our problem and conduct further research to better understand our project. We learned the importance of thoroughly understanding the problem at hand and that research is not just limited to the beginning stages of a project but should be continuously built upon.

Furthermore, we eventually narrowed down the scope of our project to just the mixing mechanism of the pyrolysis design instead of the entire pyrolysis reactor. This allowed our team to focus on the aspect of the reactor that was most interesting to us and where we could contribute the most as mechanical engineers. From this experience, we learned to set realistic expectations for ourselves and learn more about our own skill sets. This allowed us to delve deeper into concepts of pressure vessels and reactor designs as we explored different research articles for reactor designs as inspiration for our own.

Although our project was heavily focused on chemical engineering as the entire pyrolysis reaction was a chemical problem, our team still consulted some professionals in the field to better our design and understanding. We were able to reach out to Monolith, a leading pyrolysis company in the field, and learned more about what their company does and how they utilize pyrolysis. In selecting an impeller design for our mixer, we also reached out to Caframo where they provided us with important insight on what to look for in an impeller as well as general reactor design recommendations. Praneet, of course, was also crucial for our understanding of pyrolysis, reactor design and learning to operate COMSOL. In general, this project taught us all to problem solve and to carefully consider who to reach out to when facing a roadblock. In the future, we will reach out to professionals as early as possible to gain more perspectives on our problem.

Reflection

The product. After the system is upscaled and commercialized, one of the potential benefits it will bring is the lowered carbon emission compared to traditional hydrogen-producing methods. In addition, because of the high-value solid carbon byproducts, the hydrogen price will be further lowered.

Despite the benefits this system could bring, there could be some social, economic, or environmental impacts associated with the manufacturing, usage, and disposal of the system. The methane pyrolysis process uses more energy per unit of hydrogen than the traditional SMR method so there will be an increased demand on energy or electricity. The generation of electricity will produce carbon emission but this can be addressed by using sustainably generated electricity to power the pyrolysis reactor. Most parts of the system will be made of metals or other recyclable materials and can be reused or recycled during disposal.

Our design is unique in many ways so there will be many parts that need to be custom-made. Since we are not mass producing them, the cost will be high. Also, the system requires many scientific instruments for monitoring the operation and some of them cost much. For example, a mass spectrometer that measures the methane/hydrogen concentration would cost hundreds of thousand dollars. The use and disposal of the system will not cause significant economic impacts.

To characterize the societal impacts of our project, we performed stakeholder analysis as described in the design context section. And we referred to other research papers and a DOE assessment for the potential social impacts of this project.

Differences between team members and the sponsor and the effect on design processes. In a diverse team, cultural, privilege, identity, and stylistic differences can significantly affect our approach to the project. Each of us brings unique perspectives rooted in our cultural and educational backgrounds, influencing the problem solving methods, communication styles, and decision making processes. For instance, our team members are from China and the US and our sponsor Praneet is from India. Praneet already had the knowledge on the topic while our team was new to it. This led us to learning from each other. In addition, the power difference between the team and the sponsor affected the design process as well. Normally, after receiving the problem statement, we would formulate the requirements and specifications that are solution neutral. However, in our project our sponsor had some predefined design parameters for us such as the type of catalysts and methane/hydrogen flow rate. We took these directly into our specifications and concept selection instead of following the usual processes. Our project is also special in the way that there are few stakeholders involved at the current stage. Our primary stakeholder Praneet is our sponsor, and he will also be one of the first end users of the product after it is completed. Plus, he is a graduate student at the University of Michigan so we had weekly meetings to discuss the project and we did not have disagreements or conflicts.

Public health and ethical concerns. Public health, safety, and welfare are all important to any design project and so are they to ours. Since this pyrolysis reactor works with flammable gasses and high temperature devices, there is much risk involved and safety becomes especially important. However, they are not the concerns at the current stage of our design process (these factors will come into concern in the future when a working prototype is ready to be built, and additional safety analysis will be performed

when this system is to be upscaled and commercialized). Due to the limitations of this class, we can only focus on certain aspects of the system. That was one of the ethical dilemmas we have faced: to focus on the safety design of the system or something else like the effectiveness of the reaction chamber. Because of the fact that we are not building a working prototype this semester, we decided to focus on the effectiveness of the main reaction chamber.

Another ethical dilemma is that the materials we use include metals or minerals that are considered conflict minerals, as explained in the design context section. If we happen to purchase these materials originated from regions burdened by civil war, it will be bad since we will be supporting groups that continue to create conflict within the region. Therefore, in the future when this reactor is to be built, it is important to know that the materials are not from these conflict areas.

Recommendations

The current background research is heavily research literature based. In order to develop a more comprehensive understanding of the project background, other further researchers could reach out directly through email to more research groups who create existing pyrolysis reactors to get a better understanding of their building process. This would further enhance the designs created and give it a stronger research backing that's not solely based upon literature.

On a system-level, we highly recommend that future teams fully design the entire pyrolysis system with a detailed design of all of the different subsystems within the pyrolysis reactor. The rest of the reactor has many subsystems, many of which are heavily researched, so future teams must make sure that the designs meet the requirements set by standard practices in the field. We also recommend creating a future project for chemical engineering students or researchers. With a stronger chemical engineering knowledge, we can further improve the design from a chemical perspective of how the reaction works and if there were any chemical effects that were not accounted for. We recommend a future project for chemical engineering students that focuses on how best to contain the created hydrogen and carbon as well as possible ways of transporting them safely and at a low cost.

Finally, we have recommendations on how our design can be improved upon. Firstly, our COMSOL model that was created made various assumptions to simplify the model, specifically with the kinetics. It is recommended that with further research, a proper kinetic equation should be implemented into the COMSOL model to more accurately model how temperature and pressure affects the methane conversion rate. Furthermore, we highly recommend future teams to build a physical prototype, specifically of the mixing mechanism and the reactor chamber with the correct components within it. It is very valuable and crucial that this design be proven with proper experimental testing because as much as modeling is important, it is never as valuable as real physical results from a prototype. This way, future teams are able to properly develop better parameters based on physical data and optimize the parameters and design off of this. All in all, this takes into account the work we have done and integrates it into how future teams can best use what we have learned and developed to bring this project to greater heights.

Conclusions

This methane pyrolysis project aims to design a reactor that decomposes biogas into usable hydrogen and solid carbon without carbon dioxide emission. Currently, at the initial stage of this project, we are assuming the biogas is filtered and the reactor will be fed with pure methane.

Given the novelty of this technology and its current experimental status, our benchmarks are primarily derived from existing research papers on lab-scale experiments. Our focus is on high conversion rate– the percentage of the methane being decomposed into hydrogen and carbon. Pyrolysis reactors can be categorized based on heating methods and catalyst types. We studied the conversion rate of different catalysts under corresponding reaction conditions. We will decide which catalyst to use based on the balance between reaction temperature and methane conversion rate.

To choose the design process, we mainly followed the ME Capstone Design Process Framework, and we followed a combination of abstract approach and procedural approaches in our literature search.

To design the design context, we firstly categorized stakeholders into primary, secondary, and tertiary groups. Primary stakeholders, including the University of Michigan, students, biogas, and catalyst suppliers, are directly involved and stand to benefit from the project's success, especially in terms of producing low-cost hydrogen and carbon. Additionally, we analyzed the social and ethical impacts of this project. We would make positive environmental impacts and reduce CO2 emission; we need to reference existing patents and research results with ethical considerations regarding intellectual property rights; we also should consider potential job losses and the responsibility to manage the transition for affected workers in a fair and just manner.

We built our requirements and specifications from four perspectives: 1) safe storage of reactants and products; 2) size of the reactor; 3) mixing requirements 4) conditions required for pyrolysis reaction to happen; 5) efficiency of pyrolysis reaction. The pyrolysis reaction involves many different gasses in a dangerous setting, so it is essential that we have proper ways of storing the gas both before and after the reaction for the safety of everyone involved in the experiment. The scale of the reactor will be on a lab scale which was specified by our sponsor, allowing people in the future to further experiment with it. The pyrolysis conditions specify the temperature, pressure that the reactor will need to be able to reach and withstand. Finally, the efficiency of the reaction details the conversion rate and catalyst regeneration as goals for our experiment.

The main challenges we will encounter as a team surround lack of resources and limited experience, if we wanted to build a full scale model it would be very expensive even at the size we desire. There is lab space and equipment that would have to be acquired as well as the process has safety concerns that must be mitigated in a lab environment. With the limited experience we have as a team it is harder to know the necessary equipment.

In order to create our alpha design, our team utilized morphological matrices and design heuristics to individually generate ideas for our design. We then divided our design into different subsystems using a functional decomposition method. By using a weighted pugh chart, we were able to weigh different options we were considering for each subsystem to come up with a final design for the methane pyrolysis reactor. These are shown in *Table 5* and *6* above.

Given the team's budget and time constraints, we decided to focus our attention on the reactor chamber and mixing mechanism of the methane pyrolysis reactor through a reevaluation of the MoSCoW method of our different requirements and specifications. From here, we worked on our alpha design of our reactor chamber and mixing mechanism.

We created an alpha design of our CSTR reactor with a motor that will provide the spinning mechanism within the molten and solid catalyst along with various pressure and temperature parameters that we set. We defined the reactor to be built with quartz and containing 3 liters of volume and heated with an induction heater furnace.

Based on our alpha design, we conducted many engineering analyses of our design. We focused on verification of our specifications and validation of our problem statement. For our verification, we focused on the fracture stress and leak before break stress analysis of our material selection, effect of methane bubble size on residence time, as well as heating power analysis. For our validation, we performed a COMSOL simulation of the effect of mixing on conversion rate, sensitivity analysis of our COMSOL parameters, validation of our rushton mixer selection, validation on motor torque, and hydrogen production rate calculations. We do these verifications and validations through a combination of research, hand calculations, and simulations to support our claims.

From here, we were able to create a final design of our reactor chamber and mixing mechanism with specific parameters that were supported by our analysis above. We defined a thickness of 20 mm and 100 mm radius. We will use a rushton mixer with baffles for our mixing mechanism. The reactor will be coated in a calcium oxide coating to lower carbon buildup on the reactor. The rushton mixer will be made with stainless steel and the reactor shell will be built with quartz. Finally, methane gas will be fed in using a quartz frit with a small bubble size of 10-15 micrometers.

With the completion of our project, we will transfer all of our findings and knowledge to our sponsor, Praneet, as he moves this project forward to the next stage. The next stages of this project will include but not be limited to securing funding for building the pyrolysis system, securing parts and building the pyrolysis system and reactor, testing the conditions we set for safety, and experimentally testing the pyrolysis reaction to confirm COMSOL results and optimize the methane conversion rate to hydrogen and carbon. There are a lot of actions that need to be completed but we have provided our sponsor with the necessary tools to move this project forward.

Next steps for the project involve evaluating all our assumptions to improve our calculations of torque, speed, and liquid behavior. This can be accomplished on studies of turbulent and laminar flow within our tank and better modeling the dynamics of different bubble sizes, heat transfer, and speed of the liquid within the tank. We also need to verify the kinetic equations of the specific catalyst we are using to better model the methane conversion and the effectiveness of the mixing on the solid catalyst as well. We will build our final design off these next steps and this will culminate in a final design with a detailed CAD model for our final design report.

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Bios

Yunjia Hu

I am from Changzhou, Jiangsu, China, a liveable city an hour away from Shanghai. I have been fascinated by mechanisms since I was a kid. I was curious about how things work, so I always took things apart. Sometimes I could put them back together, but sometimes I could not. I have worked as a research assistant on the prosthesis hand project in the Precision Systems Design Laboratory since 2021. This research raised my interest in biomechanics–a study of the structure, function and motion of the mechanical aspects of biological systems. I am currently planning on getting a job and I am very interested in the medical device and equipment industry. A fun fact about me is that I have two cats: one can hide in any corner of the house, and the other can sneak out of the house whenever she wants.

Zhenzhuo (Leo) Liu

I am from Beijing China where I have lived until after high school. I have been loving cars since I was a kid and my dream job then was to be a race car driver. I also found that building race cars would be interesting so that eventually led to my choice of mechanical engineering for college (and I always wrote about this in my college applications). Future plan is to enter the automotive industry, and before that maybe getting a Master's degree. I also need to find something to do for this summer, either an internship or research. Last summer I was doing an internship in Lansing. I thought I would do some design work for the exterior panels of the cars but ended up painting them by programming robots. Fun facts: I also like sports and music, (and video games). I was part of an A cappella group in high school. I have tracked my car a few times and one time I boiled the brake fluid and completely lost the brake force. However, I was so smart that I noticed it before it was gone and slowed down. But it was still a little scary.

Enzhong Wang

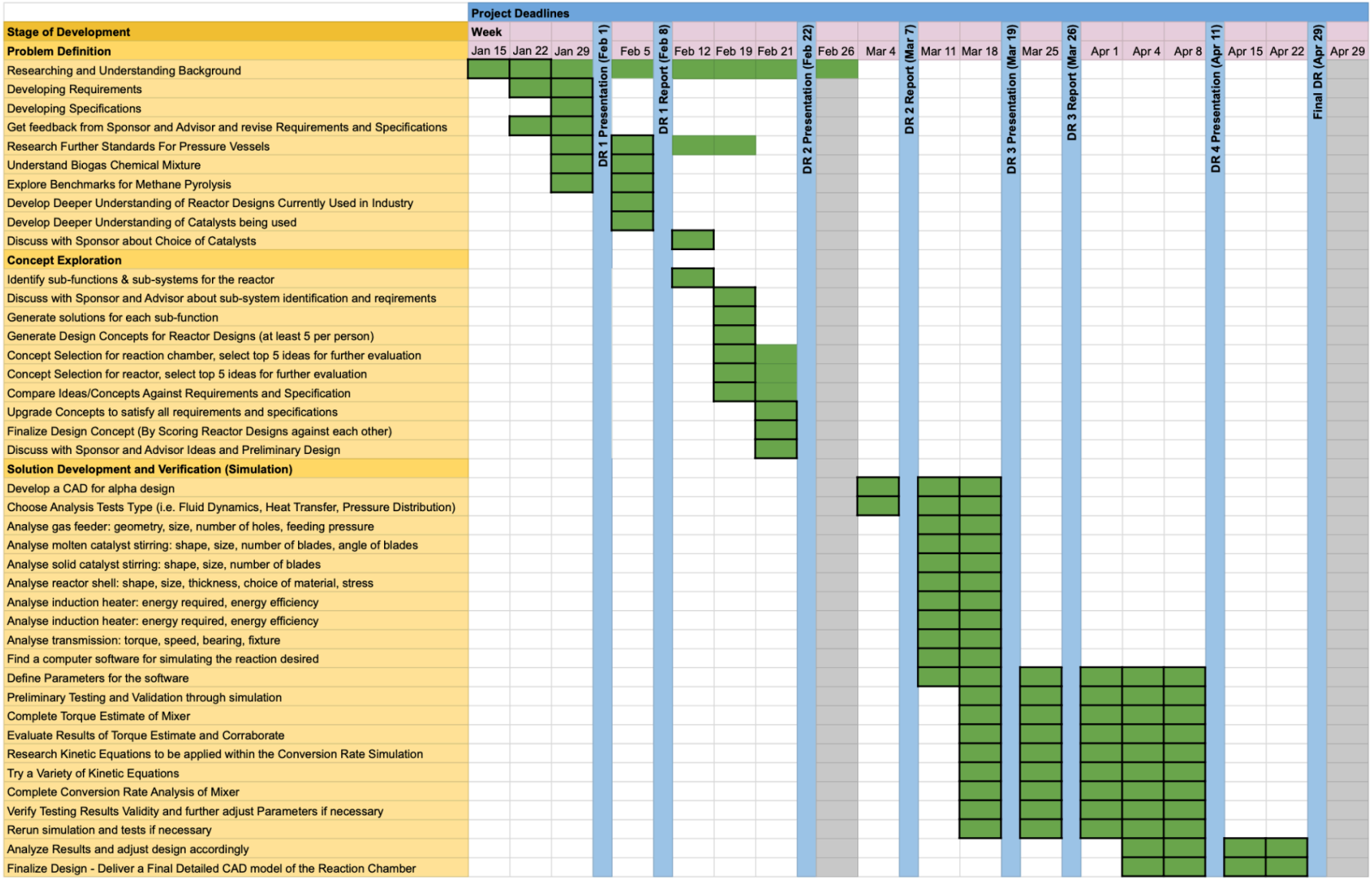
I am from Centerville, Ohio in a suburban area of the city. I have always had an interest in science, so in high school I joined our school's Science Olympiad team. In the team, the "build events" caught my interest and I became more interested in the hands-on aspect of engineering. I've grown to really enjoy learning different softwares and new concepts within mechanical engineering. Recently, after taking a class in Controls, I grew really interested in the field and am aiming to delve deeper into the subject. Currently, my future plans are to do graduate school next year through the SUGS program and after that I hope I can join the automotive industry and make an impact there. A fun fact about me is that I can recite the Chinese beaver meme in both mandarin and cantonese.

Abigail Zoetewey

I am from Grand Rapids, Michigan on the west side of the state. I lived there my entire life up until moving to Ann Arbor for school. My interest in mechanical engineering started when I was younger, I was very into taking things apart and putting them back together. I think now what I like doing in engineering is learning new and interesting software and getting to the point where I feel proficient with them. I took a class about lithium batteries last semester and I learned quite a bit about using simulink and functions in matlab I hadn't used before, and it was really cool to apply that to real technology. I am

currently planning on getting a job right after college and possibly graduate school after a bit of time in the field to get a better sense of what I like doing within engineering. I would like to work in renewable energy in some capacity, not sure yet if I would specifically like to work in wind, solar, or what specifically, but I would like to feel like I am making a positive impact on the world. I am not sure if I have any facts that are too fun, but one I can come up with is that as far as I am aware, I have never eaten a bagel.

Appendix A: Project Plan



We employed a Gantt chart to present our project plan. The full project has three stages–problem definition, concept exploration, and solution development and verification. We listed comprehensive tasks identified through detailed preliminary research and discussions with stakeholders. Additionally, we organized the project timeline on a weekly basis, which each design review deadline highlighted in blue. We used colored cells to mark the expected task completion dates. Finished tasks are marked green, unfinished tasks are represented in pink. Tasks spanning multiple cells represent that it may be a complicated task that requires more than one week to finish, or something we need to do repetitively such as sponsor meetings. We have reached the end of this project plan and updated it based on project progress and stakeholder feedback and all the tasks have been completed.

Our project plan differed from our original plans due to the change in scope of our project. Our initial plan was to build a prototype system of the entire pyrolysis system and simulate the pyrolysis reaction to confirm the validity of our design and parameters. However, we quickly realized that this was way outside of the time and budget we were provided for the project, so the scope and timeline of the project plan was changed multiple times as a result of this. We ended up deciding that going down the simulation route was the best course of action for our team in how we could bring value to the goals of the project. Although our actions differed from what our original plan was, the core of our mission stayed the same. Our goal was ultimately to improve the methane conversion rate and we were able to achieve this with what we were given and successfully create a model through our research.

Appendix B: Methane Pyrolysis Subsystem Concept Evaluation Matrices

		Do not work	May not work	May work	Do work
CH4 storage					
Option No.		Temperature <30C	Pressue =26MPa	Continuous supply	Anti-leaking
1	Tanks at high pressure (CNG)				
2	CH4 cylinder and reactor in seprate rooms				

Gas Flow						
Option No.		Flow rate	Gas leakage	Ease of monitoring	Durable	Can create desired pressure (700 kpa -> want to be higher than reactor pressure)
1	Scroll pump					
2	Gear pump					
3	Piston pump					
4	Rotary vane pump					
5	Diaphragm pump					

Methane Pretreatment				

Option No.		Able to reach 700 ℃	Heat Transfer Rate	Heat Loss	Energy Efficiency
1	Furnace				
3	Microwave Radiation				
4	Solar Heating				
5	Infrared Heating				
6	Electricity (Resistance)				
7	Electricity (Inductance)				
9	Heat Pump				

Flushing				
Option No.		Manually operated	Flushes all harmful gas out	Cost
1	Vacuum			
2	Nitrogen batch mode flushing			
3	Air batch mode flushing			
4	Helium batch mode flushing			

Methane Feeding/Inlet							
Option No.		Flow rate	Ease of monitoring	Durable	Can create desired pressure	No backflow of molten catalyst	Big contact area of CH4 and catalyst or longer residence time
1	Multi directional						

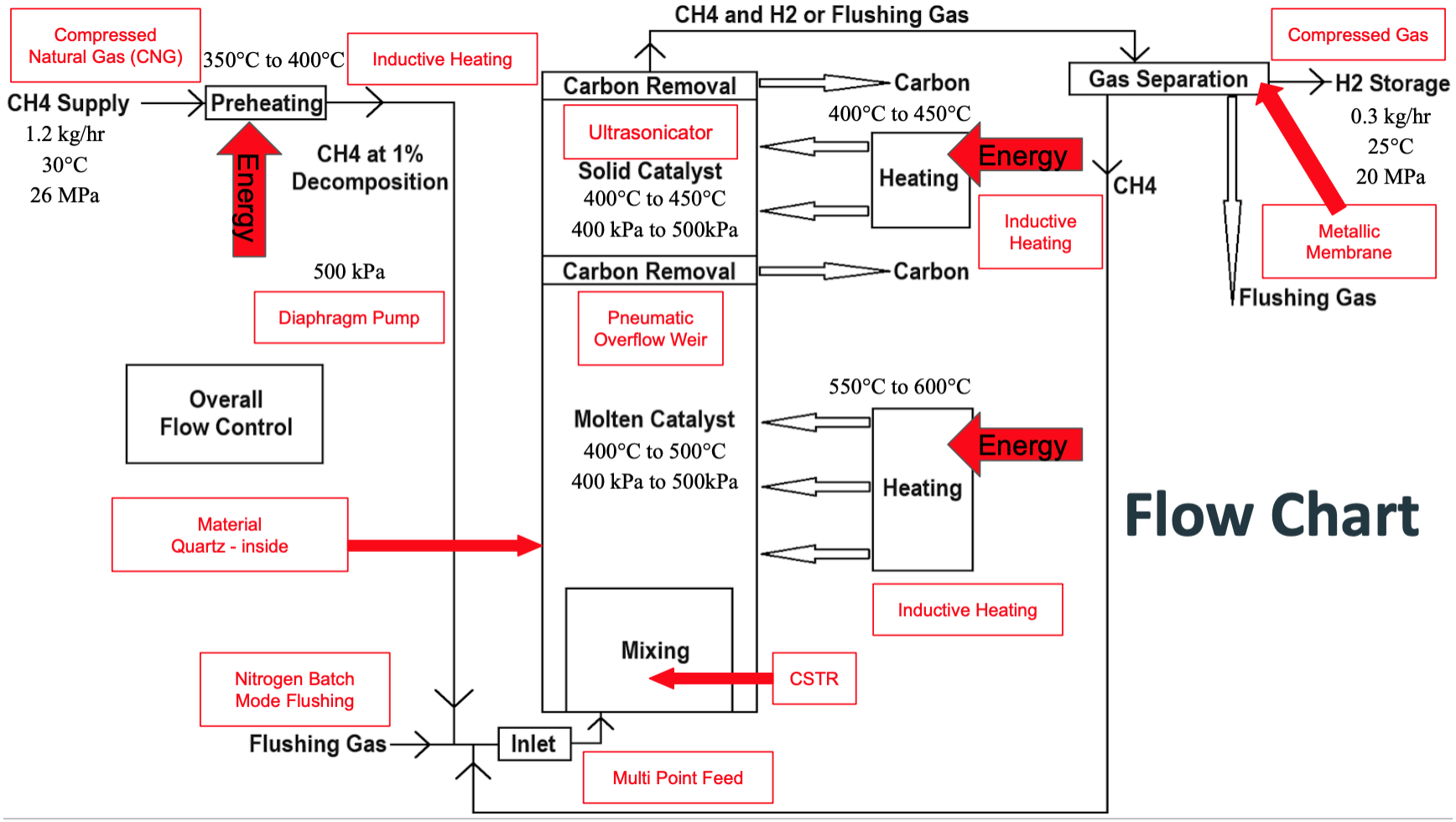
	feed						
2	Single point feed						

Hydrogen Storage							
Option No.		Temperature =25	Pressure =20MPa	Continuous supply	Possible leaking	Cost	Energy
1	High pressure gas cylinder (800 bar)						
2	Liquid Hydrogen in cryogenic tanks (21K)						
3	Stored as ammonia						

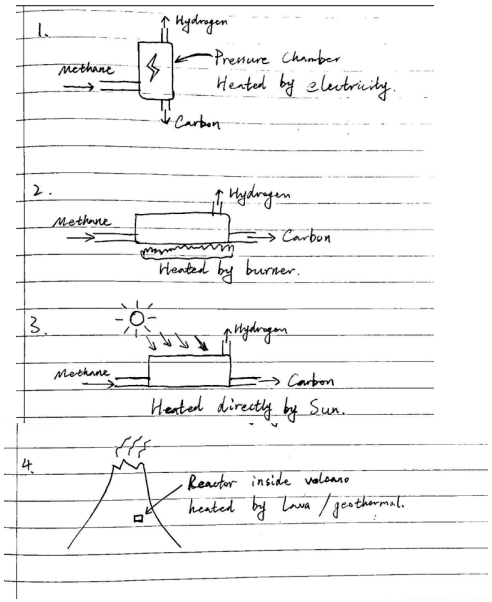
Collection of Carbon (molten) - continuous removal					
Option No.		no clogging	carbon should be pure and uncontaminated	quick collection	catalyst not damage/contaminated
1	Skimming mesh/manual/auto				
2	Recirculation of molten catalyst, filter during recirculation				
3	Blower blows the carbon off the reactor then collect				
4	Vacuum				

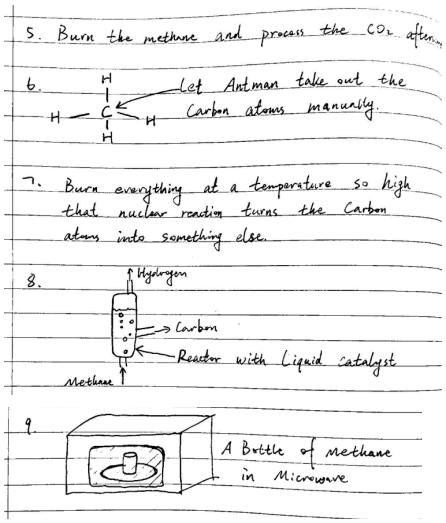
5	Pneumatic conveyance				

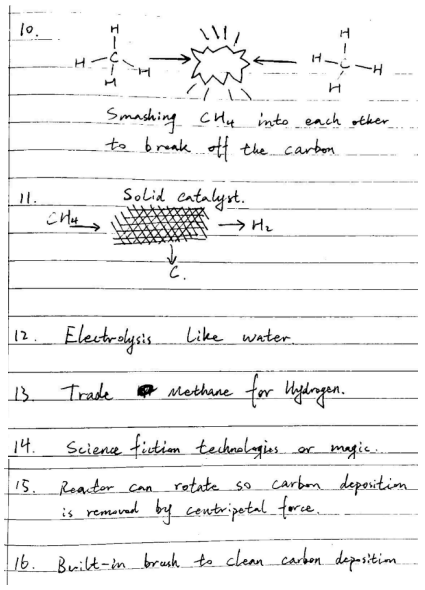
Appendix C: Methane Pyrolysis Detailed Flow Chart

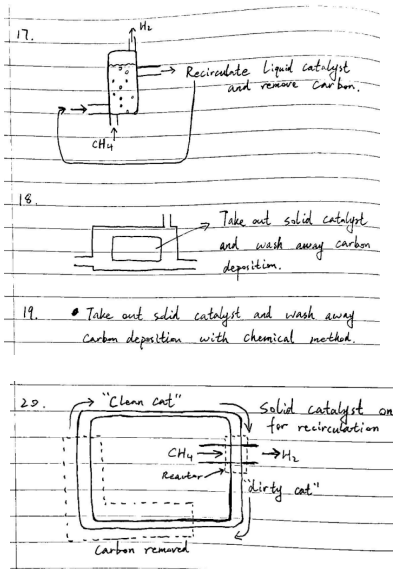


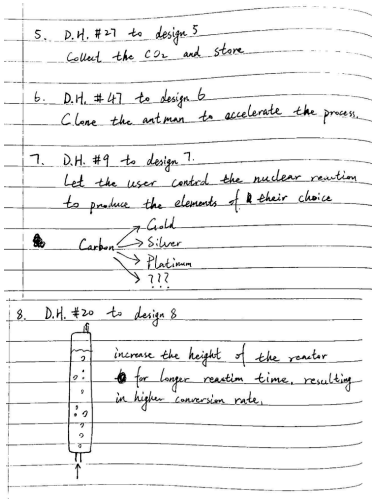
Appendix D: Concept Generation - Brainstorming

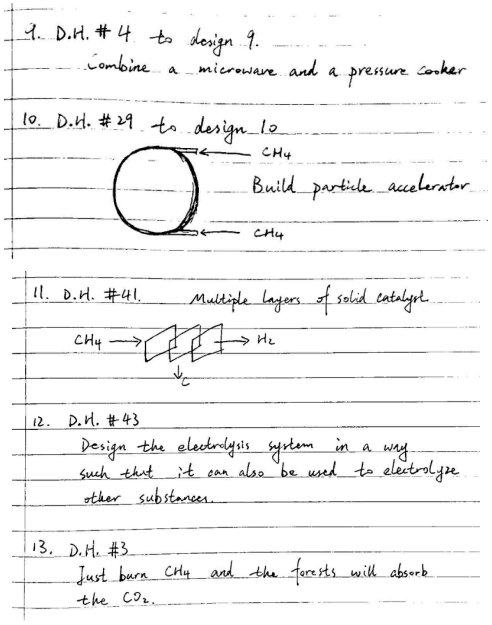


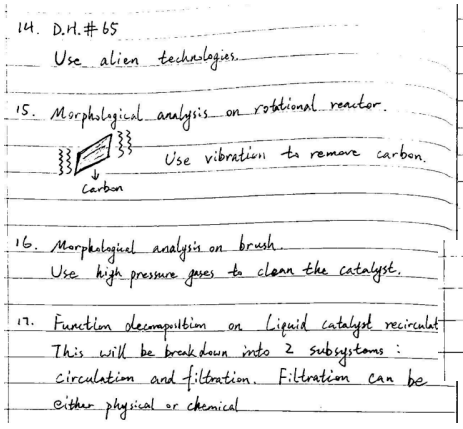


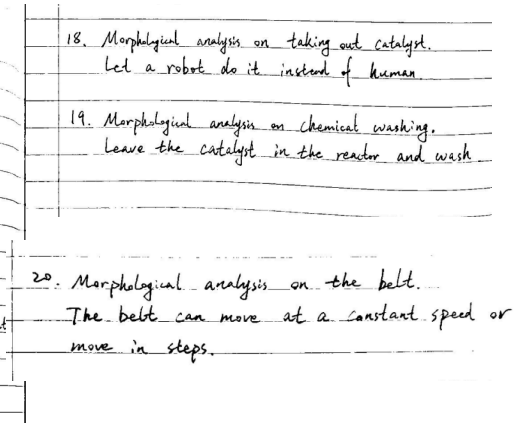






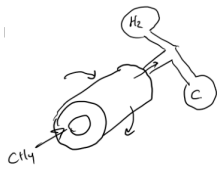




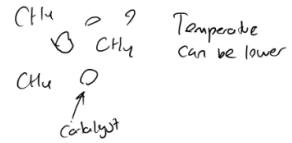


Appendix D: Concept Generation - Brainstorming Cont.

2) Brainstorming
   a) 1 - Rotating pyrolysis reactor with furnace as heat source



   b) 2 - Heat the methane in an oven
   c) 3 - Bring the methane to a chemical lab and have them do it
   d) 4 - Explode the methane with dynamites
   e) 5 - Catalyst in reactor for faster reactor

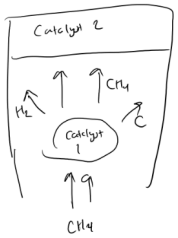


   f) 6 - Normal pyrolysis reaction in a reactor
   g) 7 - Bring the methane to space and chuck it into the sun
   h) 8 - Put methane in pressure chamber
   i) 9 - Put methane in small tube for fast reaction
   j) 10 - Burn the methane with fire

   k) 11 - Store Hydrogen as ammonia for ease of transport

$$H_2 + N \rightarrow NH_3$$

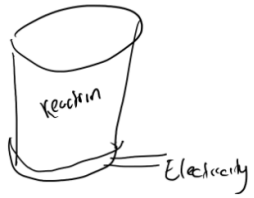
   l) 12 - Nuclear reaction
   m) 13 - Put the methane in a combustion chamber
   n) 14 - Use 2 different catalyst (1 for initial reaction with methane and second catalyst for any unreacted methane)



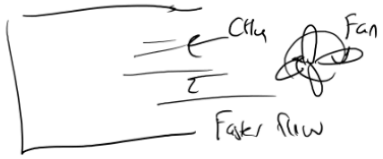
   o) 15 - Go to the bottom of the ocean for high pressure and temperature
   p) 16 - Put the methane on a stove
   q) 17 - Use high pressure gas with methane for faster reaction
   r) 18 - React methane with other chemicals
   s) 19 - Use a laser beam to shoot the methane
   t) 20 - Put it in a vacuum chamber for high pressure and heat with a furnace

1) Iteration using Design Heuristics and Morphological Matrix
   a) 21 - Using a graduated cylinder for spinning the catalysts
   b) 22 - Using the sun as a heat source for the reaction

   c) 23 - Use electricity for heating of the chamber for reaction



   d) 24 - Using heat pumps to generate heat
   e) 25 - Using solar heating to generate heat for reaction
   f) 26 - Using a boiler to heat up water to the desired temperature
   g) 27 - Using different gasses (propane) to create the temperature needed
   h) 28 - Use geothermal heating for pyrolysis reaction
   i) 29 - Using a PCB pipe and applying pressure and temperature to it
   j) 30 - Using pressure tank to apply all the pressure and temperature
   k) 31 - Using fan to increase the flow of the methane, hydrogen, and solid carbon within the reactor

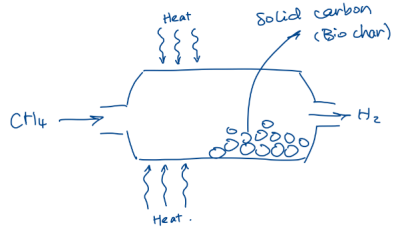


   l) 32 - Use a pressure tank to store hydrogen after reaction
   m) 33 - Gas tank for faster air flow in reactor
   n) 34 - Humidifier to keep the air around the reactor cool
   o) 35 - Using different chemicals to complete reactor cycle
   p) 36 - Pressurized gas to increase pressure of reaction
   q) 37 - Metal container to contain the pressure and temperature
   r) 38 - Radiator to create the temperature
   s) 39 - Natural gas heating for temperature
   t) 40 - Hydrogen heating for reaction temperature

Concept	Quality	Novelty
1	This idea meets the quality and requirements well because it offers a viable solution for how to effectively use the catalyst as well as clearing the carbon from the catalyst	This idea is rather novel because it is not widely used for rotating systems in a pyrolysis process. Compared to my other idea it is also rather unique and is a rather unprecedented idea. Rating of 2.
14	This idea also meets the quality and requirements. The main purpose of the process is to be able to split methane to carbon and hydrogen so having two catalysts would make the process more effective	This idea isn't very novel. It is quite common to use catalysts in reactions and having 2 isn't all that unique either. Compared to my other ideas it is rather straightforward and common. Rating of 8.
20	This idea is good but am not sure if it's a viable solution with all the requirements because although it may be able to provide the temperature and pressure needed it may not allow the reaction to happen simultaneously or allow steady flow	This idea is more novel because it's a unique way of getting the pressure and temperature needed. Compared to my other ideas it is also unique. Rating of 3.
27	This idea is good and viable because it allows the reaction to complete successfully and also have all the requirements checked. It allows steady flow and should not have any reaction with the propane gas.	This idea is rather common and used a lot in everyday pyrolysis companies. Compared to my other ideas it is not unique but very viable. Rating of 7.
40	This idea is very useful and viable because it allows the reaction to complete with a reliable heating method. It should fit all the requirements no problem	This idea is rather unique. By using hydrogen the product of the reaction for the heating, it allows a very effective method. Compared to my other ideas it is also very unique. Rating of 3.

Appendix D: Concept Generation - Brainstorming Cont.

11.



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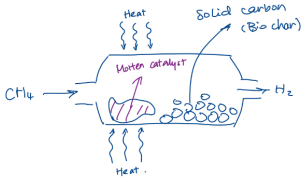

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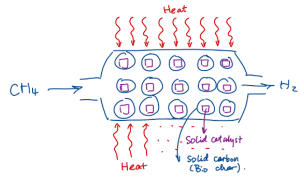

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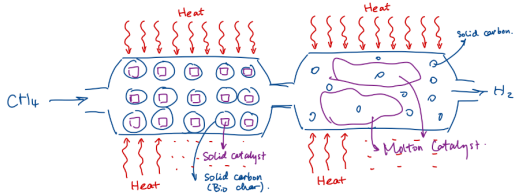

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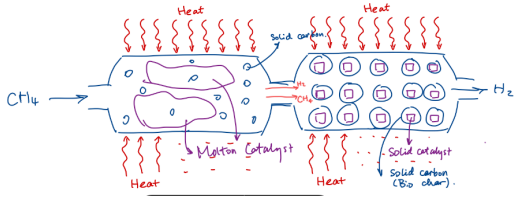

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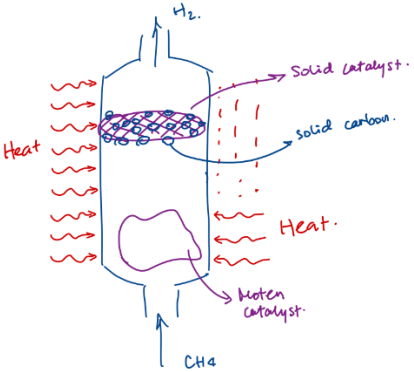

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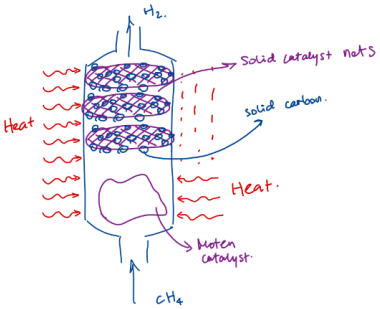

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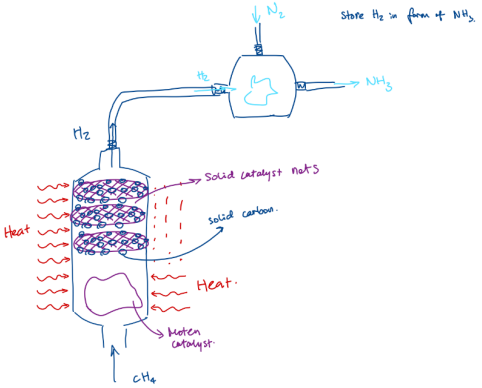

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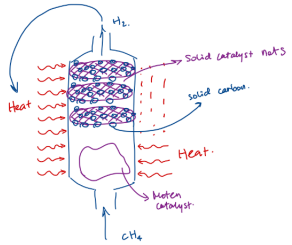
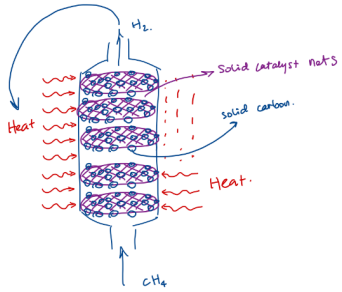


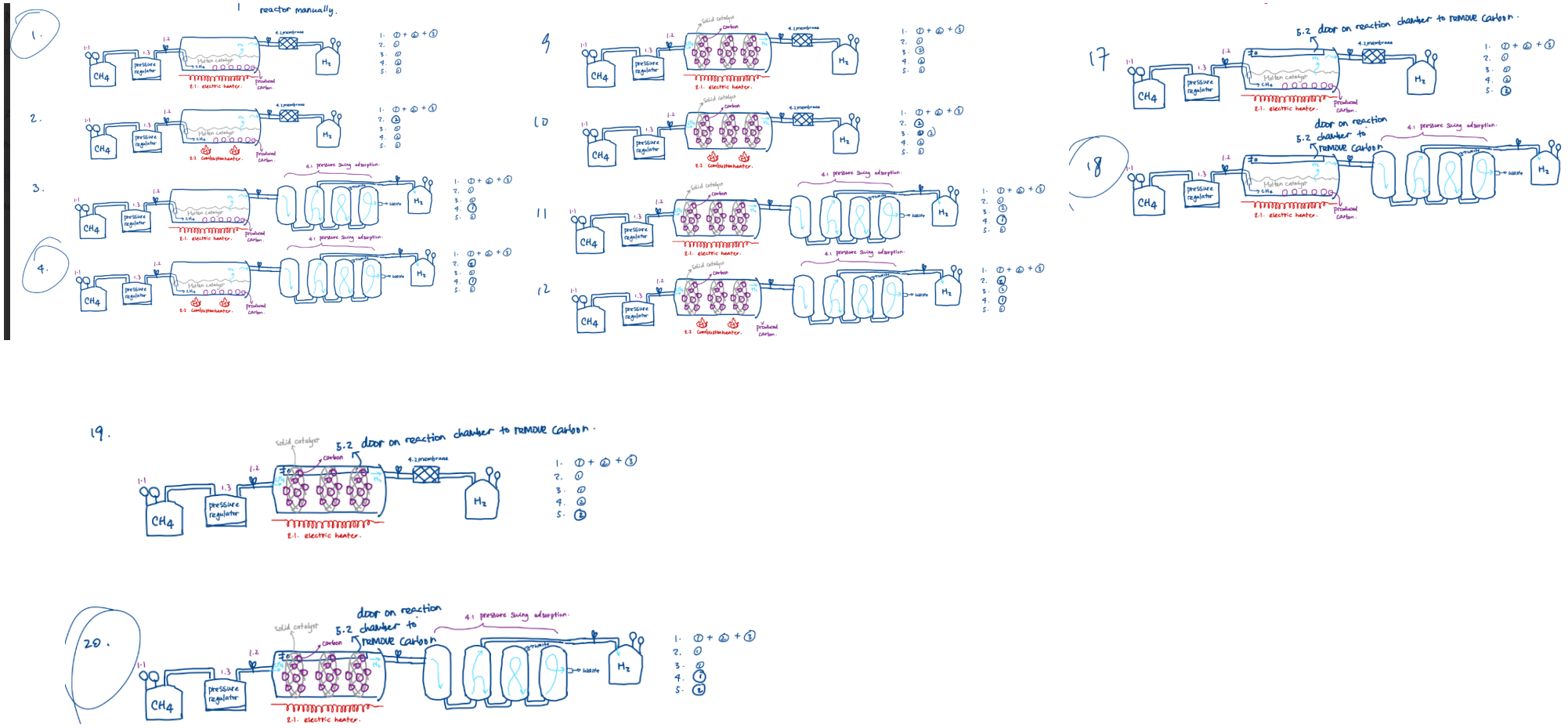
Use generated H_2 as a supplimentary heat source instead of storing it.

20.



II. 1. Morphological Matrix.

Subfunctions	Solutions →
1. Safe storage & feeding of CH_4	① Temperature & pressure monitor ② Flow control system (mass flow controller). ③ pressure regulator
2. Heat source for pyrolysis	① Electric heater ② Combustion heater ③ Microwave heater
3. Low thermal decomposition temperature.	① Molten catalyst. ② Solid catalyst ③ Mixed catalyst
4. Gathering of produced H_2 (gas)	① pressure swing adsorption ② membrane separation
5. Gathering of produced carbon (solid)	① put a collector at bottom of the reactor that produced solid carbon could fall into the collector ② Design a batch mode reaction chamber. The chamber can be opened, so carbon deposition can be removed from the reactor manually.

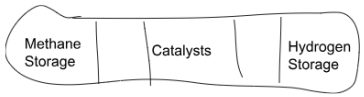

1. reactor manually.
2.
3.
4.
9
10
11
12
17
18
19.
20.
CH4
pressure regulator
Molten catalyst
solid catalyst
carbon
2.1. electric heater.
2.2 Combustionheater.
Produced carbon.
4.1 pressure Swing adsorption.
4.2 membrane
waste
H2
5.2 door on reaction chamber to remove carbon.

Appendix D: Concept Generation - Brainstorming Cont.

Heating the methane through electricity

Cold plasma heating

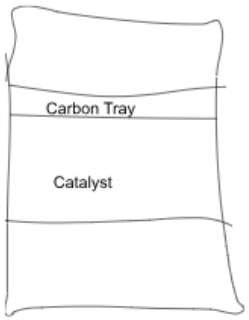
All of the process in contained within a small compact unit



Tube is very long and thin but methane takes longer time going through so more is converted.

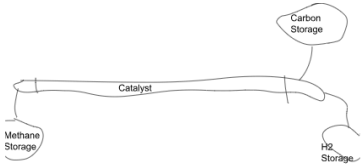
Carbon is removed with moving gas

Carbon is collected in a separate tray



Carbon is collected manually by opening it up

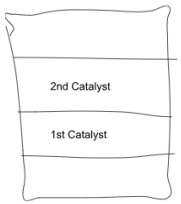
Carbon is collected with a robot arm



Microwave heating

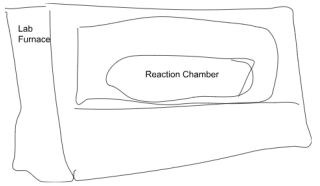
Large wide opening gas is pumped in at a slower rate

Use a 2 stage catalyst



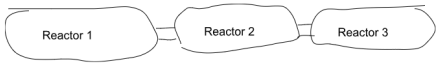
Use a three stage catalyst

Reaction Tube is very small to minimize cost for data



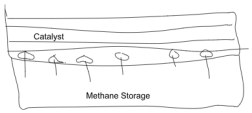
Thinking about the Align components around center card we could focus on the center of the reactor to align the flow of the methane so it works with the reactor

Mirror or Array card, maybe we could repeat a pattern of catalysts create a several stage reactor not just two or three stage but force the gas into a new chamber



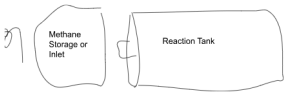
Design Heuristic Ideas:

Thinking about the Flatten heuristic card what if the device was longer and the surface area for methane to come out wider.



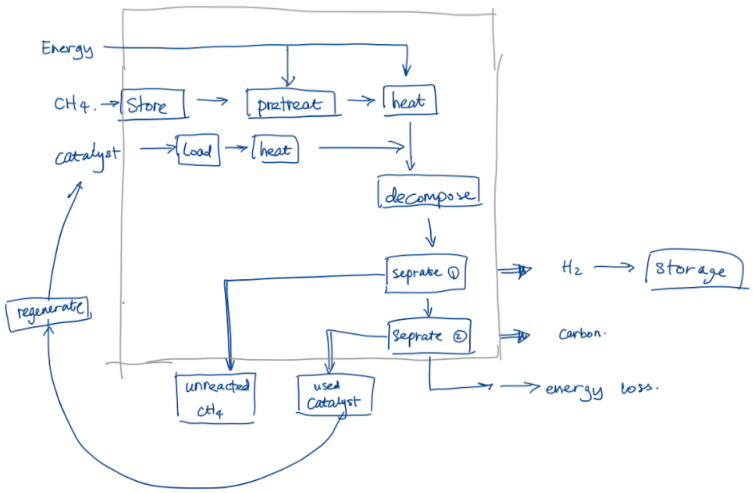
Thinking about the Adding motion card the device could also be turning

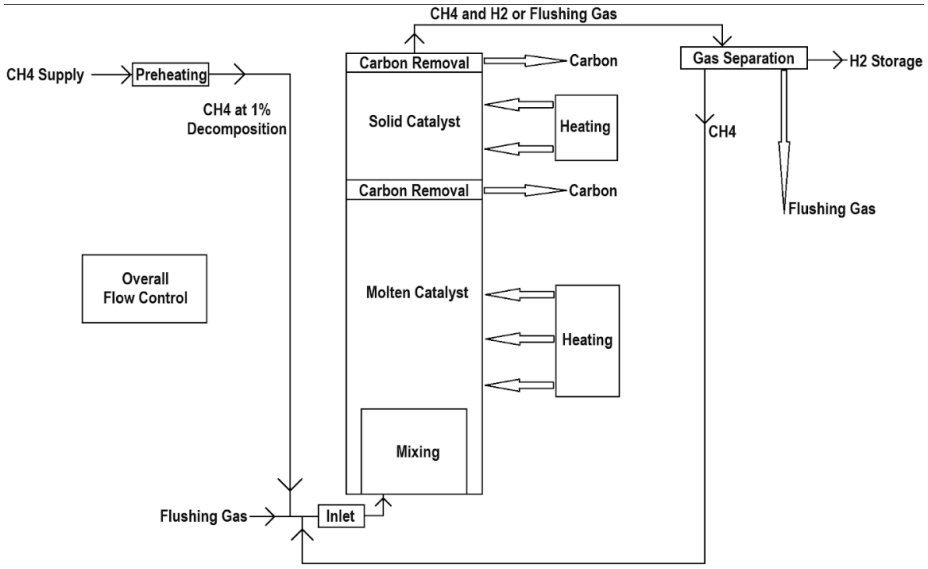
With the Twist card It makes me wonder if we could have the methane entrance port twist off

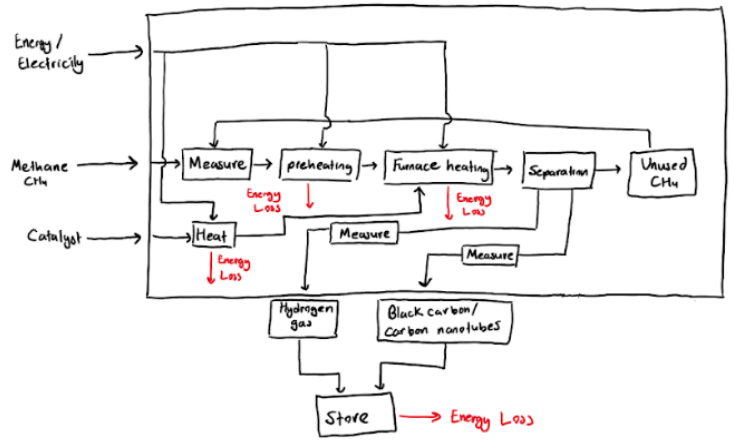


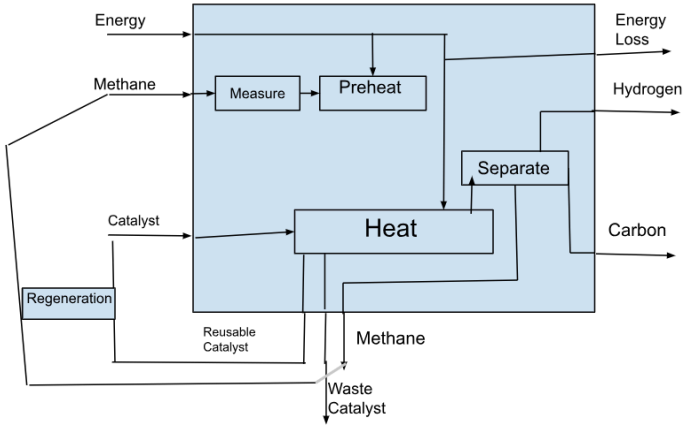
I see the Use continuous material card, I can think of doing this with some of the pressure vessels that may contain the gases.

Appendix D: Concept Generation - Sub Function Decomposition









Appendix D: Concept Generation - Individual Morphological Charts

	CH4 supply	CH4 preheat	Reactor heating	Gas flow	Collection of carbon (from molten catalyst)	catalyst regeneration (remove carbon from solid cat)	H2 filtration	H2 storage
1	natural gas pipeline	electricity (resistance)	electricity (resistance)	lobe pump	skimming mesh	vibration	distllation (different boiling point)	compressed gas
2	pressure tanks	electricity (inductance)	electricity (inductance)	radial flow pump	recirculation of molten catalyst, filter during recirculation	rotation	membrane separation	liquified
3	liquified natural gas	microwave	microwave	scroll pump	blower blows the carbon off the reactor (since carbon is lilghter then met	compressed air	molecular sieve	metal hydride
4	temperature & pressure	heat pump	heat pump	gear pump		chemical wash		chemical (ammonia)
5	flow contro system	burner	burner	piston pump		recirculation (like a tape, clean the cat during recirculation)		
	pressure regulator	solar	solar					
		waste heat from reactor						

Subsystems	Method 1	Method 2	Method 3	Method 4	Method 5
Methane Storage	tanks at high pressure (CNG)				
Methane Pretreatment	Heating coils	Direct thermal	microwave radiation	solar heating	infrared heating
Reactor Heating	furnace	Direct thermal	microwave radiation	solar heating	infrared heating
Fluid Flow (gas)	Valve system	pump	impulse pump	root-type pumps	
Collection of Solid Carbon	Ultrasonic	Use solid catalyst mesh	Use membrane since carbon is bigger than hydrogen		
Catalyst Regeneration	Steam	air	chemical treatment	Treatment with H2	
Hydrogen Filtration	hydraulic filters	introduce electric current then memb	boiling point	molecular sieve	nano-layers of graphene
Hydrogen Storage	High Pressure Gas Cylinder (	Liquid Hydrogen in Cryogenic Tanks	Stored as ammonia	adsorbed hydrogen on mat	Absorbed on interstitial sites i
Recycle Reusable Methane	pipe back to methane storage	pipe back to furnace			

Functional Deco	Method 1	Method 2	Method 3	Method 4
Methane Storag	Pressurized Tank	Pumped in through tube, tank not stored	Methane stored in colder temp storage area	
Methane Pretrea	Lab Furnace	Electric Heating	Microwave	
Heating	Electric Heating	Microwave	Lab furnace	
Fluid Flow (of th	Narrow Nozzle	bubble flow for perfect drop size of gas		
Collection of Sol	Grate to catch carbon	Arm to collect it	Top carbon rises to top and runs out a tube	
Catalyst Regeneration				
Hydrogen Filtration				
H2 Storage				

Appendix D: Concept Generation - Final Morphological Charts

Subsystems	Methane Supply/Storage	Methane Pretreatment	Reactor Shell (molten part)	Membrane	Reactor Shell (solid part)	Reactor Heating
Concepts	tanks at high pressure (CNG)	Heating coils	ceramics	Ni/MoS2 membrane	ceramics	furnace
	Utilizing the biogas and production of methane	Direct thermal	stainless steel	molten metal membrane/bubble column reactor	stainless steel	Direct thermal
		microwave radiation	super alloys	Membrane reactor design to avoid metal loss	super alloys	microwave radiation
		solar heating	glass	Sucrose Precursor	glass	solar heating
		infrared heating	stone (Quartz?)	Carbon membrane	stone (Quartz?)	infrared heating
	natural gas pipeline	electricity (resistance)	plastic		plastic	electricity (resistance)
	pressure tanks	electricity (inductance)	Alumina		Alumina	electricity (inductance)
	liquified natural gas	microwave				microwave
		heat pump				heat pump
		burner				burner
	temperature & pressure monitor	solar				solar is it a concentrator or PV?
	flow contro system	waste heat from reactor				Plasma
	pressure regulator					

Collection of Solid Carbon (Molten Catalyst)	Flushing system	Solid Catalyst Regeneration (Carbon Removal)	Hydrogen Filtration	Hydrogen Storage
	vacuum	Steam	membrane	High Pressure Gas Cylinder (800 bar)
	nitrogen batch mode flushing	air	hydraulic filters	Liquid Hydrogen in Cryogenic Tanks (21K)
		chemical treatment		Stored as ammonia
		Treatment with H2		adsorbed hydrogen on materials with a large specific surface area (<100K)
		Ultrasonicator		Absorbed on interstitial sites in a host metal
skimming mesh/manual/auto		vibration	distllation (different boiling point)	compressed gas
recirculation of molten catalyst, filter during recirculation		rotation	membrane separation	liquified
blower blows the carbon off the reactor (since carbon is lighter then metal) then collect		compressed air	molecular sieve	metal hydride
vacuum		chemical wash		chemical (ammonia)
benchmark 1 design and their approach		recirculation (like a tape, clean the cat during recirculation)	pressure swing adsorbtion	
no clogging			filtration purity rate	
continous removal vs batch removal			cost	

Gas Flow	Methane Inlet	Methane Feeding	Liquid Gas Mixing
Valve system	bubble column (bubble frit)	cstr	Stirring (rotating paddle mechanism within the reactor)
pump	Nozzle	plug flow reactor	Baffles within the
		Multi directional feed	Rotation of Reactor with (belt drive?) mechanism
			Variation of mechanism with the turning reactor
lobe pump			
radial flow pump			
scroll pump			
gear pump			
piston pump			
rotary vane pump			
	Gas - Liquid Reactors | PDF (slideshare.net)		
	simple bubble column		
	plate column		
	packed column and trickle bed		
	mechanically agitated vessels		
	dough mixers		

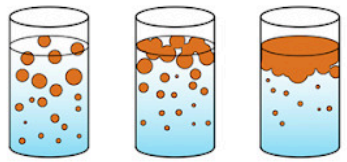
Appendix E: Excerpt from DOE Environmental Assessment on Monolith Olive Creek Facility

Table 1. Allowed Air Pollutant

Regulated Air Pollutant	Quantity (tpy)
Particulate matter <10 micrometers in diameter (PM_{10})	28.22
Particulate matter <2.5 micrometers in diameter ($PM_{2.5}$)	22.01
Oxides of Nitrogen (NOx)	85.06
Oxides of Sulfur (SO_2, SO_3, and combinations thereof)	0.85
Volatile Organic Compounds (VOC)	6.46
Carbon Monoxide (CO)	54.01
Lead (Pb)	$3.35E^{-04}$
Greatest Individual Hazardous Air Pollutant	8.95
Total Combined Hazardous Air Pollutants	13.03
Carbon Dioxide Equivalents (CO_2e)	121,753

Table 2. Life Cycle Analysis

Direct Emissions	Monolith	Business As Usual
	kg of CO_2e per kg of product	kg of CO_2e per kg of product
Monolith Production of Carbon Black, Ammonia, and coke	0.19	0
Conventional Ammonia Production	0	1.52
Conventional Carbon Black Production	0	2.53
Conventional Coke Production	0	0.1
Total (direct emissions)	**0.19**	**4.15**
Indirect Emissions (upstream and supply)		
Fuel Oil	0	1.43
Electricity - Grid Mix	0	0.32
Electricity - Solar PV	0.17	0
Natural Gas	1.0	0.97
Additives and other consumables	0.02	0
Total (indirect emissions)	**1.19**	**2.72**
Total of Direct and Indirect	**1.38**	**6.87**
Monolith percent CO_2e reduction over BAU	**80%**	



Natural separation of Gas

Appendix F: Stress Analysis Calculations

Fracture Stress Analysis:

P=500kPa, outer radius = 100mm, thickness = 5mm

$\sigma_{hoop} = P*r/t$

=(500,000)(.095)/(.005)

= 9,500,000 = 9.5MPa

Leak Before Break Analysis:

$K_I = \sigma_{axial}*\sqrt{\pi}a$

$=(Pr/2t)\sqrt{(\pi 2t)}$

$=(((500{,}000*.095)/(2*.005)))*\sqrt{(\pi*2*.005)}$

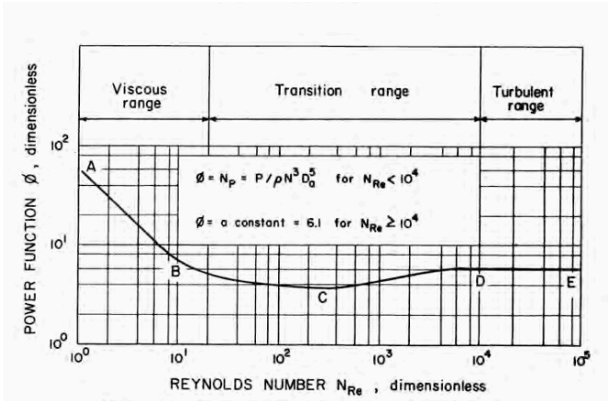
=841.92 kPa

Appendix G: Torque Calculations

$$Re_i = \frac{N_i D_i^2 \rho}{\mu}$$

$$Re_i = \frac{(600rpm)^* (200/3^*10^{-3})^2 9800.5kgm^{-3}}{0.00271476m^{-1}kgs^{-1}} = 2406.7198$$

log(2406.7198) = 3.38129



Using this graph to determine Np

$P = N_P \rho N_i^3 D_i^5$ this equation is used as we are in the transition range

$$P = 3.98 * 9800.5kgm^{-3}(600 * 1/60)^3(200/3 * 10^{-3})^5 = 51$$

Torque = $M = P/2\pi N_i$ = 51/(2π*(600*1/60)) = 0.81773 Nm

M/0.2 = 4.0886 Nm