

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

**UTILIZATION OF AN AMMONIA CRACKER FOR
GENERATION OF NH₃/H₂ FUEL MIXTURE**

HARETH MOTHANNA RASHED ALFEEL
A THESIS SUBMITTED FOR THE DEGREE OF
MASTER OF SCIENCE
DEPARTMENT OF MECHANICAL ENGINEERING

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T.C.
GEBZE TEKNİK ÜNİVERSİTESİ
FEN BİLİMLERİ ENSTİTÜSÜ

AMONYAK KIRILMASININ NH₃/H₂
YAKIT KARIŞIMI ÜRETİMİNDE
KULLANILMASI

HARETH MOTHANNA RASHED ALFEEL
YÜKSEK LİSANS TEZİ
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YÜKSEK LİSANS JÜRİ ONAY FORMU

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İMZA/MÜHÜR

SUMMARY

Recently, ammonia has been utilized to store hydrogen in a form that is simple to separate and use as a renewable source of things like energy production. When fuel is produced from ammonia has a variety of benefit of H_2 in term of ease of use and handling, as well as in terms of cost, including greater density, less complicated storage, transportation, as well as lower price. But because of its extremely limited gas turbine and other device velocity of flame, Ammonia is particularly challenging to be used directly in gas turbines and standard ICEs. Although, a few tests have shown that ammonia may be burned with reasonable grades of effectiveness if it is just partly split into H_2 and N_2 , producing a fuel which mixture of H_2 and NH_3 . This article describes a form and analysis of an ammonia cracker and splitter system which utilizes the heat produced during the burning of the fuel combination. We will look at how an ammonia cracker works to produce the appropriate NH_3/H_2 combination using various designs and geometries. In this work, a CFD model was created that takes into account fluid movement inside the burner as well as chemical reactions and energy balancing. To explore the individual phenomena in the cracker and in the jet burner, two different models have been used. It is acknowledged that the position of the cracker bluff body within the burner. Ammonia decomposition rates vary according to the position of the bluff body, which affects how hydrogen and ammonia combine in the fuel mixture. It has been established that the amount of hydrogen production in the final fuel combination depends significantly on preheating ammonia before it enters the cracker.

Key Words: Ammonia, Combustion, Bluff Body, Syngas Jet Burner

ÖZET

Son zamanlarda, amonyak, enerji üretimi gibi şeyler için sürdürülebilir bir yakıt olarak ayrılması ve kullanılması basit bir biçimde hidrojeni depolamak için kullanılmıştır. Bir yakıt olarak amonyak, daha yüksek yoğunluk, daha az karmaşık depolama ve nakliye ve daha düşük fiyat dahil olmak üzere, maliyet ve rahatlık açısından hidrojene göre çeşitli avantajlara sahiptir. Bununla birlikte, son derece düşük gaz türbini ve diğer cihaz alev hızı nedeniyle, yeşil amonyağın geleneksel içten yanmalı motorlarda ve gaz türbinlerinde doğrudan kullanımı özellikle zordur. Bununla birlikte, birkaç test, amonyağın kısmen hidrojen ve nitrojene ayrılarak amonyak ve hidrojen karışımı olan bir yakıt üretmesi durumunda makul verimlilik seviyeleriyle yakılabileceğini göstermiştir. Bu makale, yakıt kombinasyonunun yanması sırasında üretilen ısıyı kullanan bir amonyak kırıcı sisteminin tasarımını ve analizini açıklamaktadır. Çeşitli tasarımlar ve geometriler kullanarak uygun NH_3/H_2 kombinasyonunu üretmek için bir amonyak kırıcının nasıl çalıştığına bakacağız. Bu çalışmada, brülör içindeki sıvı hareketinin yanı sıra kimyasal reaksiyonlar ve enerji dengelemeyi dikkate alan bir CFD modeli oluşturulmuştur. Parçalayıcı ve jet brülördeki bireysel olguları keşfetmek için iki farklı model kullanılmıştır. Brülör içindeki kraker blöf gövdesinin konumu kabul edilir. Amonyak ayrışma oranları, yakıt karışımında hidrojen ve amonyağın nasıl birleştiğini etkileyen blöf gövdesinin konumuna göre değişir. Nihai yakıt kombinasyonundaki hidrojen üretim miktarının, amonyağın krakere girmeden önce ön ısıtmasına önemli ölçüde bağlı olduğu tespit edilmiştir.

Anahtar Kelimeler: Amonyak, Yanma, Bluff Body, Syngas Jet Brülör

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LIST OF ABBREVIATIONS AND ACRONYMS

<u>Abbreviations and Acronyms</u>	<u>Explanations</u>
A	: Area
A_i	: Pre-exponential factor
β_i	: Temperature exponent of the i th reaction
E_i	: Activation energy of the reaction
H	: Enthalpy
h_k	: Specific enthalpy of the k th specie
k	: Kinetic energy of turbulent fluctuations per unit mass
R_c	: Universal gas constant
S	: Entropy
T	: Temperature
V	: Reactor volume
V_k	: Ordinary diffusion velocity
W	: Width of the bluff body
W_k	: Thermal diffusion velocity
x	: Coefficients of reactants in NH_3/H_2 / Air chemical reaction
Y_k	: Mass fraction of the k th species
AFC	: Alkaline Fuel Cell
CFD	: Computational Fluid Dynamics
CNG	: Compressed Natural Gas
CR	: Compression Ratios
DME	: Dimethyl Ether
DNS	: Direct Numerical Simulation
FVM	: Finite Volume Method
ICEs	: Internal Combustion Engines
LHV	: Lower Heating Value
LPG	: Liquefied Petroleum Gas
MCFC	: Molten Carbonate Fuel Cell
MEMS	: Micro-Electro-Mechanical System
NH_3	: Ammonia

NO _x	: Nitrogen Oxides
PAFC	: Phosphoric Acid Fuel Cell
PEMFC	: Proton Exchange Membrane Fuel Cell
PFR	: Plug Flow Reactors
PSR	: Perfectly Stirred Reactors
RANS	: Reynolds-Averaged Navier-Stokes
SCR	: Selective Catalytic Reduction
SI	: Spark Ignition Engine
SOFC	: Solid Oxide Fuel Cell



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1. INTRODUCTION

1.1. Background

One of the most important contemporary scientific topics is on the rise in rising temperatures and environmental pollution caused by global warming gases; problems that are thought to be harmful to the general public's health. The rising need for transportation-related fuel, power production, and regional demand might make these issues worse. Currently, the majority of fuels used in transportation and power generation are petroleum-based fuels. These fuels are composed of a range of hydrocarbons that, provide fuel as well as additional gases like CO and CO₂, among others. Both CO and CO₂ are regarded as main air pollution pollutants that have a negative impact on both human good health and the ambience.

Animals that live in Cold regins, it will be only found in zoos as a result of carbon dioxide emissions, and the effects of global warming, and it will be very difficult to live in hot climates like the Arab world or low lying areas like Nepal and the Philippines are expected to be destroyed as the sea levels rise. As a result, the quest for scorbutic fuel substitutes has expanded in the direction. NH₃ is important one of the alternate fuels which a lot of researchers from india, German, Japan, the Arab world, Amarica, and the United Kingdom has been searching to in recent years. Ammonia (NH₃) is a chemical hydrogen storage molecule that is easily dissociable and may be utilized as a possible fuel for (GT) gas turbine energy production as well as to power hydrogen fuel cells, has recently been employed [1].

The sluggish flame velocity of NH₃/air mixtures is the main issue with using ammonia as an engine fuel. Ammonia can also be challenging to inflame lead to its lengthy ignition latency, very high automatic inflammation temperature, and restricted flammability. Ammonia presents a problem in that full combustion must occur at the proper moment in order to realize effective engine functioning without emitting significant amounts of NH₃ into the exhaust.

Although the characteristics of NH₃ as a energy are not fully known yet, there are tremendous need for systems that can use ammonia effectively a consistent path of deliverable fuel when figuring out of basic principles of it is combustion [2]. The goal of this effort has been to provide fresh perspective on these difficulties.

1.2. Produce fuel from Ammonia

Ammonia has numbers of benefits over H₂ in terms of price and appropriateness as a fuel. This is brought on by its greater density, comparatively simple distribution and storage, and accessibility, ammonia separates into its component nitrogen and hydrogen:



Fritz Haber and Carl Bosch, both German chemists, shared the chemistry Nobel Prize at the beginning of the 20th century. Bosch improved Haber's method of manufacturing ammonia from hydrogen and nitrogen into an industrial process that produces enormous amounts of ammonia from high pressure catalytic reaction of N₂ from the air and H₂. When temperature of 773 K and pressure value equal 200 bar, this is commonly carried out with an iron oxide catalyst. Although there have been several advancements throughout the years, the Haber-Bosch method continues to form the foundation for contemporary ammonia production [3].

Ammonia created by humans can be manufactured using water, air, nuclear power plant waste heat, or heat from another renewable energy source like: wind, hydro, geothermal etc.). Natural ammonia substance is derived from decomposing organic matter. Man-made ammonia can be produced using any type of the fossil fuel as a feedstock (natural gas, gasoline, coal, ... etc.). The primary materials are water and air. As a result, ammonia is completely recyclable since it can be created from elements that are found practically everywhere in nature (water and hydrogen), and because the byproducts of its burning are primarily water and nitrogen with no carbon [4].

As previously indicated, ammonia may be converted into hydrogen by thermal cracking or chemical cracking. Other recent research [5,6] examined the potential of NH₃ as a fuel, despite the fact that it can be poisonous when handled incorrectly, NH₃ represent an appealing energy for the following reasons:

- Regarding it is flammability, explosive natural and the diffusivity, it is less dangerous than other fuels and hydrogen [5].
- Its relatively high octane rating make it potential energy for gas turbines and internal combustion engine (ICEs) [6].

- It thermally split into H_2 and N_2 . Some research [7] have produced hydrogen for fuel cells using only around 12.7 percent of it is lower heat value (LHV of ammonia= 18.6 MJ/kg).

1.2.1. Using NH_3 (Ammonia) as a fuel source

Ammonia was first thought of as a hydrogen provider; in this sense, the supply line includes its breakdown into H_2 and N_2 in the hydrogen delivery points. However, in recent years, direct fuel consumption has been added to the list of ammonia's uses. Ammonia is flammable and since it contains no carbon, it emits no carbon dioxide during combustion, reviving interest in using it as a fuel. This is evident from the sudden rise of ammonia combustion-related scholarly papers. Figure (1-1) shows the manufacturing, transportation, and many uses of carbon-free ammonia. [8].

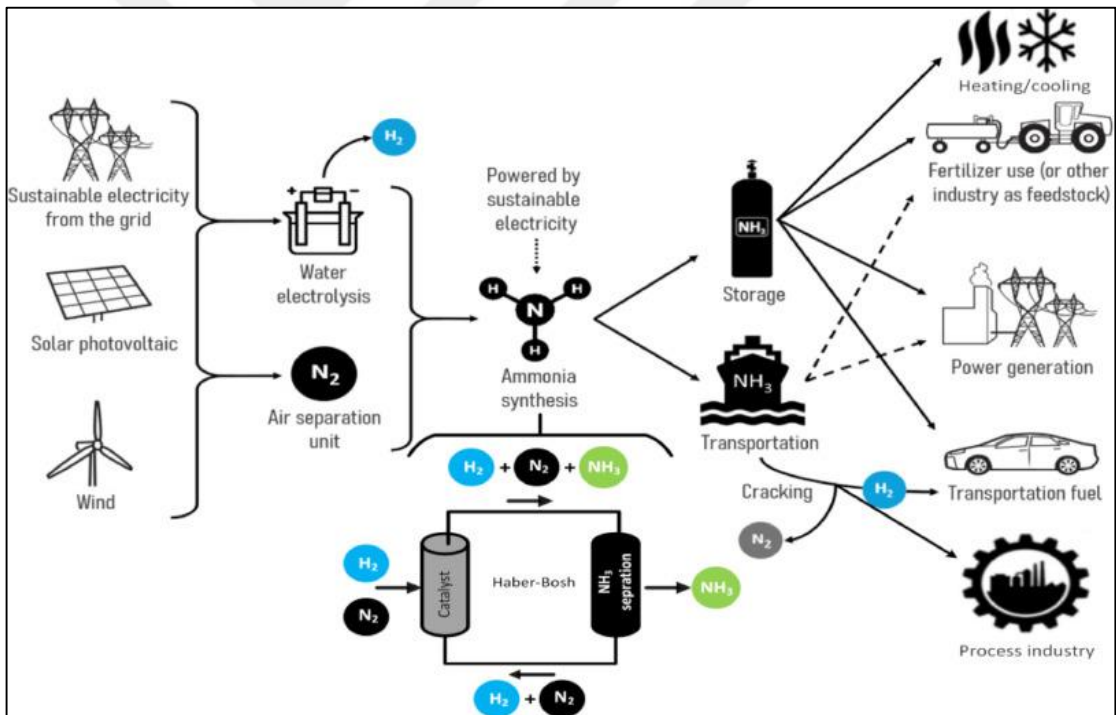


Figure 1.1: Manufacturing, transportation, and many uses of carbon-free ammonia.

1.2.2. Ammonia Specifications

A colorless gases with the pungent smell. Boiling limit of Ammonia is 239.72K and a freezing points of Ammonia is 195.44K, and an automatic ignition temperatures

of 924K when exposed to the atmosphere. It may be managed as a liquid in containers with insulation and has a higher heat vaporization (23.3 kJ/mole at its boiling limit), Reasonably high octan amount (130). The molecule of ammonia has a tetrahedrally pyramidal structure, 3 hydrogen atom, and a nitrogen atom contains a pair of unshared electrons, Nitrogen gas and water are produced during the burning of ammonia, with a weighted stoichiometric air to fuels concentration of 6.06 [9]. The characteristic of ammonia is presented in Table 1.1 [9].

Table 1.1: Ammonia Specifications.

Molecular mass	17.0312 kg/mol
Molecular volume (at 273 K, 1 bar)	22.081 mol-1
Gas constant (R)	0.48818 kJ/kg K
Liquid density (at 273 K, 1 bar)	0.6386 g cm-3
Gas density (at 273 K, 1 bar)	0.7714 gl-1
Liquid density (at 239.72 K, 1 bar)	0.682 g cm-3
Gas density (at 239.72 K, 1 bar)	0.888 gl-1
Critical pressure	112.8 bar
Critical temperature	405 K
Critical density	0.235 gcm-3
Critical volume	4.225 cm3 g-1
Critical compressibility	0.242
Critical thermal conductivity	0.522 kJ K-1 h-1 m-1
Critical viscosity	23.90 × 10-3 mPa s
Melting point (triple point)	195.44 K
Heat of fusion (at 1 bar)	332.3 kJ kg-1
Vapor pressure (triple point)	0.06077 bar
Boiling point (at 1 bar)	239.72 K
Heat of vaporization (at 1 bar)	1.37 MJ kg-1
Standard enthalpy of formation (gas at 298 K)	-46.22 kJ mol-1
Standard entropy (gas at 298K, 1 bar)	192.731 J mol-1 K-1
Free enthalpy of formation (gas at 298 K, 1 bar)	-16.391 kJ mol-1
Net heating value (LHV)	18.577 MJ kg-1
Gross heating value (HHV)	22.543 MJ kg-1
Electrical conductivity (at 238 K), very pure	1×10-11 Ω-1cm-1
Electrical conductivity (at 238 K), commercial	3×10-5 Ω-1cm-1
Ignition temperature according to DIN 51794	924 K
Explosive limits:	
NH3/O2 mixture at 293 K, 1 bar	5–79 vol% NH3
NH3/air mixture at 293 K, 1 bar	16–27 vol% NH3
NH3/air mixture at 393 K, 1 bar	15.5–28 vol% NH3

1.2.3. Aspects of Ammonia Shipping, Consumption and Collection

For portable fuel cells, the problem of energy storage is a considerable obstacle. Only hydrogen-based fuel appears to have the energy conversion efficiency necessary to justify the shift in technology needed in the field of vehicle propulsion [10]. Ammonia is being examined as a possible hydrogen transporter in this scenario to address the issue of in-cabin storage. Although Ammonia isn't like a H₂ compound, it may be kept readily in a liquid state at ambient temperatures 288K by applying an approximate pressure 10 bar.

Zamfirescu and Dincer [10] contrasted NH₃ with accustomed fuels (petrol, LPG, CNG, hydrogen and methanol). They specified fuel and method of storages as indicated in Table 1.2 from the viewpoint of fuel storage density at unit of volume or mass, as well as the prices at unit of tank volume, Ammonia is around three times more efficient than pure hydrogen as a term of energy density at unit volume. according to their research, which also showed that ammonia is simple to store in a liquid condition. NH₃ values as a fuel is shown in the table below, both economically and environmentally.

Table 1.2: Comparison of hydrogen and ammonia as fuel sources.

Fuel/storage	P [bar]	ρ Density [kg/m ³]	HHV [MJ/kg]	Energy density [GJ/m ³]	Specific volumetric cost [\$ /m ³]	Specific energetic cost [\$GJ-1]
Gasoline, C ₈ H ₁₈ /liquid	1	736	46.7	34.4	1000	29.1
CNG, CH ₄ /integrated storage	250	188	42.5	10.4	226	28.2
LPG, C ₃ H ₈ /pressurized tank	14	388	48.9	19	548	28.8
Methanol, CH ₃ OH/liquid	1	786	14.3	11.2	421	37.5

Table 1.2: Continue.

Fuel/storage	P [bar]	ρ Density [kg/m ³]	HHV [MJ/kg]	Energy density [GJ/m ³]	Specific volumetric cost [\$/m ³]	Specific energetic cost [\$GJ ⁻¹]
Hydrogen, H ₂ /metal hydrides	14	25	142	3.6	100	28.2
Ammonia, NH ₃ /pressurized tank	10	603	22.5	13.6	181	13.3
Ammonia, NH ₃ /metal amines	1	610	17.1	10.4	183	17.5

Additionally, as indicated by Klerke et al [11], ammonia be carried to the locations of consumption and utilized as a fuel, chemical, fertiliser, refrigerant, and more. These delivery methods include pipelines, railroad carriages, auto-cisterns, and ships.

1.2.4. Ammonia Safety

Access to a lot of NH₃ may be lead to serious body is burning. In extreme circumstances, such access maybe also result in mortality, lung damages, blindness, heart attack, and lung injury. NH₃ is classified as an absorption danger rather than a pollute to despite these safety issues. Nevertheless, all ammonia-based hydrogen generators must be designed, tested [12].

Ammonia is categorized as a non-flammable liquid and presents little danger of fire in the event of open flames or sparks. Compared to other gases, it has a far reduced risk of fire and explosion, and it may be made as safe as required [13].

Due to the following characteristics, ammonia is regarded as being better than other fuels:

- Because ammonia has a lighter weight than air, if it is released into the air, it evaporates quickly.
- It is self-alarming since any leakages may be recognized by its fragrance in quantities less than 5 ppm [10] due to its strong smell.
- It causes little explosive risk when carried properly because of its small flammability range and general lack of flammability.

So, using fuel of Ammonia in devices like gas turbine, which has its difficulties, is one alternative to its use.

1.2.5. Benefits of Using Ammonia

The data collected by Pfromm [14] show that an estimated 174 million metric tonnes of ammonia were produced globally in 2017. Ammonia was used as fertilizer in agriculture to the tune of almost 85%. In 2016, the price of ammonia was roughly \$600 per ton, with a minimum price of 500 dollar a ton in place since after 2008.

- Compared to liquid hydrogen, anhydrous liquid ammonia saves more energy per volume.
- Ammonia storage, use, and transportation technologies are well founded and readily accessible.
- Generating hydrogen from ammonia may be used in gas turbines devices, which are the most inexpensive and produce fewest air pollutants.
- Ammonia may be held at modest pressure and shares many of the same physical characteristics as liquid propane.
- Ammonia does not emit CO₂ during burning when used as a fuel in power plants.
- Only 12.7% of the ammonia stored energy is required for the gas to split into nitrogen and hydrogen.
- Methanol has a lower energy density (11.2 GJ/m³) than pure ammonia (13.6 GJ/m³).
- Because ammonia has a strong smell, it is easy to identify leaks, which lowers certain storage hazards.
- The contaminants in flue gases like NO_x can be captured post-combustion using its potential solvent characterisation.
- Ammonia is a very simple liquid to manage since it contains a lot of hydrogen.

1.2.6. Challenges of Using Ammonia

It's essential lowering the ammonia dissociation temperature and price for applications requiring cost-effective power production. Additionally, while utilizing ammonia for combustion, great attention should be paid for health, safety and environment of site employees as well as any surrounding human settlements and environmental variables. As a result, there are several obstacles to be solved before ammonia combustion may be fully adopted.

Under and over, the burning of ammonia produces nitrogen oxides (NO_x), primarily NO and NO₂. Nitrogen oxide are recognized to just be gases with high chemical and radiative activity that contribute significantly to the global warming effect. Also they are the primary cause of acid rains [15].

Ammonia is damaging to several metals, including plastics, nickel and copper. hence its use presents a technological problem. The inability of ammonia to ignite lead to high automatic combustion temperature (924K) in comparison to another fuel (gasoline, 713K, diesel, 498K) presents another obstacle to employing ammonia as a fuel [6]. There are strict ignition restrictions for burning of ammonia in CIEs: 16-25% by volume in air is needed. Additionally, utilizing ammonia in spark-ignition engines results in a power output that is around 20% lower than when using regular gasoline. Only engines can burn ammonia using proper ignition techniques due to having a low energy content, low energy content, a low boiling limit [6].

The use of NH₃ as a flexible fuel in GTs has been made possible by a variety of various strategies. However, a number of difficulties, such as low flame temperatures and delayed kinetics, have been encountered when using combustion of liquid of ammonia in gas turbines with steady, effective of combustion. Ammonia may burn in combustors in the vapour phase, however devices that can vaporize the ammonia or crack the moles are needed to boost flame velocities and burning ratio. Different injection tactics and a low swirl number were recommended by Valera-Medina et al. [16] to optimize gas turbine power output, but these strategies still require improvement.

1.3. Methodologies for Ammonia Cracking

Any process that breaks down more complex molecules into simpler ones, whether it involves heat, solvents, catalysts or both, is referred to as "cracking." There are several cracking techniques based on factors including temperature, pressure, and the presence of catalytic elements. A number of experiments [17] have shown that for ammonia to be used as a fuel, the ammonia must typically be hydrogen-doped, that maybe acquired by breaking the ammonia moles. Hydrogen can be added to the ammonia by cracking it. Fast flame rates can achieved for usage in high power devices.

1.3.1. Thermal Method

Entropy (S°) at Gibbs free energy equation is greater than enthalpy (H°) because thermal cracking causes the fragmentation of a single big molecule into multiple smaller components at an exceptionally high temperature:

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ \quad (1.2)$$

1.3.1.1. Thermal Cracking

Both high and low pressures can occur in thermal cracking. High pressure thermal cracking is using for separate heavy fraction into light fractions at absolute pressures of roughly 70 bar. Homolytic fission, the actual process, provides the basis for the commercially feasible manufacture of polymers. In 1891, a Russian engineer named Vladimir Shulkhov developed the first thermal cracking technique [18].

According to Hacker and Kordesch [9], at ambient pressure and at a temperature around 703 K. ammonia completely decomposes. To just be able to break down ammonia into H_2 and N_2 created thermal cracking technique for ammonia combustion cracker units in 2011. This process uses heat produced by the burning of some of the ammonia utilized. It was discovered that when the wall temperature of a silicon carbide tube reaches about 1573 K, ammonia begins to dissolve down [17].

1.3.1.2. Vapor Cracking

Facilities named steam cracker units employ a feedstock to make lighter fractions by thermally cracking material decomposition reactors in a an utilizing steam. The feedstock composition, the ratio of fuel to steam, the temperature at which cracking occurs, and the burner residence time affect of the products that are produced [19].

In the process of Vapor cracking, a vapor is mixed with liquid or gaseous fuel and heated in an oxygen-free burner. The reaction occurs at an extremely high temperature roughly 1123 K but only for a brief period of time.

1.3.2. Catalytic Methods

Availability of catalysts like iridium, platinum, nickel and silica-aluminum, that used the heterolysis breakdown of bond generating couple of ions of opposing costs, is necessary for catalytic cracking [17]. To solve the issue of hydrogen storage, a hydrogen producing facility might be built using hydrogen produced from ammonia dissociation [9].

1.3.2.1. Fluid Catalytic Method

Petroleum refineries frequently employ fluid catalytic cracking, which is more effective than conventional thermal cracking. Around 1942, a low activity alumina catalyst was utilized as the foundation for the first fluid catalytic cracking process [20]. Alkanes and alkene studies are still conducted in high school and university laboratories using alumina-catalyzed cracking devices. The "riser" is a vertical or upward-sloping pipe where cracking occurs utilizing a particularly active zeolite-based catalyst over a brief contact period in more recent designs [21].

1.3.2.2. Hydrocracking

By mixing hydrogen gas with ammonia, the hydrocracking process catalyzes cracking. The hydrocracking process may occur at a variety of extremely high pressure between (70-140 bar), reasonably high temperature between (673K-1073K), in the

presence of hydrogen, and under certain catalysts conditions, based on the circumstances of the reaction (temperature, pressure, catalyst activity) [18].

Therefore, it is crucial to create cracking systems utilizing thermal approaches that allow the use of hydrogen to occur the highest potential effectiveness as well as the lowest Probable NO_x emissions to help the actions of decarbonization in the energy generating industry.

1.4. Summary of This Section

Although the potential the effectiveness of a H₂ powered engines which uses onboard ammonia decomposes has been the subject of several research, there are still a number of issues that need to be resolved before the technology can be fully commercialized. According to certain studies, it would be feasible to increase a power engine's overall efficiency by using catalyst or thermal cracker to break down NH₃, producing a combination of the ammonia and additional hydrogen to ignite improvement. New cracking techniques are therefore required to alter the combusting mixture's composition for improved flame stability, increased engine performance, decreased NO_x emission. and superior energy loading for employment of the use of chemicals in gas turbine.

2. LITERATURE REVIEWS

2.1. Producing Power by using Ammonia

Despite the widespread discussion about alternative fuels to coal, oil, and gas, there is still a dearth of knowledge on the usage of nitrogen-based fuels to meet energy demands, as previously noted. Therefore, in order for fuels like ammonia to be useful in power generation devices in the near future, development must be sped up.

Ammonia has received a lot of relevance recently as a useful energy sources for fuel cells which may burn either NH_3 directly or the H_2 produced by cracking NH_3 with the aid of catalysts or promoter schemes [22].

2.2. Using ammonia in ICEs

One of the most popular and economical methods for converting energy into power is through internal combustion engines (ICEs). Prior until now, only a small number of research have looked the use of NH_3 as a fuel in ICEs, either in diesel engines or in (SI) spark ignition engines. Although it is commonly recognized that ammonia may be used to store hydrogen, ammonia is currently underutilized as a fuel because of its drawbacks. Table 2.1 reproduces some of the NH_3 and other transportation fuels' qualities [23].

Table 2.1: Ammonia Compared To Other Fuel Sources

Fuel	Molecule	Boiling Point K	(Air/Fuel)s	Latent Heat (kJ/kg)	Energy Content (MJ/kg-fuel)	Energy Content (MJ/kg-stoichiometric mixture)
Methanol	CH_3OH	337	6.435	1203	20.0	2.6900
Ethanol	$\text{C}_2\text{H}_5\text{OH}$	351	8.953	850	26.9	2.7027
Gasoline	C_7H_{17}	---	15.291	310	44.0	2.5781
Diesel	$\text{C}_{14.4}\text{H}_{24.9}$	---	14.322	230	42.4	2.7660
Ammonia	NH_3	239	6.046	1371	18.6	2.6414

However, ammonia burns at a slower rate and has a greater ignition temperature than gasoline and diesel, 924K compared to 713K and 498K, respectively. Before ammonia can be utilized as an ICE fuel, a number of technical concerns need to be investigated further [23]. However, recently, many researchers have begun to recognize ammonia as a potential fuel for use in ICEs, either by combining it with other fuels (such as gasoline, diesel, methanol, kerosene, etc.) to promote combustion or by partial decomposition of ammonia by H₂ and N₂ cracking in order to better start the combustion process. [10].

Pearsall and Garabedian [24] looked at the usage of NH₃ in a diesel engine with pilot injection under a variety of loads. They discovered which the engine could function effectively if the load was managed by varying the intake pressure via turbocharging and throttling, while maintaining a steady ammonia/air equivalency ratio. However, it was discovered that under loads equivalent to throttled operation, this engine exhibits backsliding combustion quality and a increasing ignition latency when intake pressures are reduced, 0.5 bar. Similar suggestions are made in favor of utilizing high compression ratios > 20:1.

Woo et al. [25] looked at the use of NH₃ as a fuel for mobile programs. They have created an idea to fully complete combustion that does not require conventional fuels, igniting NH₃-air mixtures. Both the compression ignition and SI engines used NH₃ as their primary fuel in this experiment.

2.2.1. Ignition engine with compression

Experimental research on the emissions and combustion characteristics of compression-ignition engines utilizing ammonia and dimethyl ether (DME) mixtures may be found in A pre-mixed air-ammonia-diesel mixture was provided for ignition by injecting ammonia straight into the manifold. Up to 95% ammonia and 5% diesel were used to try to run the system. Following the introduction of vapour ammonia, engine torque increased abruptly. Direct injection was shown to have far lower exhaust ammonia emissions than other methods, and adding more ammonia might enhance output power. In the previous dual-fuel operation, diesel fuel was replaced with ammonia to provide the same amount of power. As would be predicted, cracking

efficiency approached 60% due to the lower burning temperature, and NO_x emissions fell as ammonia levels declined [26].

2.2.2. Spark - Ignition Engines

NH₃ as a fuel for SI engines has very seldom been the subject of investigations in the past. A lot of studies on this topic. However, have been conducted recently as a result of the actual worries that oil sources were running low and this environmental problems connected to CO₂ emissions posed a major threat to public health [27]. Recent research has demonstrated that a SI engine typically can't operate at an adequate level when powered only by NH₃; instead, additional fuels must be combined with ammonia to produce a suitable power reaction [27].

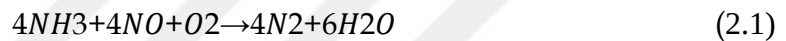
Nitric oxide, CO, hydrocarbons and NH₃ emissions from the engine after the catalyst and after it has shut down. Grannell et al. [27] measured and nitrous oxide as well. They found that a typical three-way catalytic converter may adequately remove these contaminants, but lean running must be completely avoided. The cleanup zone was found to reside between the crystalline form and the 0.2 percent rich fuel conditions. The quantity of ammonia in the fuel mixture at intake was precisely reflected by the engine's exhaust emissions when the engine was operating appropriately in terms of burn stability and overall thermal efficiency. It was recommended that the use of a post catalyst oxygen sensor is essential since lean and rich operation have a greater impact on post-catalyst NH₃, NO and Nitros emissions [27].

Due to its low auto-ignition capability and low flame speeds, ammonia cannot be used as a fuel in SI engines without being combined with other fuels as combustion boosters. This was tested in IC engines using ammonia and other doping agents [28]. It was demonstrated that the air-ammonia mixture requires the addition of an accelerant to increase ignition, speed up burning and provide a wide flammability range. One such accelerant is hydrogen, which has the advantage of being carbon-free.

A SI engine may be able to run on hydrogen and ammonia, with the hydrogen acting as a combustion promoter and coming from an on-board catalytic reactor, according to recent study. The hydrogen produced when ammonia is split is kept at its operational temperature by the heat from engine exhaust gases. The approach turned

out to be far more beneficial than injecting merely pure ammonia. On the other hand, greater combustion temperatures led to an increase in NO_x emissions. Studies on emissions have examined the mechanisms of NO formation in ammonia-hydrogen-fueled SI engines. Analyzing the unburned ammonia in the exhaust, it was found that the emissions varied from 10 to 25 ppm [29].

To use SCR (selective catalytic reduction) system may be required to try to decrease the NO_x, according to more recent research [30]. The ability to employ ammonia makes the SCR valuable. Despite being exothermic, the SCR reaction wouldn't have a negative impact on the ammonia desorption procedures. It wouldn't take much ammonia to use selective catalytic reduction to convert the NO_x emissions to water and N₂, as shown in Equation (2.1):



The key difficulty in using SCR on a vehicle, meanwhile is figuring out how to prevent significant ammonia slip under a variety of load scenarios.

2.3. Cracking of Ammonia

It is not a novel idea to utilize ammonia as a hydrogen transporter and there are several techniques to "crack" or create hydrogen from ammonia for use as fuel. To ensure an efficient cracking process, NH₃ cracking is often conducted under pressure, at a certain temperature or with a catalyst present. Only a few papers discuss thermal breakdown in the literature that is currently accessible, which is mostly focused on the catalytic breaking of ammonia. At temperatures below 698 K, catalytic breaking of NH₃ into H₂ is around from 98 to 99 percent efficient. Ammonia begins thermally cracking at temperatures 773K or higher than this limit without the need for a catalyst. In reality, the use of catalysts, pressure and temperature all affect how quickly ammonia is converted [31].

2.3.1. Catalyst Cracking

Human-produced ammonia has become more and more the focus of recent research on catalytic ammonia breakdown. Ammonia kinetic energy for cracking method been examined by using materials and some of types of iron with another material oxides [32].

The shape of the micro reactor components, the addition of a randomly choosing precursor and the employment of a catalytic promoter was all demonstrated to have an impact on the reactor's performance. At 873 K, the reactor transforms 99% of the ammonia into 60 W of hydrogen. This amount of hydrogen generation would be adequate for a variety of uses, including gas turbine, internal combustion engine and fuel cell applications [33].

2.3.2. Thermal Cracking

America Patent Office released information on Burke "Apparatus for decomposing ammonia" in 1933, marking the first significant attempt to thermally split ammonia [34]. Ammonia gas was created by heating liquid ammonia in tubes and this gas was then heated even more in a separate chamber before flowing through heated pipes more a suitable catalyst. Burke said that his innovation allowed for 90 percent ammonia breakdown between 823 K and 923 K. A technique for producing H₂ and N₂ by breaking gaseous NH₃ and reusing and cleaning an environment that has already been produced and consumed is described in a Normand patent that was registered in 1978 [17].

An oxygen-air mixture was added to waste gas that included at least 50% by volume of ammonia in a later invention by Graville (see Figure 2.1 [35]). The combustion zone is where both cracking and combustion occur, and the process is so powerful that, according to Graville [35], "no ammonia remains". To supply Oxygen is required to be the percent of oxygen (90-75)% from all percent of fuel that combusted. NO_x generation may be reduced by managing the combustion conditions.

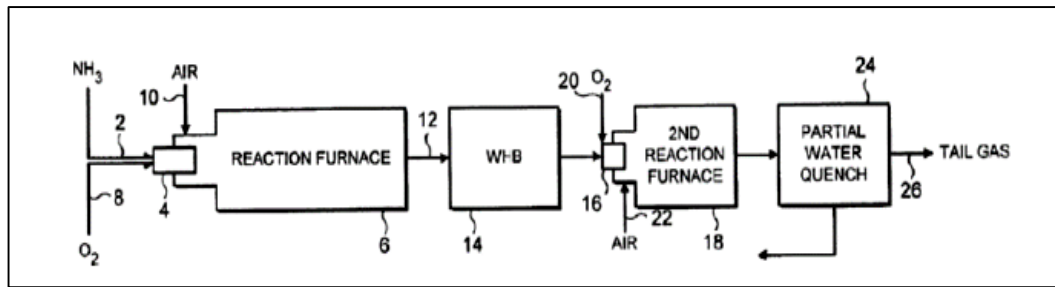


Figure 2.1: Destruction of waste gas

Goetsch et al. [36] filed a patent for a method of "generation of hydrogen by autothermal cracking of ammonia" to create high purity hydrogen. This innovation supplied a fuel cell with the hydrogen it generated. The creators discovered that it was possible to make the ammonia decomposition reaction autothermal, requiring no additional heat from any external source. When an exothermic process may continue to fuel itself and any linked endothermic reactions, auto-thermal operation is taking place stoichiometrically. This is accomplished by burning a portion of the hydrogen produced in the same reaction zone as the ammonia cracking process. However, this autothermal reformation of ammonia still needed catalyst bed technology.

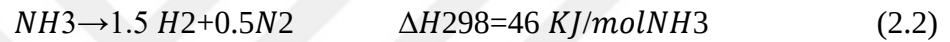
Arana et al. recorded the first incidence of high-temperature ammonia burning and breaking without the usage of electrical power, in a MEMS device [37]. Thermal characterization has demonstrated that intrinsic heat loss (conduction in the material) is exceptionally low for the reactor, which can operate up to about 1173 K. Based on experimental results, these losses are estimated to be less than 0.1 W at 1073 K. Other losses (such as those from radiation, natural convection via the surrounding air and conduction) can be considerably reduced with the appropriate packing, as a result of butane combustion that is catalytic and auto-thermal.

A conference presentation on the conversion of ammonia into a hydrogen gas mixture was given by Grannell et al. [38]. Within a conduit, a process for decomposing a part of an anhydrous ammonia mixture is started. The gas mixture is mixed with the hydrogen that is created and the combustion reaction is finished using the heat that was generated. The reaction produces a combination of gaseous products, including non-combusted hydrogen gas, which is released out the conduit's exit and may be utilized for other purposes. Based on the LHV, a product with an NH₃ and H₂ thermal conversion efficiencies like 97.3 % and about 52% H₂ by volume was produced at the

theoretical performance limit of an ammonia flame cracker with zero losses. At an equivalency ratio of 6.66, full cracking took place.

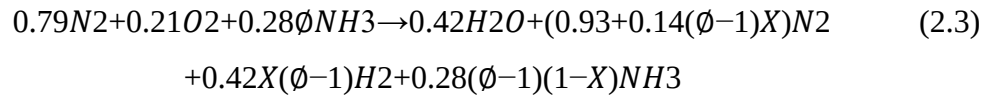
Engbaek developed an ammonia cracker for the manufacture of hydrogen for PEMFC power devices [39]. Methods for hydramine catalyst-based ammonia cracking that use counter-current flow heat exchangers to provide ammonia to the cracker were also evaluated. with an output of 800 ppm NH₃.

According to a US invention, Page et al. Alkaline membrane fuel cells used a hydrogen fuel supply from an ammonia thermal digester with a combustion compartment. approximately 75% H₂ and 25% N₂ produced by the cracker and residual ammonia concentrations ranged from 1 ppm to 20 000 ppm [40]. During the power generating process using the cracker's waste heat, ammonia from the stored material is discharged. The endothermic reaction Equation states that (2.2):



By assisting in the burning of fuels or by providing electrical heating, this heat may be put to good use. However, if the system doesn't have a battery, electrical heating is not only costly but also unavailable when the system first starts up. As a result. Ideally, this heat should be generated by burning a suitable fuel, such as ammonia or hydrogen, as in Grannell and Gillespie's [42] innovation that involves cracking ammonia into a hydrogen gas combination. Anhydrous ammonia and air are combined beforehand and flowed through a conduit as part of this ammonia cracking process. The reaction's byproducts, including the unburned hydrogen it produced, can subsequently be utilized for other things.

The total NH₃ and the air reaction is shown by the equation:



Where

ϕ : NH₃/air equivalence relation, and $\phi > 1$.

X: unburned ammonia's output of decomposition, and $0 \leq X \leq 1$

Brandenburg came up with a productive method for cracking ammonia [43]. A dielectric diaphragm separated two compartments within a resonant cavity. As seen in Figure 2.2. One of the sections was filled with ammonia gas. Electromagnetic energy is released into the opposite compartment using a microwave antenna. A plasma discharge is produced when the signal is at the right level and frequency, as seen in Figure (2-2). Anhydrous ammonia that has crossed the membrane and is leaving the cavity through an outlet can be broken down by the plasma discharge in an efficient manner.

Any metal which is a good electric conductor should be used to build the microwave's exterior walls. The interior surface coating should be made of stainless steel or nickel metal to avoid chemical corrosion during ammonia cracking. It was said that a plasma cracker could break a litre/second of NH_3 with electrical use of 2 kW and that little heat escapes from the system. The generated hydrogen might be used right away or burned in a fuel cell to generate 12 kW of electricity with an efficiency of approximately 80 percent [43].

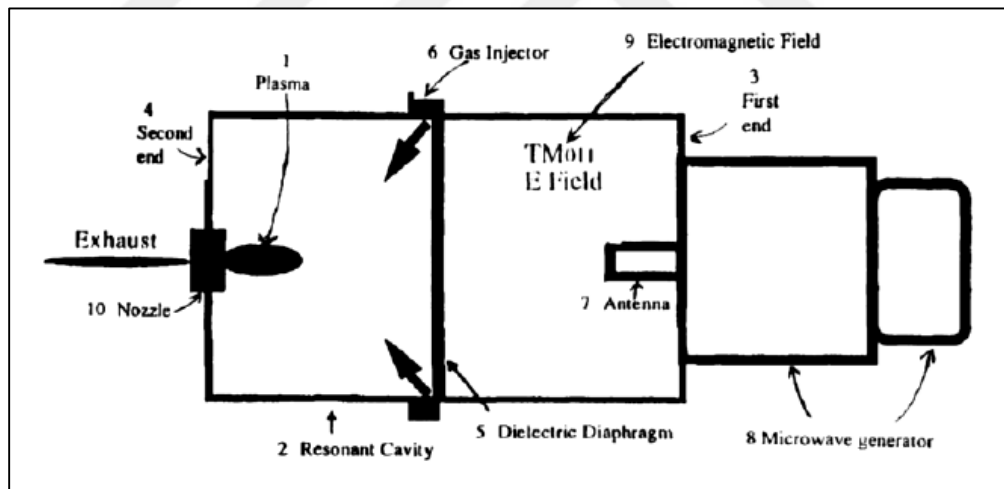


Figure 2.2: Plasma Reactor for H_2 and NH_3 Production.

2.4. Ammonia Fuel Combustion

Various experimental and numerical studies have been conducted on ammonia combustion since 1960s. Many studies can be found in ammonia flames at various conditions [44]. The fundamental objective of these research was typically to comprehend the function of hydrogen and ammonia in the synthesis and consumption

of nitrogen oxides. Other researchers gave up on the topic due to ammonia's extremely low combustion efficiency until the end of the 1980s, when several investigations on the chemistry of the air pollutant N-C-O-H revealed different thermal NO and induced NO routes.

In an adiabatic well stirred reactor, Pratt and Starkman [45] investigated a semi gaseous phase complete combustion using ammonia and air. They came to the opinion that the Arrhenius equation might adequately characterize the complete reaction rate for ammonia-air combustion. In contrast to fast reactions, they discovered that contacts with the reactor wall are crucial to the kinetic process for sluggish reactions. Therefore, more research into the dynamics of ammonia burning was necessary.

Sullivan et al [46] were below flame temperatures included both experimental and modeling research. The results of the experiments were taken into consideration in terms of plug-flow, a condensed mixing reactor and a 2-D direct numerical simulation. It was shown that the post-combustion gases might mix with the end products of the process. Ammonia oxidation occurred in a pre-mixed reaction zone at low temperatures. A non-premixed reaction zone that produces considerably less NO than the comparable premixed system may, nevertheless, be generated at high enough temperatures.

Prior research generally demonstrates that fuel bound N₂ more than thermal NO_x generation by ambient N₂ is the major factor in NO_x creation in ammonia flames [46]. For fact prediction of emissions owing to fuel bound N₂, a thorough understanding of ammonia combustion chemistry and a thorough investigation of NO_x production pathways are necessary.

2.4.1. Models of Reaction Mechanisms in Ammonia Combustion

To analyze ammonia oxidation and NO_x generation processes, a number of chemical kinetic models have been created and put into use. Tian et al. [47] carried out pertinent experimental and modeling research the combustion of low-pressure ammonia (0.04 bar). They used molecular-beam mass spectrometry in conjunction with tuneable synchrotron vacuum ultraviolet photo-ionisation to examine the stoichiometric equivalency ratios of 11 premixed NH₃/CH₄/O₂/Ar flames and their flame structures. To determine the main CH₄ and NH₃ oxidation reaction routes and how they interact, this study evaluated as well the function NO-to-NH₂ conversion

responses and flow sensitivity. Tain's mechanism [47] has recently been used often to a variety of circumstances.

Skreiberg et al. [48] created a complete chemical kinetic model for the oxidation of ammonia in the presence of hydrogen, carbon monoxide, and methane using the SENKIN and CHEMKIN programs. NO concentrations range from 0 to 2500 ppm, temperatures range from room temperature to 1330K and stoichiometries range from moderately lean to excessively fuel-rich conditions. Since several processes within it were more thoroughly defined, its use was advised for calculating the possible reduction of NO during the combustion of gases derived from biomass. It is praised for its usefulness in assessing NO created during the burning of coal gasification byproducts. Following is a summary of the findings: High temperatures promote the NH_3 , NH_2 , NH and N_2 reaction pathway.

A technique for mimicking hydrocarbon/ NH_3 and H_2 / NH_3 oxidation processes has been established in several experiments on the combustion of ammonia, this process has proven to be a reliable predictor of NO_x emissions [49].

Numerous studies that use laser-induced/saturated fluorescence to measure the creation and removal of NO_x and ammonia from flames in a flow reactor, shock tube or other environment have been reported [50]. Impact of high CO_2 levels on the chemistry of ammonia during flow reactor methane oxidation. The experimental investigation was given at temperatures between 873K and 1773K, with fuel stoichiometric ratios ranging from rich to lean, and under circumstances of atmospheric pressure. The kinetics of the model were based on the Tian mechanism [47]. It was found through route analysis that $\text{NH}_2 + \text{O}$ plays a key role in the link between HNO and NO production. In addition, direct interactions between N-radicals and CO_2 are what lead to high CO_2 concentrations effects on ammonia conversion.

The effects of raising the oxygen content in the air on the combustion of ammonia-air blends were quantitatively assessed by Li et al. [50]. By increasing the oxygen from 21% to 30%, they concentrated on improving NH_3 combustion by focusing on ignition, flame speed and temperature and prospective improvements. The rate of formation of N-related intermediate species such as NH_2 , NH , N and HNO is significantly increased when the O_2 level rises due to the increasing rate of the processes attacked by H, O and OH. The results show that increasing the oxygen content of combustion air has a positive effect on the temperature and laminar burning

velocity of the ammonia flame. Since it improves NH_3 combustion, this approach is probably favored.

It has been widely studied how to define $\text{NH}_3/\text{H}_2/\text{air}$ mixtures at various pressure, temperature and equivalency ratios using combustion processes using an ammonia-sub mechanism [51]. These tests demonstrated that the low-temperature ignition delay durations recorded in shock tubes could not be correctly predicted (below 1000K). The results show that variations in the equivalency ratio have minimal effect on delay times, but that an increase in pressure results in a large decrease in delay times. Therefore, it is crucial to compare the results of experiments performed in flow or jet stirred reactors and burners in order to strengthen the validity of these mechanisms. Mathieu and Petersen [51] studied the oxidation of ammonia under various situations, such as high temperatures (1560-2455 K) of 0.5, 1.0 and 2.0. The models that had been proven successful in forecasting the ammonia oxidation ignition delay periods under circumstances relevant to numerous industrial applications were compared to the documented chemical processes.

Recently, Skreiberg et al. [51] used laser-saturated fluorescence and sensor sampling to study methane/air flames spiked with ammonia on a plate burner at atmospheric pressure. The NO levels in the post-flame zone were measured. It was discovered that the ammonia conversion findings in rich flames were at odds with certain earlier studies. The discrepancies were attributed to the ammonia storage cylinders used by earlier researchers not having a sufficient protective covering. Additionally, it was hypothesized that flame models that included the ammonia conversion process in both lean and rich flames accurately reflected NO_x production experimental results.

Using laser-based diagnostics, the composition of ammonia-air flames premixed on a porous cork burner at atmospheric pressure for thin, stoichiometric, and rich mixes has also been studied [52]. The radical concentration profiles of NH, OH and NO in the reaction and post-flame zones showed a good agreement between the suggested kinetic model and the actual data in terms of temperature and flame front position, with the exception of NO concentration in the rich flame. It was determined that this model should be enlarged to incorporate other combustion processes, such as flame propagation and ignition and that more tests should be conducted to assess it.

Chemical models that were first created for hydrocarbon fuels can be adapted to research on the combustion of ammonia. For instance, the GRI Mech 3.0 program was

created and is frequently used to model natural gas combustion. It covers the processes involved in NO_x production and re-burn chemistry. Zieba et al. [53] likewise employed these processes with successful outcomes. For flameless oxidation technology, The interaction of the ammonia molecule with methane was studied by Zieba et al. The radicals needed for ammonia conversion are created during hydrogen oxidation. The results showed that whereas ammonia reacts slowly in lean environments and when there is natural gas, causing substantial NO_x emissions, it reacts completely and completely quickly under fuel-rich conditions.

Molecular-beam mass spectrometry was used by Shmakov et al. [54] to illustrate experimentally how the chemistry of hydrogen flames changed when NO and ammonia were added. They used premix codes from CHEMKIN-II to simulate numerically and compare the findings with those from the experiment. They then gave a thorough review of several groups' analyses employing various molecules in lean ($\phi=0.47$), almost stoichiometric ($\phi=1.1$) and rich ($\phi=2$) hydrogen blends with oxygen and nitrogen. Their research revealed that when the hydrogen proportion in the mix was raised, laminar burning velocity rose rapidly. At lean and almost stoichiometric mixes, the flame structure exhibited good agreement, but in rich flames, there was a large disparity between the measured and modelled NO concentration profiles.

2.4.2. Hydrogen - Ammonia Combustion

Several studies describing the impact of blended hydrogen on ammonia combustion have recently been published by academics. For example, Kumar and Meyer [55] conducted a comparative analysis of laminar flame speeds for premixed H₂/NH₃ combustion that included experimental and modeling data. This experiment was done using a jet flame setup under ambient air circumstances. For equivalency ratios between 0.5 and 1.1, the NH₃ component in the fuel was changed in small steps that increased the delivered energy up to a maximum of 80%. The Tian [47] reaction mechanisms using CHEMKIN-PRO and GRI-Mech 3.0 computational models were employed. The creation of the OH radical was demonstrated to be a crucial performance variable in modeling laminar ammonia breakdown since it produced greater agreement with experimental data than the GRI-Mech 3.0.

Numerous research, including [56], have supported the idea that ammonia may be a helpful ecologically friendly additive for boosting hydrogen safety. Despite this,

there are still challenges because of the relatively slow chemical reaction rate of NH_3 -air mixtures and fuel bond NO_x emissions. A co-flow non-premixed flame configuration was used by the Sungkyunkwan University team to characterize the stability restrictions and emission profiles of blended H_2/NH_3 flames.

This investigation was carried out under ambient air circumstances and simulated data created with the help of the commercially available CFD programs like Comsol 5.6 were compared. According to the findings, adding ammonia dramatically lowered the non-premixed flame stability limitations. Due to the respective diffusivities of each fraction, the CFD model predicts that NH_3 is consumed more upstream and closer to the burner than H_2 [56]. Nozari and Karabeyoglu [57] created a simplified chemical process for ammonia/hydrogen combustion. It was determined that running under fuel-rich conditions will significantly lower the overall NO_x generation of ammonia-doped flames and reduce it to minimal levels close to an equivalency ratio of 1.2, as illustrated in Figure (2-3). By contrasting the performance of the entire mechanism and experimental data with that of the reduced mechanism, they were able to arrive at these conclusions. These demonstrate the capacity to forecast the combustion properties under a variety of fuel situations [57].

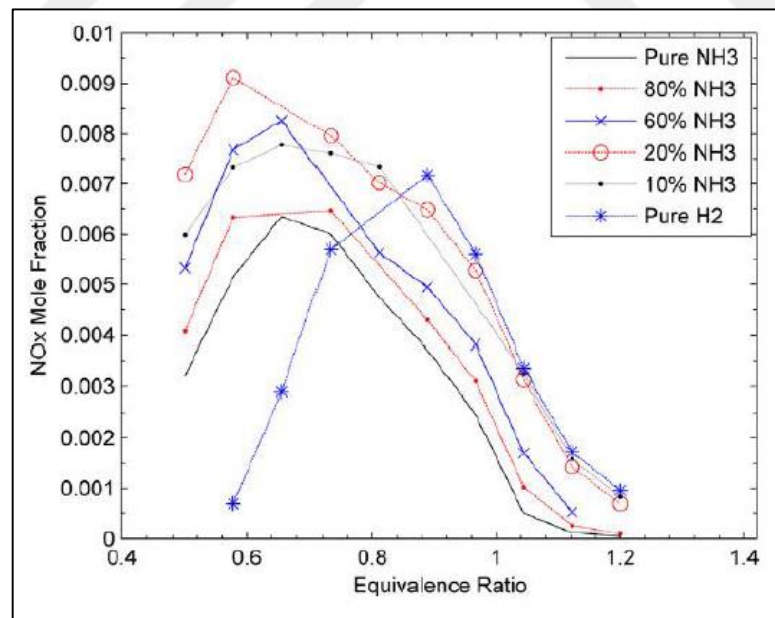


Figure 2.3: Function of equivalency ratio for overall NO_x molar concentration.

Concerns concerning hydrogen-enhanced ammonia fires at high pressures were expressed by Hayakawa et al. [58]. (up to 5 bar). They hypothesized that adding hydrogen would enhance the ammonia reaction and that the whirling flow present in

actual gas turbine combustors would boost flame stability. It was shown that the ammonia/hydrogen/air premixed flame's laminar burning velocity rose exponentially as the hydrogen ratio increased and decreased as the initial mixture pressure increased.

2.5. Ammonia Combustion Emissions

Most of the research listed above have demonstrated that burning ammonia The main exhaust pollutants are unburned ammonia and nitrogen oxides, unless the process additionally employs a mixture of carbon-based fuels like methane, gasoline or diesel, in which case CO₂ emissions must be taken into account (NO_x). Nitrogen oxide (NO_x) emissions, nitrogen monoxide (NO), nitrogen dioxide (NO₂) and nitrous oxide are the main contributors to urban smog and other kinds of acid precipitation (N₂O). Nitrogen monoxide (NO) is formed in ammonia fires by two main processes: thermal NO, which is created when nitrogen in the air is oxidized and requires a high temperature and lengthy production time, and fuel NO, which is produced by the following reaction. [59]:



Where An oxygenated species is OX, while a radical is NH_i.

Several studies The authors Nam and Gibbs [60] have written in the literature that NO_x emissions may be successfully controlled and reduced. One of the most common methods is the use of an SCR system. Ammonia or urea must be fed into the exhaust as part of SCR before a catalyst. Ammonia and NO mix in the presence of the catalyst to form molecular nitrogen and water. A range of ceramic carriers are used to make these SCR catalysts. Low NO_x reduction (10–40%) in the actual exhaust emissions and inadequate catalyst durability, however, remain problems. Therefore, for the reduction of diesel NO_x, we have investigated alternate homogeneous gas-phase selective non-catalytic reduction methods using NH₃ and Air. Due to the lack of extra equipment needed to minimize emissions, both strategies provide reduced system costs. Additionally, they offer improved fuel efficiency but necessitate the storage of a reductant inside the vehicle.

According to recent study [61], the homogeneous charge compression ignition approach may provide 40–50% efficiency at compression ratios higher than 40:1. In

various mixes of hydrogen and ammonia. The burning velocity of ammonia was demonstrably proven to rise as the flame hydrogen atom content rose. In the combustion of H_2/NH_3 and air, fuel- NO_x plays the dominant function and thermal- NO_x a small one. The findings demonstrated that using H_2/NH_3 as a fuel gas in the right combinations might improve combustion efficiency with just a little amount of NO_x production.

Woo et al. [65] used 1-D and 2-D numerical simulations to further analyze the experimentally observed NO_x generation characteristics in co-flow, non-premixed CH_4 jet flames at various oxygen, hydrogen, and ammonia concentrations. The intricate chemical kinetics found in GRI Mech 3.0 were used in the numerical simulations. According to the findings, NO_x emissions rose for oxidizers with both relatively low and high oxygen ratios. While ammonia promoted the generation of NO in the interior layers while acting as a NO_x inhibitor in the exterior layers, NO_x emissions actually dropped across the two ranges of the oxygen ratio. This phenomena appeared to be caused by a decrease in reaction rates at the same time. As was previously mentioned, this chemical reaction model performed less well when analyzing fuels based on ammonia [64].

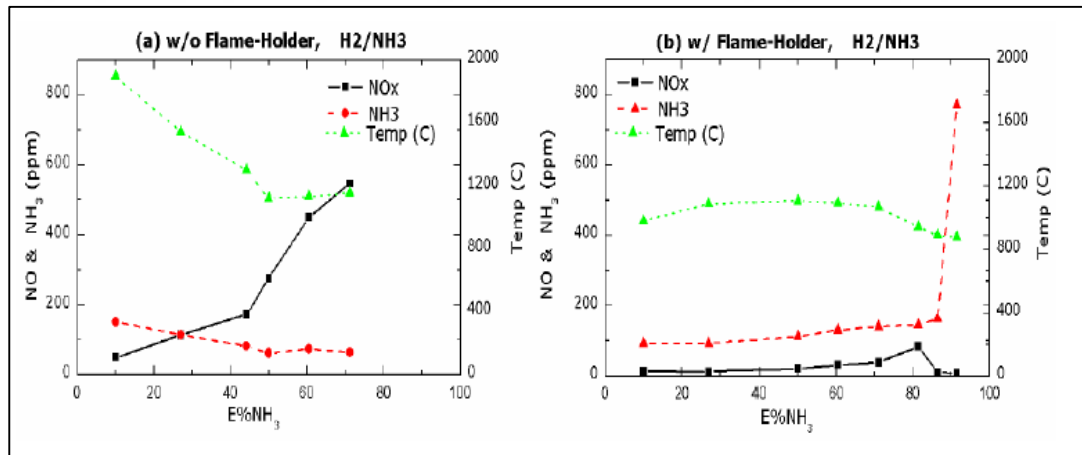


Figure 2.5: Comparison of the flame temperature and NO_x and Ammonia concentrations in the Fuel mixture.

Xiao et al. [66] carried out a 1-D numerical simulation of ammonia/methane combustion in gas turbines using Chemical Reactor Network theory. They carefully evaluated the four different techniques (Tian, Teresa AA, Konnov) to experimental research to identify which best captured reaction kinetics in real gas turbine combustor

situations. The results suggested that the Tian mechanism was the best choice for figuring out how temperature and pressure influenced NOx production. Results indicated that burning a little bit more gasoline under pressure might dramatically cut NOx emissions..

Li et al. [67] used perfectly stirred reactors (PSR) and plug flow reactors (PFR) with the Tian mechanism to predict the features of NOx production in an NH3/CH4 fueled combustor. Lower NOx emissions were discovered to be possible in a straightforward two-stage combustion process for a fuel-rich = 1.5 situation with 40% NH3. The NHi and N2O routes, as well as an increase in residence duration in the post-combustion zone, can be used to further reduce NOx in the post-combustion zone under fuel-rich condition Figure 2.6 [67].

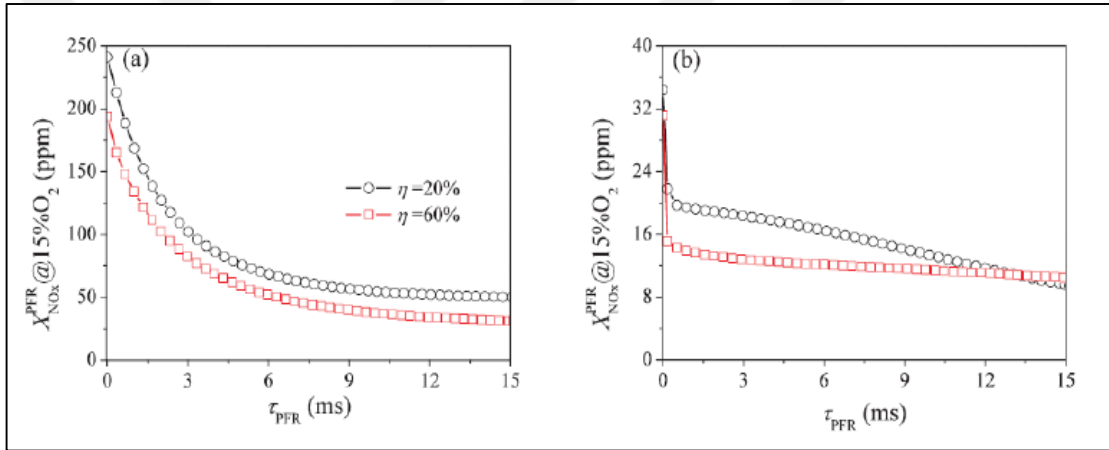


Figure 2.6: The change in NOx with initial concentration in the first stage's flow plasreactor.

2.6. Summary of Second Chapter

The use of ammonia as a replacement fuel for power production, either directly or after cracking, is covered in this chapter examination of the literature on the subject. A summary of ammonia combustion-related technologies for gas turbine applications is also provided in this chapter, with a focus on the processes used to analyze ammonia oxidation and NOx production reactions as well as strategies for lowering ammonia-related emissions.

One may have noted that there are a number of notable patents related to the use of ammonia as a fuel for various purposes accessible. These patents were obtained by

private people and/or business organizations to safeguard their intellectual property rights in anticipation of using ammonia as a green fuel in the near future.

- Compared to hydrogen, ammonia has the benefit of being extensively manufactured worldwide and having an established infrastructure for transportation and storage. It has been demonstrated to be an affordable rival to hydrogen storage. Ammonia requires less energy than hydrogen. Furthermore, the cost of power over its whole life cycle is cheaper than that of methanol or hydrogen.
- Due to ammonia tendency to liquefy in the injection line, direct injection of liquid diesel and gaseous ammonia into engine cylinders in diesel applications requires considerable injection pressure to overcome in-cylinder pressure. It will be exceedingly difficult to directly inject liquid ammonia into a cylinder in engines. However, in gasoline engines, the direct injection of gaseous ammonia might be accomplished by utilizing the small injection window prior to the increase in cylinder pressure.
- Low flow rates are not appropriate for use with gas turbines. However, it was discovered that there isn't a chemical model that can faithfully represent the wide range of ammonia burning circumstances. Before a generalized model can be suggested and put into practice, there is still a significant amount of work to be done, especially in situations when little NO_x is observed.
- For the time being, each combustion situation has shown varying degrees of reactivity, making it crucial to create explanations for certain circumstances and fuel mixtures. The maximum flame speed is reached around an equivalency ratio of 1.1, and promising experiments have shown that NO_x and CO emissions are reduced at high equivalence ratios 1.10.
- Although ammonia thermal decomposition requires a high temperature of 873 K or more, contact decomposition with a catalyst may be carried out at a temperature range of between 673 K and 873 K.
- Ru or Ru/Al₂O₃ is the best catalyst for decomposing ammonia, but they are expensive. Ni-based hydrogen-producing catalysts are favoured, but they need more contact time to achieve the same conversion efficiency as Ru-based catalysts.
- Because of their high conversion rate of ammonia at lower temperatures, potassium CNT with ruthenium catalysts appear to be the most promising. choices among all reported catalysts For the actual conversion of ammonia under industrial

circumstances, a low cost yet highly active catalyst is required due to the high costs of metals and their preparations.

- An all-purpose gas-solid phase contact reaction device made of a conversion-resistant metal, such as stainless steel, nickel steel, nickel, nickel-copper, nickel-chromium alloy or a similar substance, can be used to accomplish the ammonia decomposition process.
- To achieve optimum power loading, flame stability, reduced NO_x emissions and increased efficiency, ammonia cracking is required. Due to improved decomposition efficiency and cost savings from not requiring exotic ingredients, the thermal cracking approach has been deemed the best. To the author's knowledge, however, there isn't a paper out there that employs thermal cracking techniques without the requirement for a catalyst. In order to determine if this approach will satisfy the criteria of the energy sector, such as fuel sustainability, decarbonization of the energy sector, boosting efficiency, and reducing emissions, this study will concentrate on the feasibility of employing a thermal method to crack ammonia.

3. METHODOLOGY

3.1. Numerical Methodology

Utilization of computational fluid dynamics (CFD) to anticipate internal and exterior flow characteristics has increased dramatically in recent years. Because of the advancement of super-powered computers in comparison to barely a decade ago, high-quality, efficient CFD software with proven precision is now accessible to deliver accurate predictions at a reasonable computational cost [68]. As a result, CFD is now widely utilized in the design and analysis fluid dynamics, heat transmission, and chemical reactions of industrial systems and processes. The technique has been applied to a variety of industrial and non-industrial applications, including combustion processes in power stations, internal combustion engines, gas turbines, diffusers aircraft and vehicle aerodynamics. ship hydrodynamics, electrical and electronic engineering, chemical process engineering and others [68].

In this experiment, COMSOL Multiphysics was utilized. Three of the procedures found in this software package were utilized in this study. The first was for geometric modeling, the second was for creating meshes, and the third was for making predictions about fluid mechanics, heat transfer, chemical reactions and combustion.

The mesh produced by COMSOL Multiphysics is subjected to the governing equations of fluid dynamics using the application Fluent. These laws lead to equations for mass energy conservation and momentum strength. These equations vary depending on the characteristics of the specific flow under consideration; it is usually necessary to solve additional equations, such as heat transfer and species transport, for flows, including turbulent flows like those investigated in this paper. To offer flow solutions or to define the necessary parameters at discrete locations within the flow field, these equations are substituted with numerical descriptions that are equivalent and are solved using the finite volume technique [69].

3.1.1. Pre – Processor

The input of a flow problem to a CFD program is pre-processed by converting entering in an appropriate form for use by the solver. The following stages are included in this [70]:

- It is necessary to establish the computational domain, modeling objectives, specified outcomes, and level of precision demanded from the CFD model.
- Choosing an acceptable grid topology.
- Choose the chemical phenomenon equations, the physical model and the flow conditions (laminar or turbulent, stable or unstable).
- Creating suitable conditions at cell borders that correspond to domain boundaries.

3.1.2. Solver of CFD

The success of the following steps is required for the numerical methods utilized by the solver to work:

- Simple functions are used to approximate the unknown flow variables.
- Manipulation of the mathematical substitution of the approximations into the controlling flow equations, Using algebraic equations to solve problems.

Three techniques are used by CFD numerical solver: finite difference, finite component and finite volume. The estimation of the flow variables and the execution of the discretization procedures are the main differences between the three strategies.

The unknown of the flow problem is characterised by the finite difference approach using point samples at the nodes of a grid of coordinate lines. Finite differences resemble the derivatives of in terms of the point samples at each grid point and its close neighbors.

The shortened Taylor series expansion is the most popular way. The governing equations derivatives are substituted with finite differences, resulting in an algebraic equation for the value of Φ at each grid point [71].

The finite element methodology uses fundamental piecewise functions on elements, either linear or quadratic, to characterize the local fluctuations of the unknown flow variable. The finite volume approach is the most adaptable discretization method utilized in CFD (FVM). The domain is initially divided into a number of control volumes or cells, with the variable of interest located at the centroids of the control volumes. The governing equations differential version is subsequently integrated across each control volume [72].

The variation of the given variable between cell centroids is described by interpolating profiles between cell centroids. The variable conservation inside a control volume is expressed by the following equation, sometimes referred to as the discretised or discretisation equation. The solution generated by the FVM fulfills the conservation equations for mass, momentum, energy and species, which is its most significant feature. Both the control volume and the entire computational area satisfy these requirements [71].

3.1.3. Post – Processor

In the field of post-processing, a lot of progress has been made recently. This is owing to the growing popularity of engineering workstations, and many software packages now include data visualization features [68].

Recent additions include animation for dynamic results display. All codes offer good alphanumeric outputs in addition to graphics and feature data export facilities for further code manipulation.

3.2. Governing Equation

Fluid molecules display little resistance to external shear forces at the molecular level. As a result, every action causes the fluid to move and it is claimed that all fluids follow the laws of motion:

- The mass of the fluid is held constant.
- The overall force exerted on a fluid particle affects the rate of change of momentum, according to Newton's second law.

- The rate of energy change is formed by adding the heat contributed and the work done on a fluid particle (first law of thermodynamics).

Therefore, for a control volume, it is necessary to maintain the conservation of mass, momentum and scalars (such as energy, species, etc.) [73].

3.2.1. Mass Conservation Equation

The net rate of mass flow into a fluid element equals the rate of mass increase in a fluid element, according to the mass balance for a fluid element (continuity equation).

The continuity equation has the following form [68]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (3.1)$$

Alternatively, in vector notation:

The first component in the equation represents the rate of change of density (mass per unity of volume); the second term, known as the convective term, represents the net flow of mass out of the item beyond its limits [81, 82].

3.2.2. Momentum Equation

Two kinds of forces may be recognized from Newton's second law:

1. surface tension (viscosity and pressure)
2. body pressure (gravity, centrifugal, electromagnetic).

The following equations [68], are produced when these are applied to a fluid moving through an infinitesimal, fixed control volume.

- The momentum equation for x-component is:

$$\rho \frac{Du}{Dt} = \frac{\partial(-P + \tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx} \quad (3.3)$$

- The momentum equation for Y-component is:

$$\rho \frac{Dv}{Dt} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial(-P + \tau_{yy})}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + S_{My} \quad (3.4)$$

• The momentum equation for Z-component is:

$$\rho \frac{Dw}{Dt} = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial(-P + \tau_{zz})}{\partial z} + S_{Mz} \quad (3.5)$$

Where,

P = static pressure.

τ_{ij} = On the surface normal to the i -direction, the viscous stress component operates in the j direction.

S_{Mi} = gravitational body force in i -direction.

The pressure bears the opposite sign to that of the normal viscous stress because the normal sign convention considers tensile stress to be the positive normal stress and since pressure is by definition a compressive normal stress.

The effects of surface stresses are explicitly taken into account; in equations (3.3 to 3.5), the source variables S_{Mx} , S_{My} and S_{Mz} solely contain contributions from body forces. As a result, for instance, the body force caused by gravity would be written as

$$S_{Mx} = 0, S_{My} = 0 \text{ and } S_{Mz} = -\rho g.$$

In a Newtonian fluid, the viscous stresses are proportional to the rates of deformation. The viscosity and dynamic viscosity, which connect stresses to linear deformations, which links stresses to volumetric deformation, are the two constants of proportionality used in the three-dimensional version of Newton's equation of viscosity for compressible flow. The components of viscous stress are connected to and. The Navier Stokes equations are produced by substituting the values of viscous stress in the momentum equations [68].

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{grad } u) + S_{Mx} \quad (3.6)$$

$$\rho \frac{Dv}{Dt} = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{grad } v) + S_{My} \quad (3.7)$$

$$\rho \frac{Dw}{Dt} = -\frac{\partial p}{\partial z} + \text{div}(\mu \text{grad } w) + S_{Mz} \quad (3.8)$$

3.2.3. Energy Equation

The first law of thermodynamics, which says that the rate of change in energy of a fluid particle is equal to the rate of heat supplied to the particle plus the rate of work done on the particle, is where the energy equation originates. represents the rate of energy change of a fluid particle per $\rho \frac{DE}{Dt}$ unit volume.

The pace at which a surface force does all of the work that it does on a fluid particle is given as[81, 82].

$$\rho \frac{DE}{Dt} = -\text{div}(P\vec{V}) + \left[\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z} \right] \quad (3.9)$$

The energy equation becomes If any energy source has SE energy for each unit of volume and time, then.

$$\rho \frac{DE}{Dt} = -\text{div}(P\vec{V}) + \left[\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z} \right] + \text{div}(K \text{grad } T) + S_E \quad (3.10)$$

Equation (3.10) might be expressed as the following in vector form:

$$\frac{\partial(\rho E)}{\partial t} + \text{div}(\rho E \vec{V}) = 0 = -\text{div}(P\vec{V}) + \Phi + \text{div}(K \text{grad } T) + S_E \quad (3.11)$$

Φ : The long-term stress is represented by the dissipation function.

The dissipation function, which only includes squared terms due to the effort involved in deforming the fluid particle, serves as a source of internal energy. For this task, the mechanical energy that causes the deformation and converts it into internal energy or heat is removed. [68].

3.2.4. General Transport Equation

It is evident that the different equations share a great deal in common, and the conservative version of all fluid flow equations may be expressed as follows:

$$\frac{\partial(\rho\Phi)}{\partial t} + \text{div}(\rho\Phi\vec{V}) = \text{div}(\Gamma\text{grad}\Phi) + S_{\Phi} \quad (3.11)$$

Equation 3.12 is a representation of the so-called transport equation of property. On the left, the terms rate of change and convective are emphasized, and on the right, the terms diffusive (where d is the diffusion coefficient) and source are highlighted, respectively [68].

3.3. Turbulence Modelling

The condition of fluid motion known as turbulence is characterized by random and chaotic three-dimensional vorticity. Turbulence often predominates all other flow phenomena, leading to an increase in energy loss, heat transfer, mixing and drag. Most academics today believe that the solutions of the fluid mechanics equations might be determined merely by their boundary and starting conditions since turbulent flows are time- and space-dependent, proving that turbulence is not truly chaotic [74].

However, similarly like nonlinear dynamical systems, the deterministic solutions to the nonlinear fluid mechanics equations exhibit behavior that appears random. Due to the chaotic appearance and seemingly random behavior of these solutions, which are referred to as turbulent, statistical approaches will be required for the majority of our research on turbulence [74].

Turbulent flows are characterized by variable velocity fields. In addition to generating variations in the carrying amounts, these variations also mix transported quantities including momentum, energy and species concentration. Because of their potential tiny size and high frequency, these fluctuations cannot be directly simulated in real-world engineering calculations due to the high processing cost. The instantaneous (precise) governing equations can be time-averaged, ensemble-averaged or modified in some other way to avoid the resolution of small scales. This results in a modified set of equations that are easier to solve computationally. To calculate these

variables in terms of known values, turbulence variables and turbulence models are required [74].

The physical properties of the flow, established methods for solving a certain class of issues, the required level of accuracy, the available computing power, and the time limitations of the simulation will all have an impact on the choice of a turbulence model. Thus, in order to create effective designs using CFD, an engineer must be aware of the presence of turbulence. The models used in this study will be explained under this topic.

Major Surge Simulation, Direct Numerical Simulation, and Reynolds-Averaged Navier-Stokes (RANS) have historically been the three primary methods used to depict turbulent combustion flow with high adaptivity (LES). Figure 3.1 shows how DNS can determine the entire range of flow fluctuation, LES can determine the flow's problem-based component and model homogenous eddies, and Reynolds Averaged Navier-Stokes (RANS) can determine the entire range of turbulence (assuming isotropy).

Less computing power is required as there is more modeling in the solution. As a result, as compared to DNS, RANS-based systems consume extremely less processing power. The resources needed for LES are determined by the cut-off wavelength choice. In other words, more processing power is required the fewer eddies that are resolved. In any case, the amount of computing power required for LES falls somewhere between that of RANS and DNS. RANS is the ideal way for academic investigations since LES requires almost as much time and computational resources as the traditional RANS approach does [75]. Therefore, RANS was used in this study to examine cutting-edge methods for effectively burning ammonia mixes.

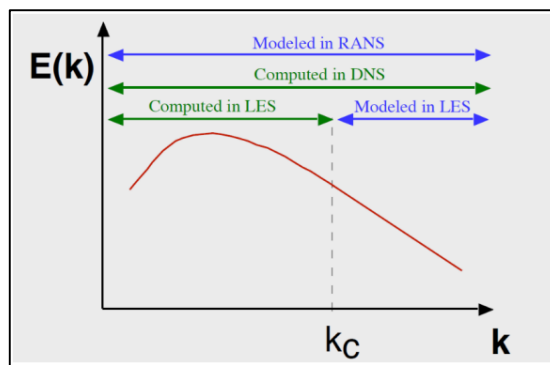


Figure 3.1: Spectrum of power generated and limit wavelength

3.3.1. Reynolds Averaged Navier and Stokes Simulations (RANS)

Because DNS requires a lot of computing power, this method was developed. Engineers have opted for a method of finding mean values and reaching a solution considerably more rapidly rather than following years of data processing, directly addressing Navier-Stokes equations and achieving solutions.

A division between average and changing data is necessary for this strategy. Reynolds Averaging is the process of treating the mean values of the flow and variations independently. As expressed in terms of Reynolds Averaging, the continuity equation is:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i) = \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i + \bar{\rho} u'_i) = 0 \quad (3.12)$$

The equation may be made simpler as follows using the constant density assumption:

$$\begin{aligned} \dot{\rho} &= 0, \rho = \bar{\rho} \\ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho \bar{u}_i)}{\partial x_i} &= 0 \end{aligned} \quad (3.13)$$

And this momentum equation is equivalent:

$$\frac{\partial (\rho \bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j + \rho u_i u'_j) = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} \quad (3.14)$$

Where the $\bar{\tau}_{ij}$ are the average components of the viscous stress tensor.

3.3.2. Standard k-epsilon Turbulence Model

Jones and Launder developed models like k-epsilon, or $K-\epsilon$, for the first time in 1972. The purpose of the model is to explain the turbulent viscosity using the turbulence's creation and destruction equations. With the aid of experimental data, empiric linkages are built.

Turbulent viscosity is defined for K - ε model [76] as:

$$\mu_t = \bar{\rho} C_\mu \frac{K^2}{\varepsilon} \quad (3.15)$$

The closure of the following two balancing equations describes K and ε :

$$\frac{\partial}{\partial t}(\bar{\rho}K) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i K) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_K} \right) \frac{\partial K}{\partial x_i} \right] + P_K - \bar{\rho}\varepsilon \quad (3.16)$$

$$\frac{\partial}{\partial t}(\bar{\rho}\varepsilon) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i \varepsilon) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{\varepsilon 1} \frac{\varepsilon}{K} P_K - C_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^2}{K} \quad (3.17)$$

The following sources provide the term P_K :

$$P_K = -\bar{\rho} \widetilde{u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} \quad (3.18)$$

The default values for the standard model constants are presented in Table 3.1. Since these default values were obtained using experimental data on basic turbulent flows, such as boundary layers, and blending layers and jets. As well as for decaying isotropic grid turbulence, they take into account shear flows that are often seen. For a variety of wall-bounded and free shear flows, the conventional k - ε model is comparatively accurate.

Table 3.1: Standard k - ε Turbulence Model.

C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_K	1.0
σ_ε	1.3

3.4. Heat Transfer Modelling

All process industries regard heat transfer to be a fundamental process. A higher-temperature fluid transmits its energy in the form of heat to a lower-temperature fluid during heat transfer. Radiation, convection, and conduction are all ways that fluids may transport heat.

From the equation for Fourier's law of heat conduction, the conduction heat transfer might be computed as follows:

$$q_x = -kA \frac{\partial T}{\partial x} \quad (3.19)$$

The following equations explain the convection heat transfer from a surface:

$$q = hA (T_{\text{surface}} - T_{\text{free stream}}) \quad (3.20)$$

Where,

q : Heat transfer rate(W).

A : Area (m²).

k : Thermal conductivity(W/m.K).

h : Heat transfer coefficient(W/m² K).

In process industries, such as heat exchangers that transfer heat between two or more fluids, conduction and convection are the most often encountered forms of heat transmission. Due to its low cost, simplicity of construction, ease of cleaning, and maximum log-mean temperature difference correction factor, shell and tube heat exchangers are frequently employed in industry. They typically have a cylindrical form and feature a collection of finned tubes through which one of the fluids flows [77].

Within the fluid and solid portions of the model COMSOL Multiphysics enables the operator to add heat transfer. To better manage the number of nodes required for conjugate heat transfer simulation, the heat exchanger has been quietly transformed into a fluid and a solid field. The absolute velocity formation and steady state solver options in this pressure-based simulation were chosen. The energy equation was selected as the model choice and the viscous model was configured to be a conventional $K - \varepsilon$ model with a standard wall function.

The heat exchanger core is handled as a fluid zone with momentum and heat transfer in COMSOL Multiphysics. Heat transmission is modeled as a heat source in the energy equation and pressure loss is modeled as a momentum sink in the momentum equation [69].

According to the simulated conditions, the flow governing equations are adjusted. Time-dependent factors are removed from the continuity, energy and Navier-Stokes momentum equations since it is believed that the situation is stable. The equations that follow are:

- Conservation of mass:

$$\text{div}(\rho \vec{V})=0 \quad (3.21)$$

- The x component of the momentum equation:

$$\text{div}(\rho u \vec{V}) = -\frac{\partial P}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \quad (3.22)$$

- The y component of the momentum equation:

$$\text{div}(\rho v \vec{V}) = -\frac{\partial P}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho g \quad (3.23)$$

- The z component of the momentum equation:

$$\text{div}(\rho w \vec{V}) = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \quad (3.24)$$

- Energy equation:

$$\text{div}(\rho E \vec{V}) = -\text{div}(P \vec{V}) + \text{div}(K \text{grad } T) + q + \Phi \quad (3.25)$$

The dissipation function may be determined using the following equation as, where:

$$\Phi = \mu \left[2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 + \lambda (\text{grad } \vec{V})^2 \right] \quad (3.26)$$

3.5. Combustion Modelling

The molecular mixture of the fuel and oxidizer is necessary for combustion. Typically, this is reliant on turbulent mixing. Combustion occurs when a fuel interacts with an oxidant, typically air, to produce heat and combustion products. These compounds always come from a series of chemical processes, not just one. For instance, the combustion of methane (CH₄), one of the most basic hydrocarbon fuels, involves more than 1000 primary processes. Additionally, it is necessary to calculate the flow and transport equations for the mass fractions m_j of each species j . The generic transport equation can be used to write the species equations [68]:

$$\frac{\partial(\rho m_j)}{\partial t} + \text{div}(\rho m_j \vec{V}) = \text{div}(\Gamma_j \text{grad } m_j) + S_j \quad (3.27)$$

The source (or sink) factor S_j in each transport equation represents the volumetric rate at which species are created (or destroyed) as a result of chemical processes. In a straightforward chemical reaction system, intermediate reactions are disregarded in favor of infinitely quick chemical reactions. The following is a possible way to express the fuel and oxygen mass fraction transit equations:

$$\frac{\partial(\rho m_f)}{\partial t} + \text{div}(\rho m_f \vec{V}) = \text{div}(\Gamma_f \text{grad } m_f) + S_f \quad (3.28)$$

$$\frac{\partial(\rho m_o)}{\partial t} + \text{div}(\rho m_o \vec{V}) = \text{div}(\Gamma_o \text{grad } m_o) + S_o \quad (3.29)$$

The species equations may be combined into a single equation for the mixing fraction f , under the supposition of equal diffusivities, $\Gamma f = \Gamma_o = \Gamma_f$:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \quad (3.30)$$

Z_i is the element i 's elemental mass fraction. The value at the oxidizer stream intake is indicated by the subscript "ox" while the value at the fuel stream inlet is indicated by the subscript "fuel." The species equations' reaction source terms cancel,

making f a conserved quantity. In turbulent flows, where turbulent convection is a considerably more important feature than molecular diffusion, the assumption of equal diffusivities is often accepted, despite the fact that it is problematic for laminar flows [69].

3.6. Chemical Kinetics Modelling

A chemical kinetic mechanism has been created which based on the fundamental reaction theory, characterizes all the processes included in the combustion process by compiling all the species, elementary reactions and reaction velocity parameters involved.. Premixed flame propagation is essential for many practical combustors, including internal combustion engines and burner-stabilized laminar premixed flames are frequently employed to investigate chemical kinetics in combustion environments. In order to interpret flame tests and comprehend the combustion process, one must be able to predict chemical kinetics and transport mechanisms in such flames. Since these flames are essentially one-dimensional (1D) and are exceedingly stable, precise experimental measurements of temperature and species profiles are made possible. Additionally, the laminar flame speed is frequently employed to describe how different fuel-oxidizer combinations burn [78].

For analyzing species profiles in flames, burner-stabilized, laminar, premixed flames with known mass flow rates have frequently been utilized. To effectively infer conclusions about the chemical kinetics, it is necessary to accurately know the temperatures because the chemistry largely depends on temperature. In this study, the freely spreading adiabatic flame was taken into account. The temperatures may be calculated using the energy conservation equation in circumstances when the heat losses are known to be minimal. Predicting the temperature distribution is an essential component of the computation for determining flame speed, which depends in part on the transmission of heat [78].

- Continuity:

$$\dot{m} = \rho u A \quad (3.31)$$

- Energy:

$$\dot{m} \frac{dT}{dx} - \frac{1}{C_p} \frac{d}{dx} \lambda A \frac{dT}{dx} + \frac{A}{C_p} \sum_{k=1}^K \rho Y_k V_k C_{p_k} \frac{dT}{dx} + \frac{A}{C_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k = 0 \quad (3.32)$$

x stands for the spatial coordinate in these equations; The mass flow rate is $\dot{m}$. (which is independent of x) The temperature is T . The mass percentage of the k th species is Y_k ; p the force; u the fluid mixture's velocity; mass density The k th species molecular weight is W_k . W is the mixture's average molecular weight R_c , the global gas constant; λ the mixture's thermal conductivity C_{p_k} stands for the mixture's constant-pressure heat capacity. C_{p_k} stands for the k th species' constant pressure heat capacity; h_k the specific enthalpy of the k th species; V_k the diffusion velocity of the k th species; and k the molar rate of synthesis through chemical reaction of the k th species per unit volume ; an The cross-sectional area of the stream tube enclosing the flame, expressed as A , is normalized by the burner area.

$$k_{fi} = A_i T^{\beta_i} \exp(-E_i/RT) \quad (3.33)$$

Where k_{fi} is the i th reaction's forward rate constant, A_i is the preexponential factor, E_i is the reaction's activation energy, and β_i is the i th reaction's temperature exponent. The user guides for CHEMKIN-III, a tool created to assess these expressions, Describe the thermochemical properties and the details of the chemical reaction equations. As demonstrated by earlier studies on combustion, which used exact chemical kinetic principles to explain how reactants convert into products at the molecular level through a staggering number of straightforward stages [79].

For instance, Mathieu mechanism is a popular reaction model for the chemistry of ammonia combustion that may be applied to practical situations like the control of NO_x formation or NO_x removal techniques [51].

4. AMMONIA CRACKING SYSTEM

NUMERICAL PREDICTIONS

4.1. Introduction

The issues with H₂ storage and transportation can be solved by building a hydrogen generation system utilizing ammonia fuel produced by thermal cracking.

Computational fluid dynamics (CFD) simulation will be a useful device for illustrating new ideas or a new design. CFD is built on numerical methods that may be applied to solve fluid dynamics issues. By applying input parameters, these solvers are given user-friendly access to the results, enabling in-depth analysis [71]. Over the past ten years, the design process has been greatly enhanced by the degree of precision provided by CFD methodologies. When CFD is used as a device in the design process, much fewer samples are needed for testing throughout the development of any system, which lowers the cost of new advancements.

The recommended design will next be subjected to a numerical heat transfer analysis after the CFD simulation of the combustion process. A unique mechanism that employs a bluff body to thermally pre crack ammonia has been added to the existing system. Figure offers a schematic of the conceptual design figure 4.1 [6] . To determine the system's form and size, numerical modeling was employed. The numerical forecasts will be given in a logical order in the subsections that follow.

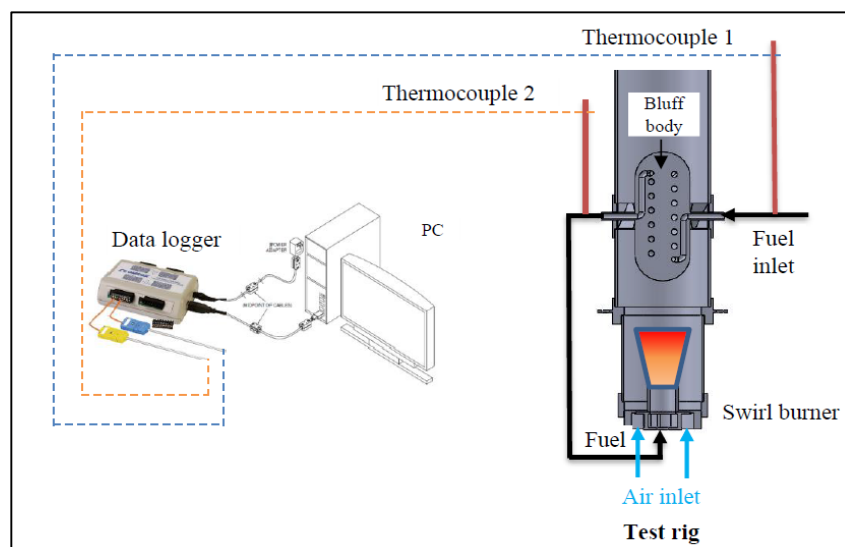


Figure 4.1: Thermal cracking process.

4.2. Combustion Simulations

4.2.1. CFD Pre - Processor Used and Models

This model imitates the turbulent burning of syngas (synthesis gas) in a basic circular jet burner. The main gases that make up syngas are H₂, CO and CO₂. Syngas gets its name from the process it uses to make synthetic natural gas. The model configuration matches that investigated by Couci and others [80].

Barlow and his team looked into the temperature and composition that result from nonpremixed combustion in a burner setup as part of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames. [81]. In COMSOL Multiphysics, the model is resolved by fusing an interface for reacting flow and one for heat transfer in fluids.

4.2.2. The Burner Design

The burner being investigated in that model is a straight pipe that is somewhat coflowed. The speed with which the gas phase fuel enters the pipe is 76 m/s, and the rate of the coflow outside the pipe is 0.7 m/s. When the pipe exits, the coflow and fuel gas come together to form an unrestricted circular jet. Three syngas-specific chemicals are present in the gas flowing through the tube: CO, H₂, and N₂. A portion of the coflow gas is air. The gasoline is ignited at the pipe's exit. The combustion that follows is of the nonpremixed variety because the fuel and oxidizer are introduced into the reaction zone separately. The reactants and oxidizer must be mixed in precise ratios for the reaction to carry on without interruption. In this configuration, the jet's turbulent flow efficiently blends the oxygen and fuel streaming through the pipe. The mixture also has to be ignited continually. The walls of the pipe being thickly constructed enables the burner to slow down the velocity of the hot product gas through the creation of small recirculation zones. The oncoming mixture is continuously ignited by the recirculation zones. These measures also help to keep the fire burning at the pipe opening. There is no ignition or burning out of the flame in one spot. [82].

The syngas combustion is currently represented in the model by two irreversible reactions:



For Ammonia combustion:



For Hydrogen combustion:



This full oxidation of the fuel assumption is in line with one of the methods employed in [80]. In order to represent the mass movement in the reacting jet, the mass fractions of six species, which include the five species involved in the reactions and nitrogen N_2 coming from the coflowing air, are calculated.

Considering the input velocity and pipe inner diameter, the jet's Reynolds number is around 16,700 suggesting that it is totally turbulent. In these conditions, the turbulent character of the flow has a substantial impact on both the mixing and reaction processes in the jet. The k- turbulence model is used to take into consideration the turbulence while resolving the flow field.

The Burner Model utilized a two-dimensional model with a cylindrical coordinate system and took advantage of the symmetry. Table 4.1 displays the values that were used in the model.

Table 4.1: Parameter of Burner Model.

Name	Expression	Unit	Description
M_CO	28[g/mol]	kg/mol	Molar mass CO
M_O2	32[g/mol]	kg/mol	Molar mass O2
M_CO2	44[g/mol]	kg/mol	Molar mass CO2
M_H2	2[g/mol]	kg/mol	Molar mass H2
M_H2O	18[g/mol]	kg/mol	Molar mass H2O
M_N2	28[g/mol]	kg/mol	Molar mass N2
M_NH3	17[g/mol]	kg/mol	Molar mass NH3
dH_CO	-26.42[kcal/mol]	J/mol	Standard enthalpy of formation CO
dH_CO2	-94.061[kcal/mol]	J/mol	Standard enthalpy of formation CO2
dH_H2	0[kcal/mol]	J/mol	Standard enthalpy of formation H2
dH_H2O	-57.80[kcal/mol]	J/mol	Standard enthalpy of formation H2O
dH_N2	0[kcal/mol]	J/mol	Standard enthalpy of formation N2
dH_O2	0[kcal/mol]	J/mol	Standard enthalpy of formation O2
dH_NH3	-316.8[kJ/mol]	J/mol	Standard enthalpy of formation NH3

Table 4.1: Continue.

Name	Expression	Unit	Description
Cp_mix	$\begin{aligned} & \text{tcs.wr_wNH}_3 \cdot \text{Cp_NH}_3(T) + \\ & \text{tcs.wr_wH}_2 \cdot \text{Cp_H}_2(T)/M_{\text{H}_2} + \\ & \text{tcs.wr_wH}_2\text{O} \cdot \text{Cp_H}_2\text{O}(T)/M_{\text{H}_2\text{O}} \\ & + \text{tcs.wr_wN}_2 \cdot \text{Cp_N}_2(T)/M_{\text{N}_2} + \\ & \text{tcs.wr_wO}_2 \cdot \text{Cp_O}_2(T)/M_{\text{O}_2} \end{aligned}$	J/(kg·K)	Heat capacity, mixture
dH_R1	$0.5 \cdot dH_{\text{N}_2} + 1.5 \cdot dH_{\text{H}_2\text{O}} - (dH_{\text{NH}_3} + 0.75 \cdot dH_{\text{O}_2})$	J/mol	Enthalpy change reaction 1
dH_R2	$dH_{\text{H}_2\text{O}} - (dH_{\text{H}_2} + 0.5 \cdot dH_{\text{O}_2})$	J/mol	Enthalpy change reaction 2

The Burner was drawn in the form of a cylinder (100 mm diameter, 400 mm length) shown in figure 4.2 with an open top to allow to smoke and gases emitted due to combustion to get out, the entry of fuel and air is also drawn from the bottom (2.3 mm, 30 mm respectively), In the middle, the Bluff Body was drawn, which will be the part in which the thermal cracking of ammonia will get.

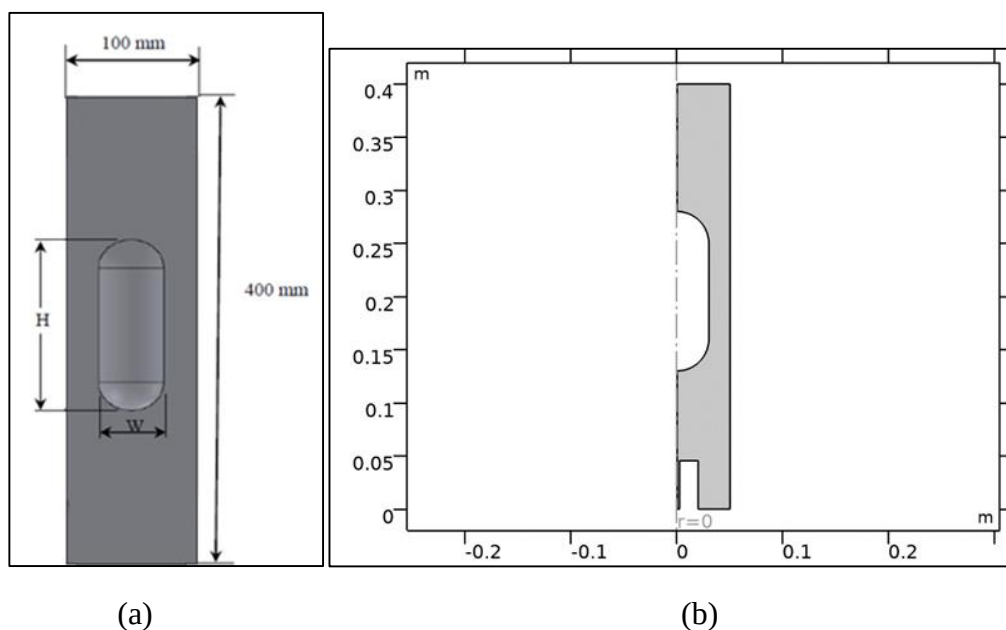


Figure 4.2: Cross section of Burner's body.

4.2.3. The Bluff Body Design

An area of turbulence or a wake will be left behind by a bluff body in the flow. Therefore, This bluff body's aerodynamic effect is necessary to separate flow across a sizeable area of its surface and create a vortex that makes the flow completely turbulent. [83].

To achieve the best results, we tried to investigate several different models. One of them was the Bluff Body with one tube, which was drawn using dimensions of 60 mm in width and 150 mm in height and an interior tube with a 6.35 mm diameter as evident in Figure 4.3.

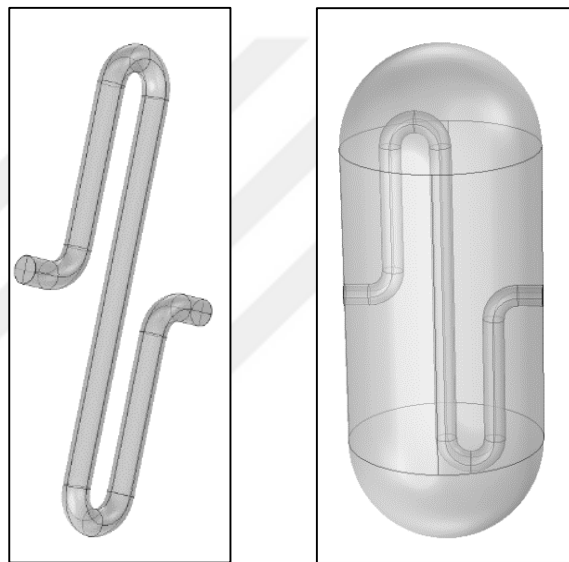


Figure 4.3: Bluff Body with 1 tube.

Another Model that we studied, Bluff Body was drawn with 2 tube (tube inside tube) with dimensions of interior tube with a 3 mm and exterior tube with a 6.35 mm diameter figure 4.4.

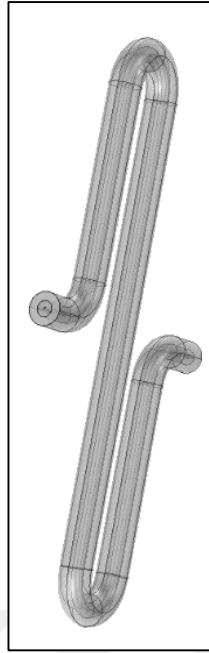


Figure 4.4: Bluff Body with double tube.

4.3. Meshing

To choose the appropriate mesh size and calibrate the outcomes, the independence mesh analysis was utilized. The element type for the unstructured cell type was a fine tetrahedron. The nodes where fluid characteristics are computed are defined by each cell. At each node, based on the data, the solution is iterated data acquired from the surrounding nodes. Therefore, a greater number of components leads to a greater amount of nodes and eventually, more computations, or higher computation costs, are needed. To prevent mesh variation from affecting the quality of the findings and to enable a decrease in processing time, a mesh independence study must be carried out.

The Mesh values applied to the Burner model using COMSOL Multiphysics are shown in Table 4.1 and Figure 4.5, and we obtained these results.

Table 4.2: Values of Mesh of Burner Model.

Mesh statistics	
Description	Value
Minimum element quality	0.1399
Average element quality	0.7524
Triangle	12588
Quad	3264
Edge element	764
Vertex element	14

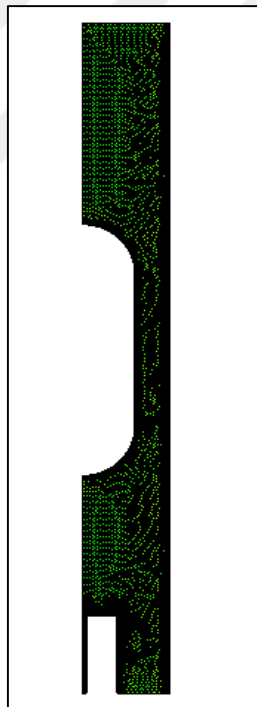


Figure 4.5: The Mesh of Burner Model.

The second model (Bluff Body with 1 Tube) was also given the mesh technique at the same time, as indicated in Table 4.2 and Figure 4.6.

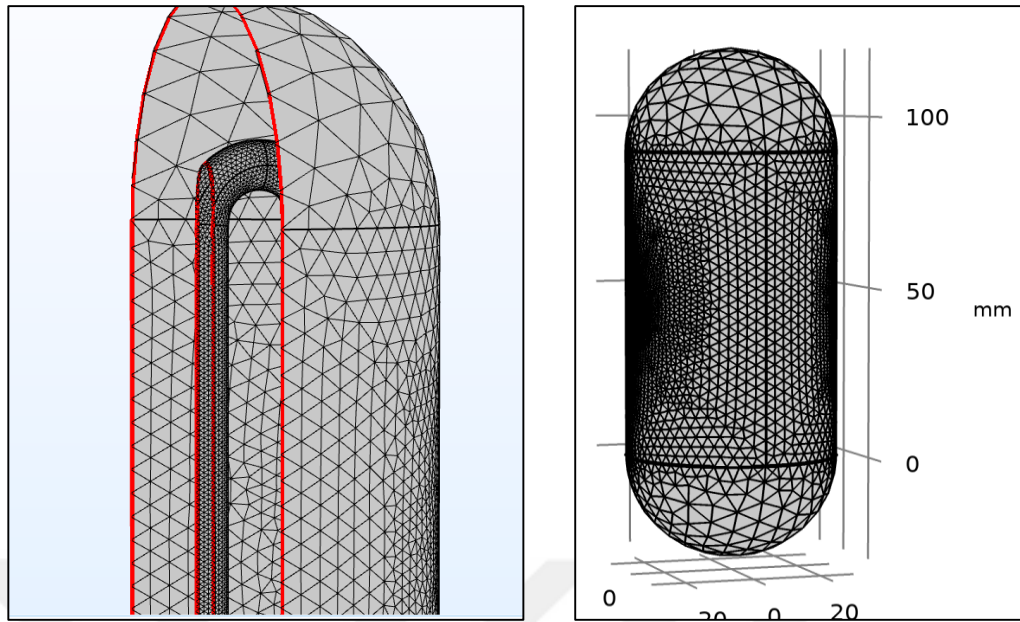


Figure 4.6: The Mesh of Bluff Body Model.

Table 4.3: Values of Mesh of Bluff Body Model.

Mesh statistics	
Description	Value
Minimum element quality	2.389E-5
Average element quality	0.6316
Tetrahedron	2856510
Prism	424080
Triangle	164300
Quad	10620
Edge element	5203
Vertex element	60

The third Model, a Bluff Body with two tubes (tube inside tube), was then given the mesh process to improve the surface contact of the heat exchanger between the heat source also the ammonia, which causes an increase in thermal cracking as shown in Table 4.3 and Figure 4.7.

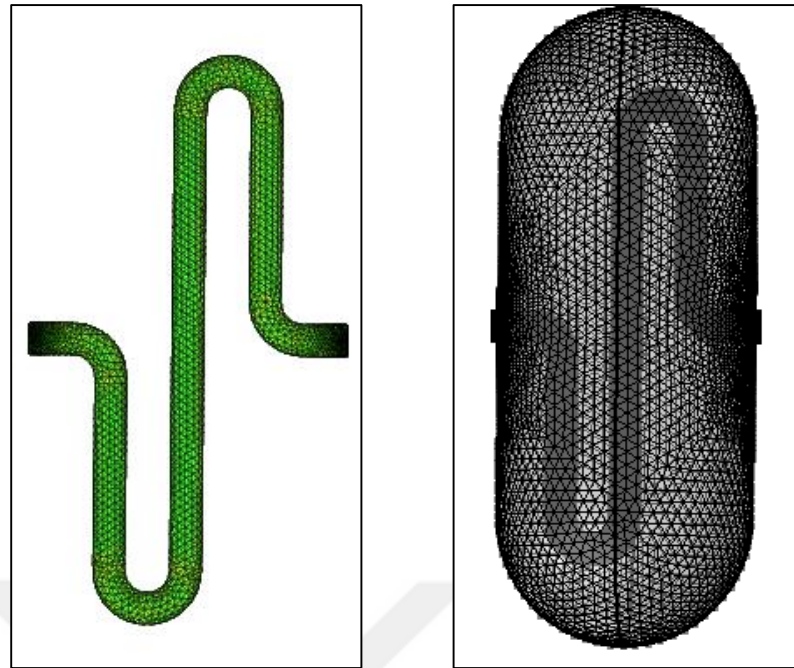


Figure 4.7: The Mesh of Bluff Body with 2 tubes Model.

Table 4.4: Values of Mesh of Bluff Body with 2 tubes Model.

Mesh statistics	
Description	Value
Minimum element quality	6.048E-5
Average element quality	0.6938
Tetrahedron	166208
Pyramid	696
Prism	44486
Triangle	14192
Quad	840
Edge element	1390
Vertex element	36

5. RESULTS AND CONCLUSION

5.1. Simulation of Bluff Body

The bluff body was examined and simulated with the experimental results of degree of Doctor of Philosophy in Mechanical Engineering (Ammonia Cracking with Heat Transfer Improvement Technology) that published by Cardiff University / United Kingdom at 2019 by using ANSYS engineering software and COMSOL Multiphysics program. which was drawn using dimensions of 60 mm in width and 150 mm in height and an interior tube with a 6.35 mm diameter.

When we compared the results that we got with experimental results of thesis that published by Cardiff University, we found that we got very close results to the real results. We were able to get very close results with an error rate about 0.84 %. Shown in figure 5.1.

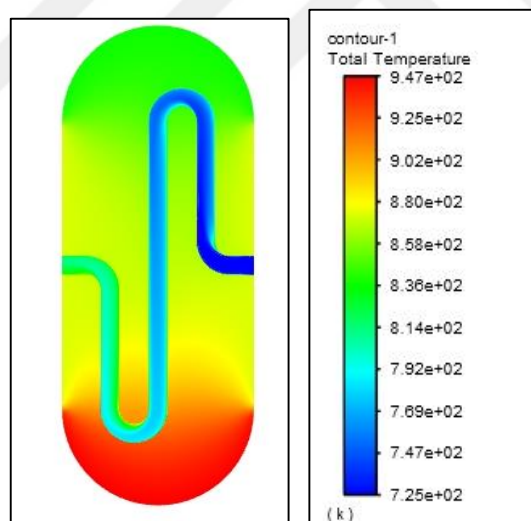


Figure 5.1: Temperatue filed of Bluff Body.

5.2. Jet Rounded Burner Model

Figure 5.2 shows the velocity field that is created in the nonisothermal reacting jet as a result. The hot free jet's growth and evolution are evident. As a result of the turbulent mixing at the jet's outermost regions, fluid from the co-flow is accelerated

and a component of the jet. The co-flow curves in the direction of the jet downstream of the orifice, which are known as entrainment and can be seen, are evidence of this.

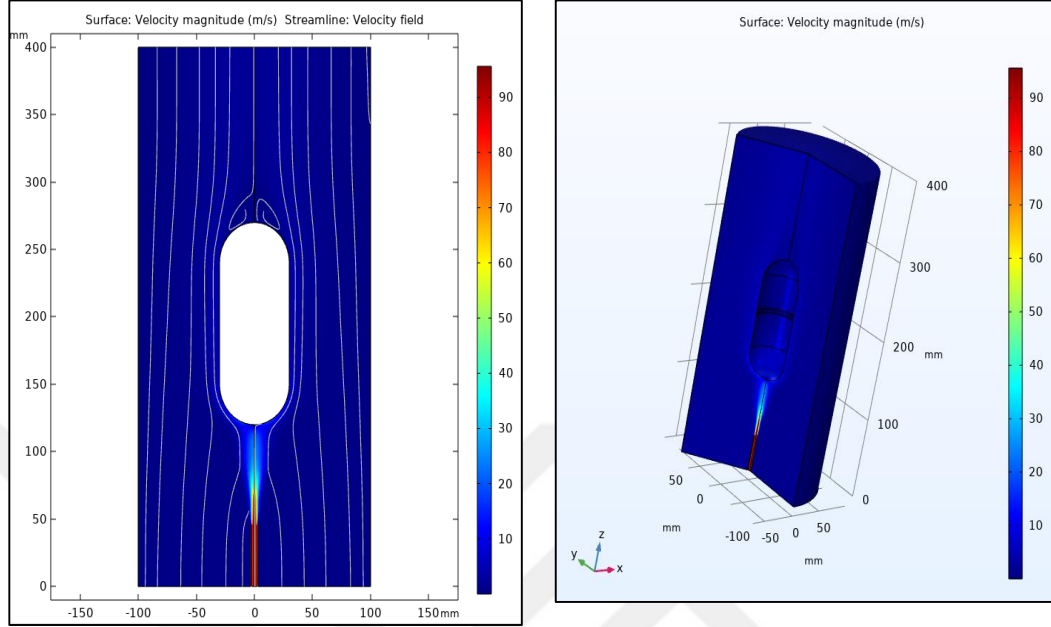


Figure 5.2: Velocity ranges.

Figure 5.3. shows a revolved dataset to highlight the circular jet's shape while also displaying the temperature of the jet. It is estimated that the jet's maximum temperature is around 2150 K. Figure 5.4 shows a visualization of the mass fraction of carbon dioxide in the reacting jet. The external layer of the jet is the site where O₂ is generated. Here, the gasoline from the pipe interacts with the oxygen in the coflow. The agitation in the jet shear layer causes an increase in the reactions. Additionally, it can be observed that O₂ generation begins just outside the pipe. This also applies to the rise in temperature seen in Figure 4. According to this, the flame is affixed to the pipe and there is no lift-off.

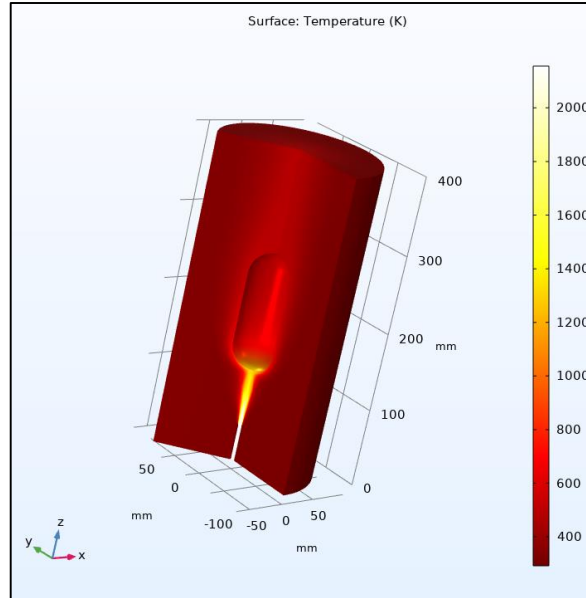


Figure 5.3: Temperature ranges.

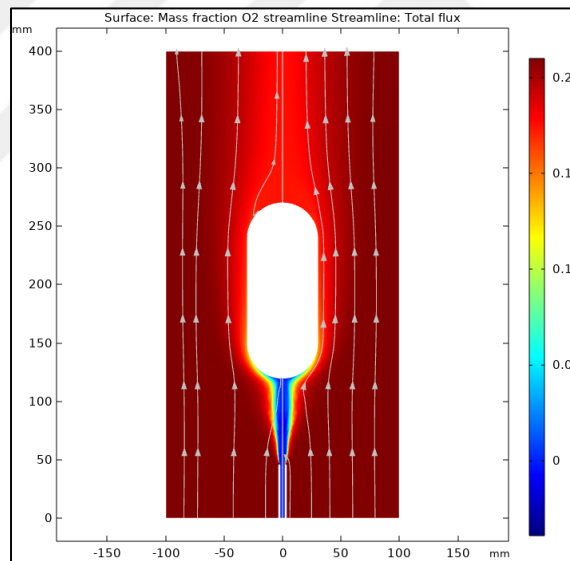


Figure 5.4: O₂ Mass fraction.

The model's outputs are compared to Barlow and colleagues' experimental findings in [91,92,93]. The model's prediction of the peak temperature is very close to what was measured in the experiment.

5.3. Bluff Body with Jet Burner Model

Figure 5.5 shows the fuel's reaction with the air caused it to travel along the flow routes in the reaction zone, thus preventing the flame from following the centerline. (i.e., the flame was placed in a circular shape above the fuel injectors, evenly distributed around the midline of the combustor). As a result, this volume's temperature increased as the majority of the combusting gases entered the flame zone. The off-center flame, however, had a respectable efficiency in this situation.

Figure 5.5 shows how the reaction zone received the majority of the hot combustion gas and became a rather evenly heated region, whereas the region of the walls stayed comparatively cold, the structure of the flame was also significantly influenced by the shape of the bluff body. In this instance, positioning the bluff body in the middle of the combustion chamber resulted in the production of a steady flame.

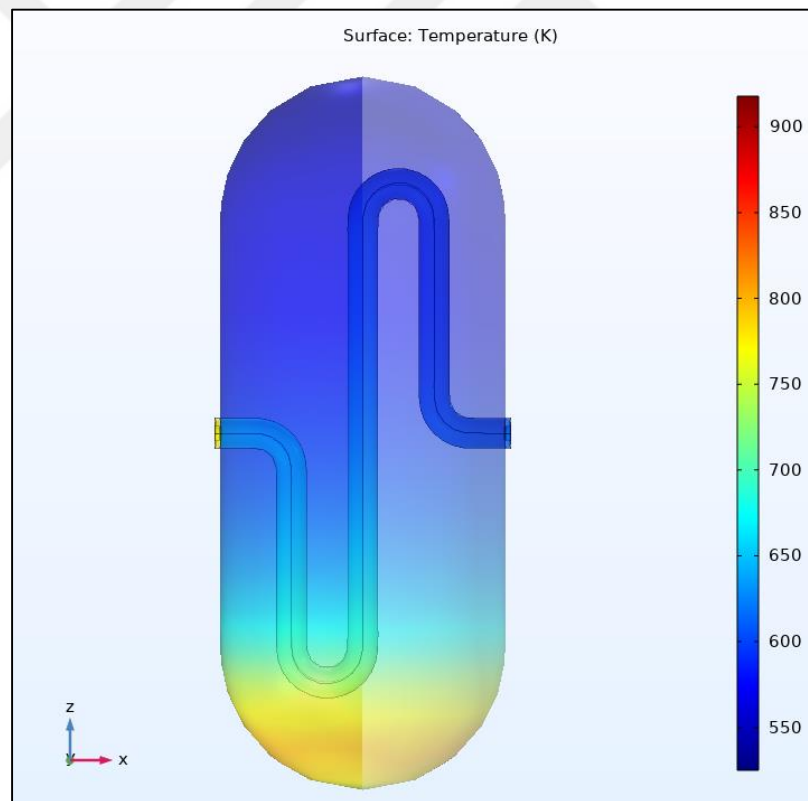


Figure 5.5: Contour Temperatures.

The turbulence intensities within the combustion zone for the bluff body are clearly seen in Figure 5.6 Turbulence shear layers are a significant source of turbulence

in turbulent jet flames. The size of the reaction zone increased due to the increased interaction between the turbulent currents within the combustor and the reaction zone, which sped up the time it took for the fuel/air mixture to react.

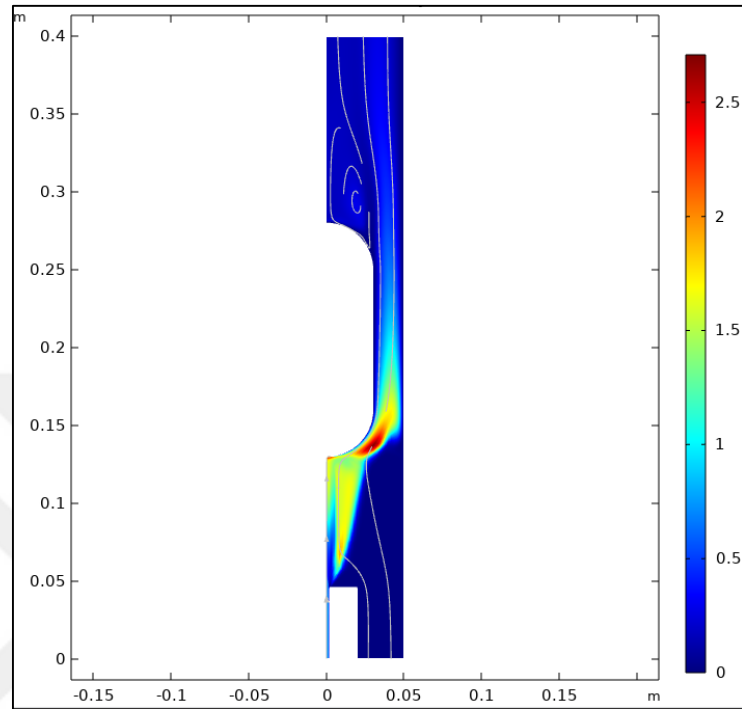


Figure 5.6: Turbulent field.

5.4. Bluff Body (tube inside tube) with Jet Burner Model

The object of using double tubes in Bluff body is to increase the surface contact between Heat and Ammonia and to get a best results of Ammonia cracking process

Figure 5.6 shows how the bluff body was constructed to be supported by a tube inside a tube, which also improved heat transfer. It was made up of two tubes, one within the other, with diameters of 3 mm for the inside tube and 6.35 mm for the external tube.

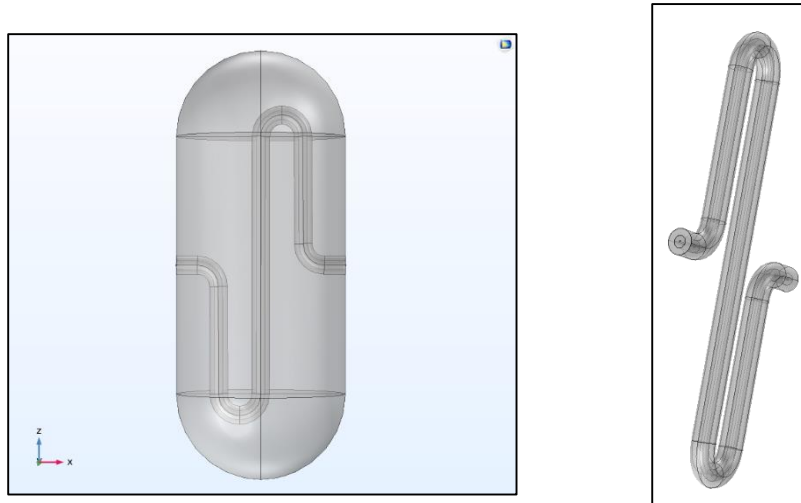


Figure 5.7: Bluff Body with 2 tubes.

This model objective was to increase the surface contact between the ammonia and heat source within the combustion chamber, especially surrounding the bluff body. The findings for the best situation, which is represented by the addition of the Bluff body model as shown in figure 5.7.

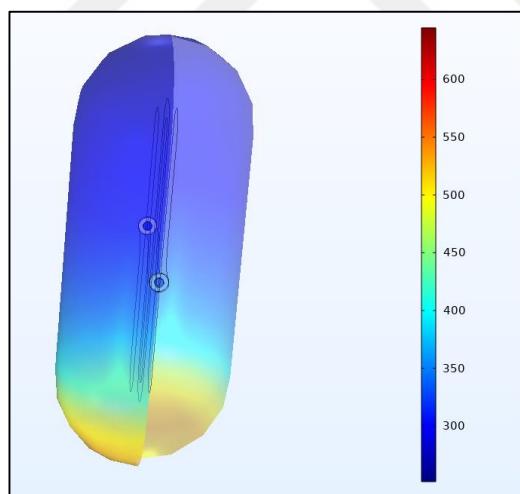


Figure 5.8: Contour Temperatures of Bluff Body with 2 tubes.

5.5. Mole fraction

The Bluff body has been injected with 100% ammonia. It was observed that the process of thermal cracking is clear after the ammonia passed through the Bluff body and was heated by the Burner because some of the hydrogen is separated from the

ammonia. As a result, we can take advantage of the ammonia leaving the bluff body and use it as a fuel used in various fields as shown as figures (5.7, 5.8, 5.9).

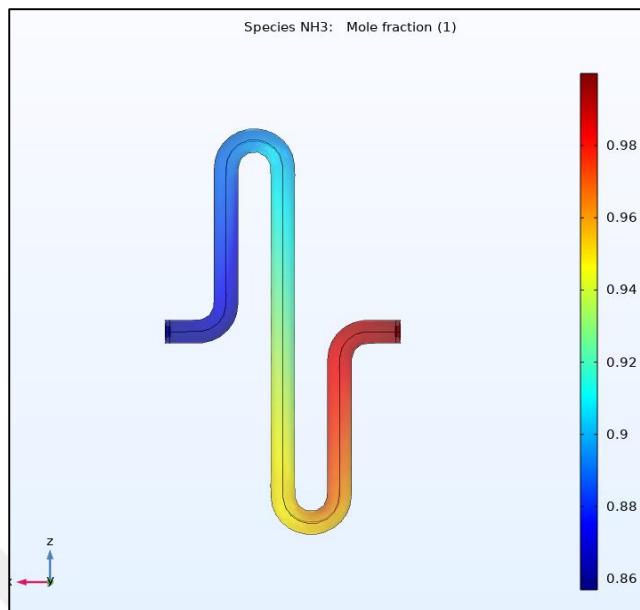


Figure 5.9: NH3 mole fraction.

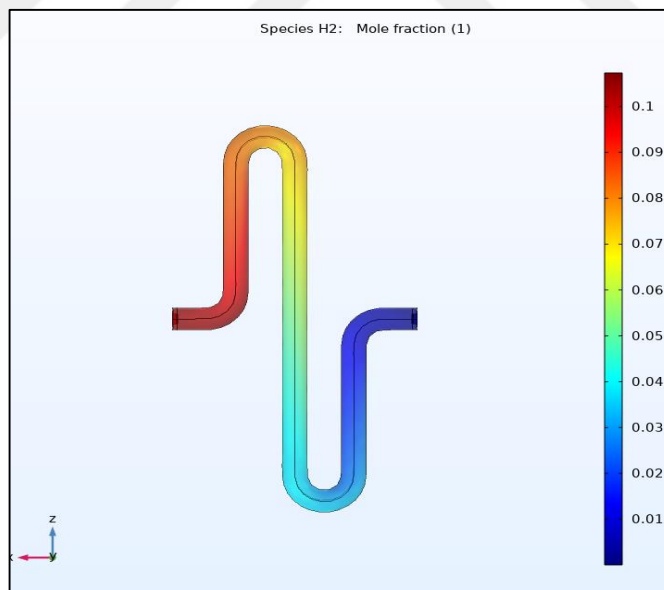


Figure 5.10: H2 mole fraction

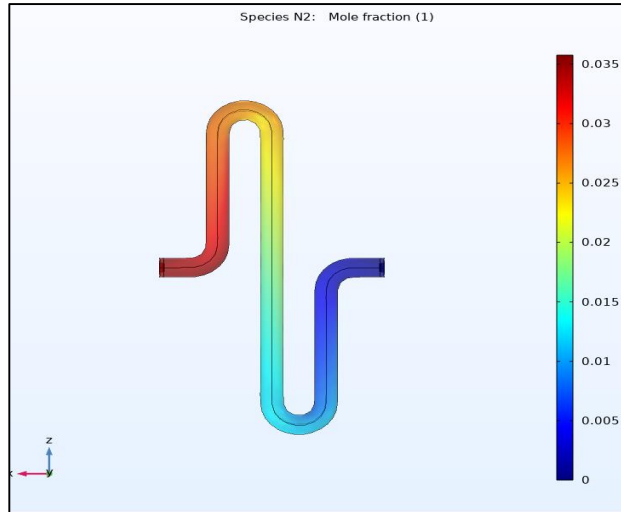


Figure 5.11: N2 mole fraction.

5.6. Result

This result shown in the Table 5.1 was obtained by integrating the syngas jet burner model with the Bluff body double tube model,

The burning model was studied alone, and then the results were taken and made as a Boundary condition for the second model (Bluff Body)

After studying the second model again, the results were taken and made as a Boundary condition for the Burner representing the fuel that we obtained after the ammonia thermal cracking process.

Table 5.1: Input and output values of Bluff Body.

Inlet Temp (K)	Outlet Temp (K)	NH3 Mole fraction	H2 Mole fraction	N2 Mole fraction
293.15	610.49	0.85756	0.1068	0.0356

5.7 Conclusion

This paper described the development of a H₂ generation system employing ammonia thermal cracking. The use of NH₃ as a fuel is possible with such a system, which also solves the issues with H₂ storage and transportation. NH₃ cracking is thought to offer superior flame stability and power loading. Due to the effectiveness

of the breakdown process, the thermal cracking approach has traditionally been regarded as the best.

Numerous experts contend that the bluff body's design must be based on a profile that permits ammonia cracking at high temperatures. So, using previous assessments (such as shape, enhanced heat exchange, manufacturing feasibility, flow patterns, etc.) and the following elements, a final design was created. It was necessary for the temperature of ammonia to be, both sufficient for cooling the bluff body and high enough to begin the cracking process once it had passed through the bluff body.

5.8. Suggestions for Future Work

Reducing the speed of the flame coming out of the burner and also reducing the space between the burner and Bluff body in order to have more contact between Bluff body and the heat source, Benefit from the heat of the gases coming out of the burner and after the body, using other forms inside the Bluff body may lead to increased thermal cracking of ammonia

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