# Alternative fuels for the maritime industry and their impact on flue gas composition

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**Abstract**: The maritime industry contributes to 80-90% of global trade and is on an increasing trend. However, it is also responsible for substantial amounts of greenhouse gas (GHG) emissions such as carbon dioxide (CO<sub>2</sub>), nitrogen oxides (NOx), sulfur oxides (SOx), carbon monoxide (CO), and hydrocarbons (HC). Therefore, industries are searching for alternative solutions to reduce GHG emissions by using alternative fuels. This study presents a novel investigation exploring the performance of various alternative marine fuels such as liquefied natural gas (LNG), methanol (MeOH), ammonia (NH<sub>3</sub>), and hydrogen(H<sub>2</sub>) in terms of combustion and emissions. Such comprehensive evaluation is limited in literature, making this study uniquely valuable in contributing to the field. The study assesses the impact of different equivalence ratios on emissions for the studied fuel profiles using Cantera and Aspen HYSYS simulations. Results show that CO<sub>2</sub> peaks at the stoichiometric ratio, with CO rising from 0.8 to 1.1. Non-carbon fuels like NH<sub>3</sub> and H<sub>2</sub> emit fewer GHGs than carbonaceous fuels such as LNG and MeOH. H<sub>2</sub> has the highest energy release at 87.21 MJ per kg, while NH<sub>3</sub> shows lower emission levels, suggesting its potential as a sustainable maritime fuel. This research emphasizes the significance of choosing the right fuel to mitigate maritime emissions, highlighting NH<sub>3</sub> and H<sub>2</sub> as promising alternatives.

Keywords: Fuel, Ammonia, Flue gas, Emissions, Aspen HYSYS, Python, Simulation, and Cantera.

# 1. INTRODUCTION

The global maritime sector is crucial in facilitating international transportation and trade. Maritime transportation, while efficient and relatively clean per unit of material transported, has gained attention due to its fuel efficiency and growth projections. It is expected to increase at an annual rate of 5.3% between 2010 and 2035. Nevertheless, it also significantly contributes to greenhouse gas (GHG) emissions, which are expected to double or triple by 2050 if no measures are taken. Other than environmental damage, these emissions can lead to health concerns, with shipping particulate matter (PM) emissions linked to thousands of cardiopulmonary and lung cancer deaths globally (Moirangthem and Baxter, 2016).

According to the International Maritime Organization (IMO), maritime transport contributes nearly 2.5% of GHG emissions worldwide and generates one billion tons of carbon dioxide (CO<sub>2</sub>) annually. Consequently, maritime industry is actively seeking alternatives to mitigate GHG emissions.

In April 2018, the IMO established ambitious targets through the Marine Environmental Protection Committee (MEPC) resolution MEPC.304(72) to decarbonize the global fleet. This strategy outlines initial goals to reduce the average  $CO_2$ emissions per transport work by a minimum of 40% from 2008 levels by 2030 and by 70% by 2050. Additionally, this target aims to decrease the total annual GHG emissions from shipping by at least 50 % by 2050. Achieving these objectives involves employing technical and operational approaches, as well as exploring alternative fuels (ABS, 2021).

In the pursuit of deconcentrating the shipping industry before 2050, advancements in ship technology primarily concentrate on newly constructed vessels. However, considering the extended operational lifespan of ships, it is evident that a substantial portion, approximately 20% of the global fleet according to certain projections, will continue to operate beyond 2050 despite being originally designed for fossil fuel propulsion as shown in Fig. 1. It is imperative to address the decarbonization of these existing vessels as a vital component of the broader maritime energy transition. One viable approach involves retrofitting these ships to operate on carbon-neutral or zero-carbon fuels. This retrofitting process may necessitate modifications to the vessel's engine, tanks, pipework, systems, and overall structure. This strategy acknowledges the importance of adapting existing vessels to align with sustainable and environmentally friendly energy sources, contributing significantly to the overall objective of reducing carbon emissions in the maritime sector (LR, 2023).

The maritime industry is currently experiencing a notable transition in fuel technology. In 2023, half of the ordered tonnage is equipped to utilize LNG, LPG, or MeOH in dual-fuel engines. This represents a significant increase compared to one-third of the tonnage on order in 2022. The shift towards alternative fuels is evident not only in new builds but also in existing vessels. Presently, 6.52% of the tonnage of

operational ships can operate on alternative fuels, reflecting an increase from 5.5% in the previous year (DNV, 2023). This trend underscores the industry's commitment to adopting more sustainable and eco-friendly fuel options across both new and existing maritime assets.



Fig. 1. Predicted marine fuel use to 2050 (ABS, 2021).

Furthermore, the production of alternative fuels has been rigorously investigated to meet the demands of the maritime industry and other sectors (Aryal et al., 2021). Renewablebased alternative fuels and chemicals are also recognized for their environmental benefits (Gadkari et al., 2021). Recently, simulation-based studies are considered to solve problems in different sectors as they enable realistic exploration of realworld problems in a safer, more cost-effective, and efficient manner (Ghimire, et al., 2021a). Further, efficiency and emissions estimation using various models for different ship types using conventional fuels are discussed in (Ghimire, et al., 2022) and (Ghimire, et al., 2024).

This study aims to investigate the emissions of LNG, MeOH, NH<sub>3</sub>, and H<sub>2</sub> as alternative fuels in marine diesel engines. In this simulation-based study, the amount of NOx, CO, CO<sub>2</sub> and GHGs are compared based on the same amount of energy produced by each fuel. Aspen HYSYS is used to model an internal combustion diesel engine, and parameter optimization is done for limiting the emissions for each fuel by changing the equivalence ratio. Cantera (Python Code) is also employed to model the combustion process and calculate the chemical potential of every element present in the flue gas.

# 2. CONCEPT AND GOVERNING EQUATIONS

In this section, the process of production emissions in an internal combustion engine (ICE) is discussed theoretically, and the effective parameters of its reduction are explained through academic concepts. To create a base for evaluating and comparing the pollution of different fuels, scientific relationships are presented, and the most important emitted gases from a marine diesel engine are defined to compare alternative marine fuels.

## 2.1 Chemical reactions in the combustion process

The combustion process is a chemical reaction between a fuel and an oxidizing agent, typically the  $oxygen(O_2)$ , from the air. This reaction releases heat and produces combustion byproducts, such as  $CO_2$ , water vapor, and other gases, depending on the composition of the fuel. The general chemical reaction of fuel and air is given by (1):

$$C_{\alpha}H_{\beta}O_{\gamma} + \left(\frac{1}{\phi}\right)\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)(O_{2} + 3.76N_{2}) \rightarrow$$

$$\alpha CO_{2} + \left(\frac{\beta}{2}\right)H_{2}O + \left(\frac{3.76}{\phi}\right)\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)N_{2} +$$

$$\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)\left(\frac{1}{\phi} - 1\right)O_{2} \qquad (1)$$

In equation (1),  $\phi$  is equivalence ratio, and it is defined as the actual FAR (fuel-air ratio) per stoichiometric FAR. When  $\phi$  is one, it means that the mixture is in stoichiometric condition, but when  $\phi$  is smaller than one, it means that there is more air available to burn the fuel and in common, the mixture is called a lean mixture in conditions where  $\phi > 1$ , the amount of fuel is more than the required air, and as a result, some fuels remain unburned after combustion. The mixture is called rich in the last situation (McAllister et al., 2011). The equivalence ratio plays a critical role in flame temperature as well as emission production. Hence, (1) is used to control the amount of feed (reactants) in an engine to control the flame temperature and flue gas concentrations. Although it shows the general chemical reaction, in practice, a series of sequential or simultaneous reactions are encountered. In hydrocarbons fuel, by increasing the number of carbons the species and steps of elementary reactions increased rapidly. For instance, combustion of CH<sub>4</sub> has 53 species in reaction mechanism and C<sub>8</sub>H<sub>8</sub> has 857 species (McAllister et al., 2011). In real-world scenarios, each of these reactions is time-dependent and is affected mainly by temperature, that will be discussed later.

## 2.2 Chemical kinetics

Chemical kinetics involves the study of the rates at which chemical reactions occur. The rate of reactions defines the speed of species consumption and production. Combustion chemistry exhibits two significant characteristics not typically seen in other chemical systems. Initially, the speed at which combustion reactions occur is highly influenced by temperature. Additionally, a considerable amount of heat is released during a chemical reaction, which affects the temperature. To elaborate it, consider (2) describe a general elementary reaction, and a, b, c and d are stoichiometry coefficient.

$$aA + bB \rightarrow cC + dD$$
 (2)

According to (2) the rate of reaction progress  $(\dot{q}_{RxT})$  is calculated by equation (3) that in which the Arrhenius rate constant k is the constant of proportionality and calculated from (4). The expression for the rate at consumption of reactant A,  $(\hat{r}_A)$  is then provided by (5).

$$\dot{q}_{RxT} = k[A]^a[B]^b \tag{3}$$

$$k = A_0 T^b \exp\left(-\frac{E_a}{\hat{R}_u T}\right) = A_0 T^b \exp\left(-\frac{T_a}{T}\right) \qquad (4)$$

$$\frac{d[A]}{dt} = \hat{r}_A = -a \cdot \dot{q}_{RxT}$$
(5)

In (3) the activation energy  $(E_a = T_a \hat{R}_u)$  is the minimum energy that required to have successful collision to result in a successful reaction. Coefficient b is for collision. As it can be concluded the rate of reaction or in other way rate of consumption or production of species is directly related to temperature. In practice, k is derived from experimental data. For instance, Figure 2 illustrates how someone can calculate the Arrhenius rate constant of some elementary reactions of burning CH<sub>4</sub> by using (6) and plotting the test data.

$$\ln k = \ln A_0 - \frac{E_a}{\hat{R}_u T} \tag{6}$$



Fig. 2. k value for different elementary reactions of burning methane (CH<sub>4</sub>) (McAllister et al., 2011).

In equilibrium condition, reaction rate is calculated by forward and backward reaction rate constants as  $k_f$  and  $k_b$ . In (7) equilibrium constant is based on concentration or partial pressure defined.

$$K_c = \frac{k_f}{k_b} \tag{7}$$

For example, the following equilibrium reaction is taken for calculation:

$$aA + bB \leftrightarrow cC + dD$$
 (8)

In this way, the reaction progress is defined by the following relation:

$$\dot{q}_{RxT} = k_f [A]^a [B]^b - k_b [C]^c [D]^d$$
 (9)

Therefore, equilibrium constant can be derived based on thermodynamics properties in the reaction as follows:

$$k_{C} = \frac{k_{f}}{k_{b}} = \frac{[C]^{C} \cdot [D]^{d}}{[C]^{C} \cdot [D]^{d}} = K_{p}(T) \left(\frac{\hat{R}_{u}T}{101.3 \ kPa}\right)^{a+b-c-d}$$
(10)

In that (10)  $K_p(T)$ , is the equilibrium constant based on partial pressures and can be defined by the following equation:

$$K_{p}(\mathbf{T}) = exp\left\{\frac{a\hat{g}_{A}^{0} + b\hat{g}_{B}^{0} - c\hat{g}_{C}^{0} - d\hat{g}_{D}^{0}}{\hat{R}_{u}T}\right\}$$
(11)

Where  $\hat{g}_A^0$ , is the Gibbs free energy and can be found in the thermodynamic tables.  $K_p(T)$  is unitless and temperature dependent.

Therefore, in a combustion process of a general fuel, the rate of progress can be computed from activation energy, temperature, and concentration by the following (12):

$$\dot{q}_{RxT} = A_0 exp\left(-\frac{E_a}{\hat{R}_u T}\right) [Fuel]^a [O_2]^b =$$
$$= A_0 exp\left(-\frac{E_a}{\hat{R}_u T}\right) x^a_{fuel} x^b_{O_2}$$
(12)

To use these equations and calculate emissions for each fuel at different temperature and pressure condition, commercial and scientific tools such as Aspen HYSYS and Cantera (Python) are developed to ease the simulation of combustion processes. In this study, authors used both software to model the combustion process in a marine diesel engine. The methods and the results will be discussed in the next chapter. In the next section the emission from combusting fuels is discussed.

#### 2.3 Emissions

Emissions in maritime industries refers to the release of GHG and air pollutants from ships that transport goods and passengers across the world's oceans. Common types of emissions are  $CO_2$ ,  $NO_x$  SO<sub>x</sub>, PM and  $CH_4$ ; They are dependent on the flame temperature.



Fig. 3.  $NO_x$  and CO concentration versus flame temperature  $(T_f)$  (McAllister et al., 2011).

Figure 3 shows the challenges of achieving lean combustion, emphasizing issues with flame stability at low temperatures. In low temperatures, less  $NO_x$  emissions is produced. Lean blow off is the condition where the combustion flame transitions from a lean to a condition where combustion cannot be sustained (McAllister et al., 2011).

The calculated emissions are the results of emissions formed in the elementary reactions. Using the Arrhenius constant (k, K,  $A_0$ ,  $E_a$ ) that is achieved from the chemical kinetics mechanism, and having pressure of chamber can calculate the combustion engine's production rate or emission rate.

## 2.4.1 Greenhouse gases (GHG) emissions

 $\mathrm{CO}_{2e},$  or  $\mathrm{CO}_2$  equivalent, is a measurement unit used to quantify the impact of various GHG on global warming and

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climate change. It allows scientists to standardize measurements of gases like  $CO_2$ ,  $CH_4$ , nitrous oxide, and synthetic gases.  $CO_{2e}$  helps in understanding the contributions of different gases to rising temperatures and environmental changes. The main GHG included in  $CO_{2e}$  measurements are  $CO_2$ ,  $CH_4$ , nitrous oxide, hydrofluorocarbons, perfluorocarbons, sulfur hexafluoride, and nitrogen trifluoride.  $CO_{2e}$  is used to create a standardized metric that simplifies the comparison of the global warming potential of various gases.

Table 1 shows the gases typically encompassed within the  $CO_{2e}$  (carbon dioxide equivalent) measurement. (13) is total sum of this  $CO_{2e}$  that is mostly reported in kg unit (US EPA, 2023).

$$CO_{2e} = \sum (GHG \ emission \ \times \ GWP)$$
 (13)

Table 1: Global warming potential (GPW) for GHG.

GHG	GPW
Carbon dioxide (CO <sub>2</sub> )	1
Methane (CH <sub>4</sub> )	25
Nitrous oxide $(N_2O)$	298

## 2.4.2 Alternative fuel selection

According to the definition of this project, fuels - LNG, MeOH, NH<sub>3</sub>, and H<sub>2</sub>- in pure conditions were selected to model in the simulation. The chosen fuels are common fuels that researchers are working on as pure or mixture fuel for compression ignition (CI) engines and they are extensively expected to be utilized in marine applications (ABS, 2021). Their distinctive properties make them adaptable options for sustainable energy solutions. NH<sub>3</sub>, renowned for emissions reduction, aligns with green initiatives. LNG, a cleanerburning natural gas, is favored for its lower emissions profile. Biofuel, derived from renewable sources, offers an ecofriendly alternative. MeOH, a liquid fuel, is valued for its versatility and low carbon footprint. H<sub>2</sub>, a clean energy carrier, stands out for its potential in fuel cell applications, promising a greener marine industry (Moirangthem and Baxter, 2016).

LNG is a promising maritime fuel, reducing  $CO_2$  emissions by 33.7%. Case studies reveal substantial environmental gains, with LNG leading in emissions, cost, and engine adaptability. However, high bunkering station costs hinder industry acceptance. Ongoing research focuses on optimizing infrastructure for improved viability (Wang et al., 2023).

MeOH emerges as a promising alcohol fuel for maritime use, offering cleaner energy and reduced emissions. Its high-octane rating, compatibility with existing engines, and ease of integration make it a viable solution. Advanced engines, like MAN B&W LGIM, showcase its potential for improved performance and efficiency in maritime applications (MAN, 2021; Tian et al., 2022; Ghimire et al., 2021b). NH<sub>3</sub> has the potential use in maritime transport for decarbonization faces challenges such as regulatory changes and the absence of ready-to-sail NH<sub>3</sub>-fueled ships. NH<sub>3</sub> engines, researched since 1900, are costlier than conventional LNG and diesel engines. Storage, safety concerns, and emission control methods impact NH<sub>3</sub> feasibility. Different NH<sub>3</sub> grades and storage types exist, each with specific considerations. NH<sub>3</sub> can serve as an energy

carrier, particularly in fuel cells, offering advantages over H<sub>2</sub>. Combustion challenges include NH<sub>3</sub>'s properties, flammability, and NOx emissions. Overall, NH<sub>3</sub>'s adoption hinges on overcoming technological, safety, and regulatory hurdles (Reiter and Kong, 2008).

 $H_2$  potential as a green marine fuel is evident, but challenges in emissions during production and low energy density complicate its viability. Grey  $H_2$ , which is generated through the processing of alternative fossil fuels or natural gas, dominates production (75%), limiting emissions reduction by producing about 70-gram CO<sub>2</sub> per MJ energy from  $H_2$ . However, its exceptional energy content could enhance efficiency, but volume challenges and cryogenic storage requirements pose obstacles.  $H_2$  blends like HLNG or HCNG offer alternatives. Key concerns include safety, storage, and development costs (ABS, 2021).

## 3. SIMULATION OF COMBUSTION CHAMBER

In this simulation study utilizing Cantera, which is opensource software, and Aspen HYSYS, the focus is on modeling the combustion chamber to assess the emissions of five alternative fuels – LNG, MeOH, NH<sub>3</sub>, H<sub>2</sub>, and Bioethanol. By considering optimal engine conditions for each fuel, the project delves into the intricate interplay of thermodynamic properties, combustion kinetics, and emissions. Cantera, with suite open-source for chemical kinetics its and thermodynamics, complements HYSYS, a widely used process simulation software. The examination of flue gas emissions provides valuable insights into the environmental impact of diverse maritime fuels, crucial for advancing sustainable and efficient combustion processes.

# 3.1 Aspen HYSIS

Aspen HYSYS is a process simulation software used to model and design chemical processes. It is widely used in the oil and gas industry to simulate various processes such as distillation, heat exchange, and chemical reactions. A built-in reactor was used to explore the scope of Aspen HYSYS for evaluating emissions from combustion. Figure 4 illustrates the set-up of the simulation, which was based on work done by (Suyitno et al., 2019).



Fig. 4. Simulation of combustion in Aspen HYSYS.

## 3.2 Cantera

Cantera is an open-source suite of software tools for solving problems involving chemical kinetics, thermodynamics, and transport processes. It is designed to aid scientists and engineers in modelling and simulating a wide range of chemical phenomena, such as combustion, catalysis, atmospheric chemistry, and materials science. Cantera provides a comprehensive set of features, including a database of chemical species and reactions, thermodynamic and transport property calculations, a solver for kinetic equations, and support for various input and output formats. Cantera version 3.0.0 was used for this project in Python as interface of Cantera (Reiter and Kong, 2008).

# 4. SIMULATIONS RESULTS

In this section, the Cantera and Aspen HYSYS simulation results for all four alternative fuels are discussed. For the simulations, the initial combustion condition considered for the simulation was taken from state-of-the-art research papers, which are shown in Table 2. The composition of LNG is considered to be the same as LNG from Qatar: 89.87% CH<sub>4</sub>, 6.65% Ethane, 2.30% Propane, and 0.98% Butane (Kanbur et al., 2017). However, as GRI30 does not contain butane's reaction mechanism and chemical kinetics, butane was not considered in the simulation; it was replaced by N<sub>2</sub>

Tab	le 2:	Initial	conditions	of th	e fuel	combustion	in	engine.
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Fuel	Temperature (K)	Initial Pressure (bar)	Reference
LNG	300	30	(Yao et al., 2022)
MeOH	513	75	(Verhelst et al., 2019)
NH <sub>3</sub>	563	39	(Reiter and Kong 2008)
H <sub>2</sub>	300	16.5	(ABS, 2021)

Moreover, as in this project the design of the engine is out of the scope of the project, the simulation considers the optimal engine conditions. In HYSYS, the reactor uses the Gibbs free energy method, but Cantera uses chemical kinetic mechanisms such as the GRI30 library database, which is based on experimental reaction rates developed by scientific institutes.

# 4.1 LNG Simulation

The CO<sub>2</sub> and CO emissions of burning LNG is shown in Fig. 5 in various equivalence ratios. The results of HYSYS and Cantera are similar, with small differences.



Fig. 5. CO<sub>2</sub> and CO from LNG in simulation.

Looking at the figures, the maximum  $CO_2$  emissions is about 90000 ppm in both simulations that produced in about stoichiometric reaction. Additionally, it is obvious that by

increasing the equivalence ratio, CO concentration rises rapidly. Whereas Figure 6 compares the emission parts of  $NO_2$ , NO, and  $N_2O$  for LNG in two simulations with HYSYS and Cantera. In lean mixture, a major part of emission from LNG is NO. It peaks at the equivalence ratio of about 0.8, producing 3500 ppm and 8000 ppm emission in HYSYS and Cantera, respectively.  $N_2O$  emission peaks at a fuel/air ratio of 0.6  $N_2O$  emission is very low in both simulations.



Fig. 6.  $NO_x$  and  $N_2O$  from LNG in HYSYS and Cantera simulation.

# 4.2 Methanol Simulation

Figure 7 illustrates CO<sub>2</sub> and CO emission of MeOH in various equivalence ratio.



Fig. 8. CO2 and CO from MeOH in HYSYS and Cantera.

The graphs are almost the same with negligible differences in quantities that would be because of the concept of solving chemical reactions in both utilized software. The maximum amount of  $CO_2$  is 110000 ppm and 103000 ppm in HYSYS and Cantera respectively. Whereas Figure 8 shows comparison between  $NO_2$ , NO, and  $N_2O$  emissions for MeOH in two simulations with HYSYS and Cantera. In lean mixture, the  $NO_2$  has the highest peak at FAR of 0.5, but as the mixture gets richer the NO, and  $N_2O$  emissions increase up to the equivalence ratio of 0.8, and after that they again decrease.

The maximum NO emissions were calculated at about 5000 ppm and 9000 ppm in Aspen HYSYS and Cantera, respectively.



Fig. 8.  $NO_x$  and  $N_2O$  emissions from MeOH combustion in HYSYS and Cantera simulation.

# 4.3 Ammonia Simulation

Simulation was based on an experiment where NH<sub>3</sub> was used in an two-stroke engine (Ichikawa et al., 2023). where initial pressure is 39 bars and temperature are 563 K. The FAR is changed from 0.1 to 1.1 to see how emissions depend on this factor. Figure 9 shows that running in a lean mixture in needed to reduce NH<sub>3</sub> slip from combustion. The combustion of NH<sub>3</sub> produces no carbon in the emissions and only NO<sub>X</sub> and N<sub>2</sub>O is considered shown in Fig. 10. NO<sub>2</sub> emissions are the highest around the equivalent ratio of 0.5, and NO emissions are the highest around FAR of 0.8, the same as the N<sub>2</sub>O emissions. Similarities of results from Aspen HYSYS and Cantera simulation are observed here, also like all other fuels. The general trend that is seen for all fuels is that the CO<sub>2</sub> emission peaks at the stoichiometric ratio, where CO starts to increase rapidly after that.



Fig. 9. NH<sub>3</sub> slip from NH<sub>3</sub> combustion in HYSYS and Cantera simulation.

NO is the major part in  $NO_x$  emission and usually peaks at about equivalence ratio of 0.8, while  $NO_2$  is usually maximized between 0.4 and 0.6 in all fuels. Generally, emissions decrease with reducing equivalence ratio.



Fig. 10. NO<sub>x</sub> and N<sub>2</sub>O emissions from Ammonia combustion in HYSYS and Cantera simulation.

## 4.4 Hydrogen Simulation

Figure 11 illustrates flue gas emission of burning  $H_2$  in various equivalence ratio.



Fig. 11. NOx and  $N_2O$  emissions from  $H_2$  combustion in HYSYS and Cantera simulation.

The similarities of graphs between Aspen HYSYS and Cantera show validation of the simulations. Generally, the emission concentrations are higher in Cantera's results than HYSYS ones. At FAR of 0.8 NO emission is maximized with about 5000 ppm in HYSYS simulation and 10000 ppm in Cantera modelling. NO<sub>2</sub> emission is always below 55 ppm in both simulations, and N<sub>2</sub>O emission is negligible. However, clean H<sub>2</sub> does not produce any CO or CO<sub>2</sub>, which is a great advantage of using H<sub>2</sub> as a fuel instead of fossil fuels. Table 2 illustrates flue gas emissions from burning H<sub>2</sub> in various equivalence ratios. The similarities of the graphs between Aspen HYSYS and Cantera show that the simulations are validated.

## 5. COMPARING FUELS AND DISCUSSION

The flue gas emissions produced by various fuels were investigated under the initial conditions specified in Table 2, with an equivalence ratio of 1 maintained for all fuels.



Fig. 12. Emissions (g/MJ) to produce 1 MJ of energy.

By standardizing the energy output across different fuels, the corresponding emissions were effectively compared.

Fuel	Required fuel (kg/MJ)	CO (g/MJ)	CO <sub>2</sub> (g/MJ)	CO <sub>2</sub> e (g/MJ)	NOx (g/MJ)
LNG	0.04	5.27	77.48	2157.18	2.35
MeOH	0.06	9.64	51.64	1444.41	4.26
NH <sub>3</sub>	0.08	0.00	0.00	11.91	1.25
$H_2$	0.01	0.00	0.00	35.14	1.72

Table 3. Emissions from fuels while producing 1 MJ energy.

Figure 12 demonstrates that carbon-based fuels exhibit the highest emissions, with LNG having the greatest impact, followed by MeOH. The results of this analysis are also presented in Table 3.





Figure 13 presents a comparison of fuels based on their  $CO_2$  equivalence. It is evident that carbon-containing fuels, such as LNG and MeOH, generate significantly higher  $CO_2$  equivalence compared to NH<sub>3</sub> and H<sub>2</sub>. However, fuel consumption also needs to be taken into consideration when suggesting fuel composition due to its effect on cost estimations.



Fig. 14: Comparison of alternative marine fuels based on required mass for producing 1 MJ energy (kg/MJ).

Figure 14 shows what amount (kg) of fuel is needed to produce 1 MJ of energy where it can be observed a quite opposite scenario. LNG overperforms other fuels in terms of fuel consumption,  $H_2$  is the only exception which seems most efficient in terms of fuel consumption too. However, fuel consumption also needs to be taken into consideration when suggesting fuel composition due to its effect on cost estimations.

## 6. CONCLUSIONS

The study sheds light on emissions from various marine fuels, contributing valuable data for sustainable energy choices in maritime industries. The comparison of GHG levels shows that when considering all the emissions, the non-carbon fuels still release fewer emissions per unit of energy. Based on different initial conditions of all the alternative maritime fuels, H<sub>2</sub> overperforms the other fuels in terms of fuel consumption. Nonetheless, the infrastructure cost of using H<sub>2</sub> should also be considered as one of the decision factors. Although, among all studied fuels, NH<sub>3</sub> shows good potential as an alternative fuel for the marine industries by producing the least emissions, attention should be given to its safety issues. However, the decision on fuel selection should also consider fuel consumption. The research can be expanded to use complex models of engines under different conditions, different ranges of fuel mixtures, and infrastructure as a future work scope. Fuel blends, for example, biofuel blends, can be explored with different compositions and sources. Emissions during the production process of the fuels need to be incorporated to reduce the overall carbon footprint. Additionally, a multicriteria decision analysis study can be conducted for optimum fuel selection based on criteria like emissions, cost, and efficiency.

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