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The N_2O production from ammonia and hydrogen as fuels for shipping purposes

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Ammonia and hydrogen are considered promising alternative fuel options for shipping purposes. However, the complete passage to these new fuels for power production is not straightforward, especially for the maritime sector. To properly address the issues related to large-scale implementation of alterantive fuels, a holistic approach including techno-economic, environmental, and societal aspects is strongly recommended. Concerning the environmental domain, a useful indicator is the emission of nitrogen oxides (NO_x), which is over 95 % derived from anthropogenic sources. In this regard, some of the oxidized nitrogen would ultimately produce nitrous oxide N_2O, which would offset some of the climatic benefits reached by switching maritime shipping fuels. For these reasons, this work evaluates and compares the emission rate of N_2O (g_{N2O}/kWh) and the corresponding emission index (g_{N2O}/kg_{fuel}) of N_2O produced by ammonia and hydrogen, in the framework of shipping purposes, by using the thermo-kinetic mechanism KIBO developed at the University of Bologna. Results give insights and technical indications on the sustainability of these tank-to-wake, zero-carbon fuels.

Keywords: Nitrous Oxide, Maritime transportation, Tank-to-wake sustainability, Zero-carbon fuels.

1. Introduction

In the view of emission reduction, anhydrous ammonia (NH_3) or hydrogen (H_2) are considered valid alternatives for a zero, or a near-zero, carbon solution on a tank-to-wake basis in maritime transportation (namely the emissions resulting from fuel use onboard a marine vessel or propulsion, energy generation, and auxiliary systems), irrespective of the origin of the fuel. In particular, NH_3 offers promising technological characteristics as a marine fuel, with flexible storage options: it can be liquefied at ambient temperature under 10 bar pressure or at ambient pressure (cooled to -34 °C), thus enabling rapid and straightforward fuelling procedures, comparable to conventional marine fuels. Furthermore, the volumetric density of NH_3 matches that of LNG, providing sufficient energy density for extended voyages on tanker vessels (McKinlay et al., 2020). In this regard, a complete reference for several practical energy systems with ammonia is given by recent essential papers, where, however, no mention of the shipping system is given (Kobayashi et al., 2019; Alnajideen et al. (2024).

While NH_3 presents several advantages over H_2 due to its simple storage conditions, it poses significant operational challenges due to its severe corrosivity and toxicity. It is also worth saying that the potential maritime demand for ammonia as a primary shipping fuel would require a substantial expansion of global production capacity. This scaling challenge introduces uncertainty about the long-term viability of fuels for international shipping, despite their attractive physical and economic properties. Indeed, the scale of the demands of maritime shipping fuel is such that the technology could significantly alter the global nitrogen cycle (Wolfram et al., 2022). Besides, the debate over H_2 as a marine fuel highlights the low energy density. Furthermore, the current high cost of (green) H_2 is a major barrier even if it may become less problematic as technological advances in electrolysis and declining renewable energy costs could make hydrogen commercially viable at competitive prices. Eventually, NH_3 and H_2 could enter the energy market relatively quickly due to the existing technologies, including the shipping system. However, the transition to sustainable energy production by using these carbon-free fuels requires careful consideration of multiple factors to ensure successful implementation, including safety, economic and environmental aspects (Wolfram et al., 2022; Zanobetti et al., 2023; Karvounis et al., 2024).

If a tank-to-wake basis is considered, NH_3 and H_2 can only produce nitrogen oxides (NO_x, mainly NO, N_2O and NO_2) either thermal (nitrogen derives from air) or thermal/fuel-derived NO_x (nitrogen derives both from air and NH_3), due to (on the spot) absence of carbon. The emitted NO_x has many adverse impacts on human health, the environment and biological ecosystems such as ozone layer depletion and acid rain. Here, it is worth noting that environmental indicators based on NO_x are intrinsically reliable, because these oxides are over 95 % from anthropogenic sources, whereas CO_2 and other GHG emissions may be affected by the biases of natural sources (Shaw & Heyst, 2022).

According to recent inventory data, ship emissions represent a significant environmental concern, contributing 13 – 15 % of global anthropogenic NO_x emissions (Hoesly Rachel, 2024). Within the maritime sector, container vessels emerge as the dominant source, accounting for over 30 % of total ship emissions annually. This is followed by bulk carriers, oil tankers, and chemical tankers in descending order of contribution. The geographic distribution of these emissions shows distinct regional patterns. The most severe NO_x emission intensities are observed in four key maritime regions: the Yellow Sea and the East China Sea, the Persian Gulf, the North Sea, and the Tyrrhenian Sea (Yi et al., 2024). In the future, the total amount of NO_x produced on ships must be compared with Nitrogen Oxides (NO_x) – Regulation 13 - Tier III, which allows for a total weighted cycle emission limit of 2.0 gNO_x/KWh, aiming at the reduction of air pollution and acid rains. Within NO_x, nitrous oxide (N_2O) is of paramount importance and a long-lived greenhouse gas (GHG). In the troposphere, it is a relatively stable compound, where it acts uninhibited as a GHG. According to the Intergovernmental Panel on Climate Change (IPCC), Sixth Assessment Report (2020) (AR6) the global warming potential (GWP) of N_2O is 298 times that of CO_2 for a 100-year timescale. Furthermore, N_2O has been recognised as a dominant ozone-depleting substance (Ravishankara et al., 2009). Indeed, when into the stratosphere, N_2O is destroyed by direct photolysis by ultraviolet radiation, thus forming

NO by reaction with excited atomic oxygen, which causes the decomposition of stratospheric ozone (O_3) and the consequent diminution of the protective role of the ozone layer against harmful effects of UV radiation (Colorado et al., 2017). It is then not surprising that in 2023, to reduce emissions from the maritime transport sector, the MRV Regulation (EU Regulation No 2015/757 on the Monitoring, Reporting and Verification of CO_2 emissions) was amended. Indeed, from 2024, shipping companies must monitor and report N_2O, together with methane and CO_2 emissions, too. Quite clearly, in the case of the fuel analysed in this work, N_2O is the only pollutant with a GWP, and its measurement allows for comparison between those fuels and the limiting values given by MRV regulation.

Despite these observations, few studies have addressed the production of N_2O in NH_3 and H_2-fuelled ships and the corresponding technology for its reduction. This work evaluates the N_2O produced by the pre-mixed burning of the two fuels through the thermo-kinetic code KIBO developed at the University of Bologna (Salzano et al., 2018; Pio et al., 2022; Pio et al., 2024). Results give clear indications of the possible effects of N_2O on global warming, giving further insights into the emission sources for the shipping system, also aiming at advanced reduction technologies (McKinlay et al., 2021; Alnajideen et al., 2024).

2. Detailed kinetic mechanism

Regardless of the investigated species or conditions, kinetic mechanisms are largely considered powerful tools for the characterization and representation of reactive systems. Different approaches can be used for their realization, resulting in different sizes, as well. More specifically, kinetic mechanisms can be distinguished as skeletal, reduced, or detailed based on the number of reactions and species included. Within the same class, the selection of species and reactions to be included can be based on expert judgment (manual reaction selection) or automated protocols (e.g., based on the estimation of the rate constants or production fluxes). Further elements on these subjects can be retrieved in the current literature (Pio et al., 2022).

2.1. *Kinetics of ammonia combustion*

From a kinetic perspective, the chemical reaction pathway of thermal processes based on the use of NH_3 is characterized by a hydrogen abstraction as the initiation reaction, activating the system through the production of the radical $NH_2\cdot$. Typically, considering the possible limitations and convenience in operative conditions, the abstracting agent is $OH\cdot$ for this initiation reaction. The consumption of $NH_2\cdot$is dominated by the reaction with NO to form nitrogen and water, with a lower but significant impact from the reaction forming $NNH\cdot$ and $OH\cdot$. A reduced relevance is attributed to the net pathways producing $NH\cdot$ and $HNO\cdot$, which are further transformed in NO_x. Although the main steps of the chemistry of NH_3 are generally accepted, a unique consensus has not been already reached for the secondary and side reactions, which represents an essential aspect for the quantification of pollutants produced in these processes. To this scope, several experimental and numerical studies have been conducted in the recent year. As an example, more than 30 kinetic mechanisms have been produced to capture the chemistry of NH_3 in the last 10 years. Additional information on the current state of the art of understanding the NH_3 chemistry is beyond the scope of this work, but can be retrieved in a dedicated literature review (Alnasif et al. 2023).

2.2. *Kinetics of hydrogen combustion*

Depending on the operative conditions, the dominant activation pathway for H_2 can be attributed to the reactions forming $H\cdot$ and $HO_2\cdot$ and the scission to $H\cdot + H\cdot$. The produced radicals can be further recombined in $OH\cdot$ or N-based radicals (Konnov 2019). The presence of small radicals produced in many reactive systems allows for the inclusion of largely studies properties and reactions within kinetic mechanisms, resulting in robust and consistent structure of models. However, significant variations can be observed within the existing models, especially once NO_x are of concern, as reviewed by several authors (McKinlay et al., 2020; Karvounis et al., 2024). In line with the reaction pathways described for the NH_3 case, the formation of $NNH\cdot$ assumes a pivotal step for the production of NO_x. In this case, it can derive from the direct reaction of nitrogen with hydrogen radicals, because of the abundance in the reactive phase. Indeed, according to the classical theory, the formation of NO can be attributed to the thermal (or Zeldovich) mechanism as well as to the chemical route, having in NNH· a key radical, and prompt mechanism. The last alternative is typically associated with the contacts between nitrogen and carbon-containing radicals, which do not apply to the investigated cases. A detailed description of the most relevant steps and kinetics for the formation of NO_x from hydrogen-containing species can be found elsewhere (Pan et al., 2023).

2. Methodology

The detailed kinetic mechanism KIBO, which includes nitrogen-based chemistry was used (Pio et al., 2019). The adopted kinetic mechanism includes 172 species and 488 reactions. The design of KIBO prioritizes final size and computational efficiency for practical implementation while maintaining accuracy, as evidenced by thorough validation documented in existing literature. A mono-dimensional reactor implemented in the open-source software Cantera (Goodwin, 2009) was utilized to simulate the laminar burning velocity of a premixed gaseous stream. This script allows for the estimation of the overall reactivity in terms of laminar burning velocity, temperature profile, and composition distribution along the axial direction until the equilibrium conditions are reached. Thermo-chemical properties are continuously updated based on the estimated temperature, employing the coefficients included within the adopted kinetic mechanism for the NASA polynomials. An adaptive grid was employed in this work to reduce truncation errors without an abrupt increase in computational time. Threshold values for the ratio between two consecutive solutions (ratio), the first derivative of consecutive solutions with respect to time (slope), and the second derivative of consecutive solutions with time (curve) were defined. More specifically, ratio = 3, slope = 0.05 and curve = 0.07 were considered for the numerical investigation. These values were defined based on a grid sensitivity analysis reported in previous work (Pio et al., 2024), which demonstrated the robustness of the collected data in combination with the effectiveness of calculation requirements under these hypotheses. Results are given in terms of adiabatic flame temperature (T_{ad}, K), specific fuel consumption (FC, g_{fuel}/kWh), molar fraction (x) and amount of N_2O produced per kWh (g_{N2O}/kWh), by varying the stoichiometric fraction φ within the range 0.6 – 1.4:

$$\varphi = \frac{\frac{x_{fuel}}{x_{O_2}}}{\left(\frac{x_{fuel}}{x_{O_2}}\right)_{st}} \qquad (1)$$

where x is the molar fraction of fuel and oxygen (O_2), and st refers to the stoichiometric ratio. The oxidant is considered as air and the initial temperature is always 300 K, future works will be devoted to higher temperatures and layouts representative of the real case conditions as those observed in technological systems.

Eventually, a specific emission index EI_{NO_2} is evaluated based on the collected data and the definition reported in the equation below:

$$EI_{N_2O} = \frac{Emission\ of\ N_2O\ [g_{N_2O}]}{Fuel\ Inlet\ [kg_{fuel}]} \qquad (2)$$

For the sake of completeness, Table 1 reports the analysed composition of the two fuels and some essential parameters.

Table 1. Heat of combustion $-\Delta H_c^o$, specific fuel consumption FC and gas composition for the fuel-air mixtures analysed in this work. Thermodynamic data from NIST (2023).

Fuel	$-\Delta H_c^o$ kJ/mol	FC g/kWh	φ	x_{fuel}	x_{O_2}
NH_3	382	193.1	0.8	0.183	0.172
			1.0	0.251	0.157
			1.2	0.101	0.189
H_2	242	25.4	0.8	0.219	0.164
			1.0	0.296	0.190
			1.2	0.123	0.184

In both cases, the FC values reported in Table 1 were calculated by assuming full combustion to water and pure nitrogen N_2, when applicable. These values were compared with the specific fuel consumption FC calculated by the detailed kinetic code KIBO, which takes into account the partial conversion of the investigated fuels as well as the production of NO_x. Furthermore, the data on the emission rate and the emission index were compared with the default values given by international organisations, such as the Intergovernmental Panel on Climate Change (IPCC) and the International Council on Clean Transportation, (ICCT), as reported in Tables 2-4 for several ship types, engine types and fossil-derived fuels. In the tables, the CO_2 parameters are also included for future reference.

Table 2. Default emission rate for European ships and boats on inland waterways as reported by the Intergovernmental Panel on Climate Change (IPCC) (Jun et al., 2001).

Engine Type	Gas	g_{gas}/kWh	EI_{N_2O}
Diesel	CO_2	4.68	3140
	N_2O	0.108	1.3
Gasoline (4-Stroke)	CO_2	68.4	873
	N_2O	7.2×10^{-3}	0.08
Gasoline (2-Stroke)	CO_2	68.4	873
	N_2O	1.4×10^{-3}	0.02

Table 3. Default emission rates for U.S. ships and boats as reported by the Intergovernmental Panel on Climate Change (IPCC) (Jun et al., 2001).

Ship Type	Gas	g_{gas}/kWh	EI_{N_2O}
Ocean-going Ships	CO_2	279.36	3212
	N_2O	7.2×10^{-3}	0.08
Boats	CO_2	270	3188
	N_2O	7.2×10^{-3}	0.08

Table 4. Default emission rate for N_2O as reported by the International Council on Clean Transportation, (ICCT) (Cormer and Osipova, 2021). SSD = Slow Speed Diesel; MSD = Medium Speed Diesel.

Engine Type	Fuel	g_{N2O}/kWh
SSD, MSD	Maring gas oil and Heavy Fuel oil	0.03
Steam Turbine	Maring gas oil and Heavy Fuel oil	0.04
Otto-MSD/SSD	LNG	0.02
	LNG - diesel	0.03
Steam Turbine	LNG	0.02

Few other references can be found for the specific marine applications. As reported by Wallington et al. (2014) and Yoo et al. (2012) reported an emission rate of 3.6×10^{-3} gN_2O/kWh for a small vessel (700 tons) equipped with a marine diesel engine not equipped with a Selective Catalytic Reduction (SCR) system. Cooper (2001) found similar values. Recently, Aakko-Saksa et al. (2023) assume that no N_2O is produced by standard fuel engines or, that data are rare because N_2O concentration is below the instrumentation thresholds in most cases, even if NH_3 could introduce some N_2O.

3. Results

Fig. (1) shows the adiabatic flame temperature and the molar fractions of N_2O for the investigated fuels and equivalence ratios, as calculated by KIBO.

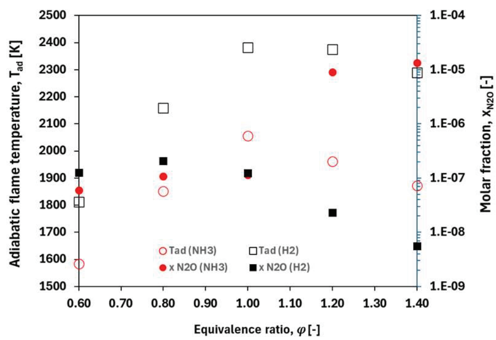

Fig. 1. Molar fraction (x, filled symbols) of N_2O and adiabatic temperature (T_{ad}, empty symbols) for NH_3 and H_2 vs equivalence ratio φ, as calculated by KIBO.

Quite clearly, NH_3 is producing more N_2O than H_2, at rich conditions (φ > 1), despite the lower adiabatic flame temperature (which directly affects the NO_x production). This aspect can be only partially attributed to the intrinsic endothermicity of the oxidation of nitrogen toward NO_x. Indeed, based on the hierarchical structure of the detailed kinetic mechanisms, the partial bond break of NH_3 to form N-containing radicals and H-containing radicals will result in two distinguishable reaction pathways. Namely, the species produced by the low-reactive N-based chemistry will act as thermal and chemical diluents, whereas the highly reactive H-based intermediates and products will result in a flame structure similar to the pure H_2 case. Hence, for any set of initial conditions investigated in this work, NH_3-containing mixtures lead to lower adiabatic flame temperature than hydrogen-containing mixtures having the same initial temperature, pressure, and equivalence ratio. The figure also shows a linear correlation of the molar fraction of N_2O with the equivalence ratio for the H_2 in rich composition, whereas an almost constant N_2O emission can be observed in the case of lean mixtures of H_2 and NH_3. Conversely, an abrupt increase in N_2O emission can be observed once rich ammonia flames are of interest. That is quite important in the framework of advanced combustion technologies, such as e.g., the MILD (Moderate or Intense Low oxygen Dilution) combustion regime, which uses recirculated heat and exhaust gases to reduce the flame temperature, thus reducing the amount of pollutants and increasing thermal efficiency. In this regard, it is worth mentioning that MILD combustion produces a dramatic decrease in NO_x emissions but is still far from being adopted for shipping purposes.

Fig (2) shows the specific fuel consumption FC (g_{fuel}/kWh) of NH_3 and H_2, and the corresponding emission rate of N_2O (the amount of N_2O expressed in grams produced per kWh).

As expected, FC is not constant with the equivalence ratio. In theory, this trend can be attributed to different factors, including the formation of NO_x, incomplete conversion of fuel, and incomplete oxidation. Considering the amount of energy associated with the involved reactions and the amount of NO_x produced, a limited impact on the produced energy can be expected for the first alternative listed before. In addition, the mole fraction of not converted fuel is > 1.0 %v only for the case of $\varphi > 1.2$, meaning that an almost completed conversion of the initial species can be assumed in most of the investigated conditions.

For what concern the remaining factor (i.e., the incomplete oxidation), it is worth noting that, although more than 99.9 %v of the exhaust gaseous mixtures deriving from the combustion of NH_3 is composed of nitrogen, steam, hydrogen, ammonia, and oxygen regardless of the investigated conditions, significant variations can be observed once different equivalence ratios are compared. More specifically, a hydrogen content > 5 %v is obtained only once $\varphi = 1.4$ is assumed. Similarly, an oxygen content > 5 %v is obtained only for the case of $\varphi = 0.6$, where a negligible amount of hydrogen can be expected. Hence, the main factor affecting the FC can be associated with the formation of stable species affecting the overall exothermicity of the reactive process.

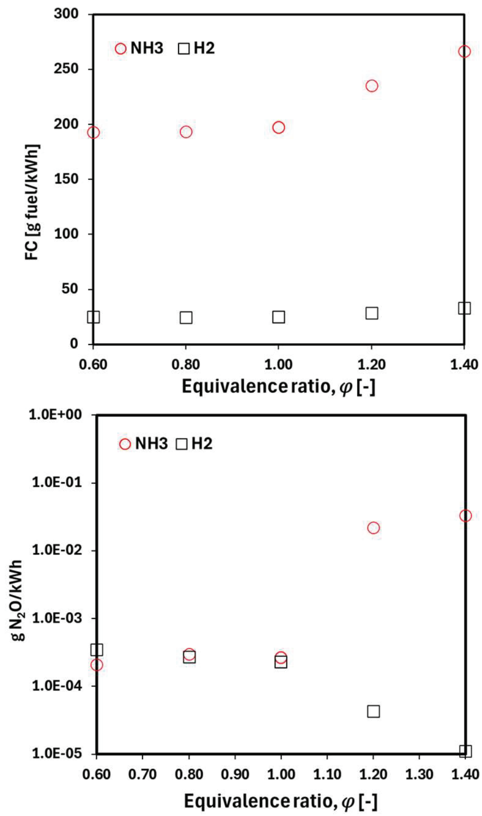

Fig. 2. Specific fuel consumption FC (g/kWh, top) and the emission rate of N_2O (g/kWh, bottom) produced by NH_3 and H_2 vs equivalence ratio φ calculated by KIBO.

Besides, the FC of NH_3 is consistently higher than that of H_2, due to its lower mass-specific combustion energy. Regarding the emission rate for N_2O, two different trends can be observed for the investigated fuels, in line with the discussion reported in the previous part of this work related to the molar fraction of N_2O. For lean and stoichiometric equivalence ratios, the calculated emission rate of N_2O is 3.0×10^{-4} gN_2O/kWh, for both fuels.

Considering the possible technological solutions based on the combustion of ammonia or hydrogen for maritime transportation, this value can be considered a reference value for comparison with other fossil fuels. Indeed, it is an order of magnitude lower than the values of gN_2O/kWh reported in Tables 2-4 for standard fuels such as Heavy Fuel Oil (HFO), Diesel, Liquefied Natural Gas (LNG), and different ship/engine types. In the same tables, the maximum index EI_{N_2O} is 0.02, which is again much more relevant than the emission index calculated either for NH_3 or for H_2 unless the very rich conditions.

Finally, Fig (3) shows the emission index EI_{N_2O} for the analysed fuels. The EI_{N_2O} reaches a maximum value at very rich (low-oxygen) conditions.

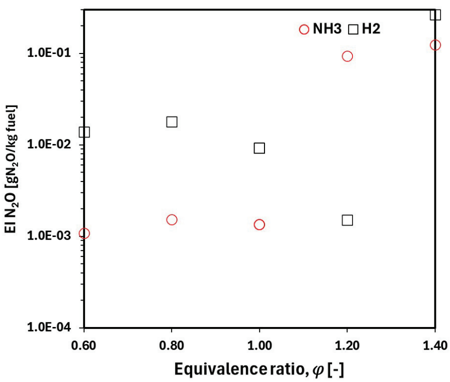

Fig. 3. Emission index EI N_2O (-) for NH_3 and H_2 vs equivalence ratio φ.

As expected, the production of N_2O is minimised at lean conditions (excess air), which are typical of low-NO_x technologies (Colorado et al., 2017). Here it is worth noting that if the flame temperature is sufficiently high, any N_2O formed in the flame zone is destroyed (Kramlich et al., 1994). That is seen for H_2. However, for rich conditions, the unreacted NH_3 prevails over the temperature effects.

5. Discussion

If used on ships, on a tank-to-wake assumption, NH_3 and H_2 produce nitrogen oxides (NO_x) with near-zero carbon emissions (Shaw, S.B., Van Heyst, B., 2022). However, the analysis reported above has confirmed that the introduction of pollution control technologies is needed for the N_2O produced by those two fuels when adopted shipping purposes. Besides, Aakko-Saksa et al. (2023) have recently discussed new exhaust after-treatment technologies for marine diesel engines, which can induce N_2O emissions. Future experimental and on-field analysis of N_2O production on ships are therefore of paramount importance. Furthermore, the detailed kinetic models adopted in this work are based on theoretical thermo-chemistry only, whereas some deviations could be analysed if the models are more deterministically applied to real shipping power generators.

6. Conclusions

The global energy demand for shipping is about $3x10^{11}$ kWh/year, about 7% of the total energy from oil and 1.9% of the world's global energy demand IRENA, 2021; IEA, 2020). This huge energy request makes the complete replacement of fossil fuels (Heavy Fuel Oil, Diesel, methane) with NH_3 or H_2 for shipping unsustainable due to production limitations if only considering the industrial request for these chemicals as building blocks for essential and inalienable products as fertilisers (McKinlay et al., 2021). Therefore, these chemicals can only be used for short-distance routes, port operations and long-term docking in urban harbours, where a local decrease in pollution can be reached. To this regard, several developments are nowadays devoted to the use of zero-carbon or near-zero blended fuels as hydrogen/ammonia or hydrogen/methan mixtures (Mashruk et al., 2021; 2022). These aspects will be covered in future works.

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