

Pollutant reporting protocols for low-carbon and carbon-free fuels combustion: A review on current challenges and progress

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ABSTRACT

This review examines existing pollutant reporting protocols and their corresponding emission metrics, focusing on their suitability for assessing pollutant emissions from carbon-free (hydrogen and ammonia) and low-carbon fuels (synthetic dimethyl ether and methanol) from an air pollution perspective. Meeting global decarbonisation targets has introduced technical challenges to the reporting of pollutants, with ammonia, hydrogen, dimethyl ether, and methanol, being the most discussed energy carriers for implementation in the transport and heat sectors, as well in hard-to-decarbonise industries such as cement and steel. Moreover, existing standards and methods were developed in a hydrocarbon-led environment, and, in most cases, are not suitable for providing comparable emission values in fuel-flexible operations. A key point of this study is the discussion on the challenges of using concentration-based emission metrics for the combustion of carbon-free and low-carbon fuels. An overview of the existing studies establishing the theoretical framework to support this discussion is also provided. A comparative analysis of existing emission metrics and standards enables a clear overview of the challenges encountered when using carbon-free and low-carbon fuels. Migrating existing standards to performance-based metrics linked to process outputs has been consistently shown to provide the fairest emission metric in fuel flexible scenarios. However, the use of appropriate conversion factors for concentration-based emission metrics has been reported as the path of least resistance for existing European standards. Finally, this review offers a general overview, to both the combustion and air pollution communities, on the challenges associated with properly reporting pollutant emissions in an ever-changing energy landscape.

1. Introduction

The world energy matrix, driven by global decarbonisation pledges, is shifting towards carbon-free¹ and low-carbon fuels,² such as hydrogen, ammonia, biofuels, and synthetic fuels with carbon capture and storage systems in their production process [1–5]. This transition presents significant technical and regulatory challenges. Their different thermophysical properties and chemical kinetics make their direct use in most existing combustion devices a challenging task. At the regulatory level, existing reporting protocols and the corresponding emission limit values (ELVs) were developed under a fossil-fuel dominant stage, whose underlying assumptions are not adequate for the range of fuels being considered by global decarbonisation efforts [6–13]. Therefore,

dedicated studies for a myriad of renewable, carbon-free, and/or low-carbon fuels have been performed at all scales across the globe to bridge this knowledge gap [14–28].

Hydrogen, in particular, has played a significant role in both the UK's domestic and industrial sectors since the beginning of the 19th century. It was initially a component of town gas (containing up to 50 % v/v of H₂). After the discovery of the North Sea natural gas (NG) deposits, a technological shift towards natural gas occurred [29]. This shift forced the retrofit of the existing gas pipeline and gas appliances to operate under a different fuel. The complete reconversion of the UK infrastructure, comprising over 14 million homes, took place between 1967 and 1977, achieving a peak reconversion of 2.3 million homes per year at its peak [30].

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¹ Carbon-free fuels considered in this study are hydrogen and ammonia.

² Low-carbon fuels consider synthetically produced carbon-based fuels with carbon capture measures in place. In this study, only methanol and dimethyl ether are considered.

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Now a similar challenge may be faced. The conversion of natural gas pipelines to operate with blends of NG and H₂, as well as pure H₂, is being assessed as a feasible path towards decarbonising the UK's energy matrix. Currently, natural gas is defined in the UK as a mixture of hydrocarbons (mostly CH₄ and C₂H₆, accounting for ~95 % v/v), inert gases (N₂ and CO₂, at ~4 % v/v), and other traces [31], with a maximum allowance of 0.1 % v/v of H₂ [32]. This definition inherently limits the amount of H₂ that can be injected into the gas pipeline, forcing an update to the pertinent legislation. Other European countries operating under the same gas standards as the UK, such as France and Germany allow up to 10 % v/v of H₂ in their natural gas. H₂ is also being considered as a replacement fuel in hard-to-abate sectors, such as the cement and steel industries, currently responsible for 14 %–16 % of global anthropogenic CO₂ emissions [33].

Among the challenges of using H₂ as a pure or blended fuel for combustion processes is the need to produce it with a low carbon footprint. In April 2023 the Department of Energy Security & Net Zero from the UK Government, published its UK Low Carbon Hydrogen Standard, where guidelines for hydrogen producers were presented to define the concept of 'low-carbon hydrogen'. This requires a greenhouse gas (GHG) emissions intensity less than or equal to 20 gCO₂e/MJ_{LHV} of the produced H₂, for a purity of 99.9 % v/v at a pressure level of 3 MPa [34]. In June 2024 the EU Directive 2024/1788 established the European definition of 'low-carbon hydrogen' as hydrogen produced from non-renewable sources with a reduction of at least 70 % in their GHG emissions, resulting in a threshold of 28.2³ gCO₂e/MJ_{LHV}, which is the same limit on GHG emissions intensity set by Japan.⁴

On the other hand, alongside the efforts to cut GHG emissions, the reduction of criteria air pollutants, particularly nitrogen oxides (NO_x, considered as the sum of NO and NO₂), has been taking place across developed countries through the application of emissions control measures in the energy and transport sectors [15]. Even though carbon-free fuels do not emit CO or CO₂ from their combustion process, they are not exempt from NO_x emissions, and in some cases, they may have greater NO_x emissions than carbon-based fuels. This is the case for uncontrolled H₂-air diffusion flames or fuel-rich premixed flames, which have a greater adiabatic flame temperature and promote thermal-NO formation mechanisms, while ammonia-air combustion is mostly driven by fuel-NO [14,15,35,36]. A thorough account of the different NO_x formation pathways, and their relation to process conditions and fuel properties, was presented by Glarborg et al. [35].

NO_x emissions are known to be responsible for serious problems for human health and the environment. Specifically, their inhalation can worsen respiratory conditions like asthma, and long-term exposure can increase the probability of developing respiratory diseases (e.g., acute bronchitis or emphysema) [37,38]. The environmental impact of NO_x emissions is linked to their interaction with existing gases in the atmosphere, producing acid rain, ozone, particulate matter, and other pollutants [39].

Policymakers have been widely relying on data from Integrated Assessment Models to support the development of international and national policy for the abatement of emissions from GHGs [40] and criteria air pollutants [41]. For the support of European policies, the GAINS model implemented by IIASA has provided the basis for the development of agreements to reduce transboundary pollution in Europe [42]. For the national policy development in the UK, the UKIAM model has helped to understand the pollutant source apportionment of different sectors and their synergies with proposed net-zero strategies. These models are highly regarded by policymakers and are expected to play a significant role in the revision of the Gothenburg Protocol [43].

³ Considering the carbon intensity of a conventional steam methane reforming plant of 94 gCO₂e/MJ_{LHV} [68].

⁴ Japan limit for Well-to-Gate GHG emissions intensity was set as 3.4 kgCO₂e/kg-H₂, which is equal to 28.2 gCO₂e/MJ_{LHV} [69].

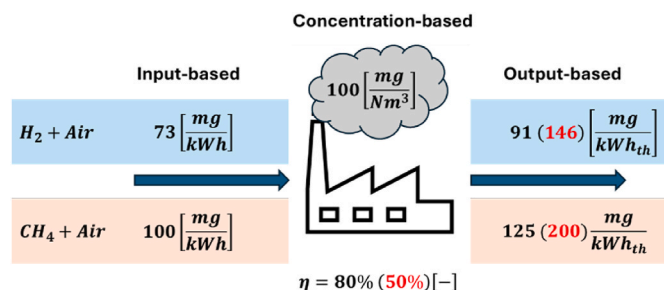


Fig. 1. Differences between concentration-, input- and output-based emission metrics for the same process operating with two different fuels and at two different efficiency conditions.

However, incorporating emissions from novel technologies, mostly proven at a pilot plant scale and recently being deployed in commercial systems, has proven to be a challenge. Therefore, properly accounting for the GHG and air pollutants emissions of the different carbon-free and low-carbon fuels considered for deployment raises the necessity to precisely assess the impact of each fuel across the different sectors where they may be used.

A key barrier to properly assessing the impact of process emissions on the environment lies in the heterogeneous reporting formats used by experimental combustion researchers [6,10–12]. In contrast, air pollution assessment researchers usually rely on emission factors (g/GJ, kt/TWh, ng/J, g/kWh, either on input or output basis or similar metrics) published by governments and obtained from long-term measurements of mature combustion plants [40,41]. While emissions from the combustion of carbon-free and low-carbon fuels can be reported on a volumetric concentration basis on a wide range of bases, such as wet, partially wet, dry, oxygen-free, air-free [21], CO₂-corrected [24], and oxygen-corrected [14,15,24,25]; and on performance-based emissions metrics based on input energy used (relative to either the lower or higher heating value of the fuel used) [16,17,19–21,24,44] or the actual work done (output-based emissions) [25]. This has proven to be an ongoing challenge in assessing the environmental impacts of using alternative fuels to decarbonise the existing energy matrix. Fig. 1 depicts the variation of emission levels obtained for two different fuels using a concentration-based metric as a reference point. When H₂ is combusted, the lower volume of products released and higher steam content per unit of energy make it more susceptible to overestimating emissions from the drying and set O₂ concentrations steps used in concentration-based emission metrics. Additionally, even though performance-based emission metrics provide an even field to compare across fuels, there are still additional factors to be accounted for to properly assess effective emissions from different processes (such as efficiency and load factor) [12,45].

To provide an extended example of the issues to be addressed, Table 1 compares the effective conversion of emission levels using concentration-based or input-based emission metrics for the combustion of both hydrogen and methane with air. It becomes apparent that to fairly compare emissions from fuel-flexible processes considering the use of carbon-free fuels, additional factors must be considered. Values were converted using the conversion method presented in Appendix A.

To the best of the authors' knowledge, there is no other review paper focused on discussing the status of pollutant reporting protocols and their shortcomings in fairly assessing pollutant emissions from both low-carbon and carbon-free fuels in a context useful for air pollution scientists and policy makers. Existing papers, like the pioneering work of Douglas et al. [6–9], present the specific impacts in the reporting of pollutants while using hydrogen or ammonia in gas turbines. Gößrau et al. [12] expanded the previous work done by Douglas et al. and studied the impact of cycle adaptations, such as exhaust gas recirculation (EGR), steam injection (SI), and water injection (WI), on the reporting of emissions from gas turbines, gas boilers, and combined heat

Table 1

Comparison of concentration-based and input-based emission levels from CH₄ and H₂ combustion.

	Concentration-based ^a		Input-based ^b
H ₂ + Air	100 mg/Nm ³	@ 3 %O ₂	73 mg/kWh
		@ 15 %O ₂	219 mg/kWh
CH ₄ + Air		@ 3 %O ₂	100 mg/kWh
		@ 15 %O ₂	300 mg/kWh
H ₂ + Air	137 mg/Nm ³ @ 3 % O ₂		100 mg/kWh
	46 mg/Nm ³ @ 15 % O ₂		
CH ₄ + Air	100 mg/Nm ³ @ 3 % O ₂		
	33 mg/Nm ³ @ 15 % O ₂		

^a On a fixed O₂ concentration and dry basis.

^b Considering LHV as denominator.

and power plants. Garan et al. [11] focused on developing a consistent emission correction method capable of providing comparable volumetric emission metrics on a fuel-flexible scenario. Moreover, Schmitz et al. [10] provided the theoretical basis for a fair discussion of the future emission limit values of NO_x emissions in a fuel flexible world, while surveying existing regulations and pertinent standards.

In this context, this review paper focuses on summarising and discussing the research conducted on the effects of using low-carbon and carbon-free fuels on current pollutant reporting protocols, surveying.

- The reporting of NO_x emissions from the combustion of these fuels across the different possible industrial and residential applications.
- The status of pollutant emissions metrics and the challenges linked to the use of adequate reporting protocols to assess the impact of using carbon-free and low-carbon fuels relative to conventional fuels such as natural gas.
- An overview of current pertinent technical standards presenting reporting methods for pollutant emissions of combustion systems within the UK, EU and USA.

Finally, this review paper aims to unify the existing discussion on pollutant reporting protocols. It provides guidance to two main groups. First, it helps the combustion research community to produce robust emission metrics for different technologies and fuels being tested. Second, it assists the air pollution community in accessing consistent emission metrics datasets. These datasets will be capable of providing a fair assessment of the air quality impact of implementing new fuels and technologies across various decarbonisation efforts globally.

2. Existing emissions metrics

Three main emissions metrics used in existing standards can be identified as: (i) output-based emission levels [45,46]; (ii) input-based emission levels; and (iii) concentration-based emission levels [11,13]. Output-based emission levels link the emissions from a process/system in relation to its useable output. This is usually found in sectors where the final use is easily quantifiable, such as in the transport sector where emissions are reported per km driven, or the production of chemicals, fuels, or electricity where emissions are reported either per kg of product or per unit of energy equivalent in the case of fuels. Additionally, output-based emission levels encourage the improvement of efficiency within the process [11,13]. Input-based emission values relate the mass of pollutants emitted to the amount of fuel used by the process, this is commonly seen in industries where the output is not easily standardised, or when environmental performance of different engines/turbines, whose flue gases are difficult to totalize, are to be compared on similar basis. Concentration-based emissions are best suited to continuous measurement systems used by governmental bodies to assess the overall operational performance of an industrial process [10,11,13].

Emission factors are usually obtained from government bodies related to environmental regulation, who in turn obtain them from

industry reports on GHG and air pollutants emissions, as well as their own continuous monitoring systems, and the activity levels from their processes. These factors follow several environmental directives, and their reporting protocols are well documented for conventional carbon fuels, such as coal and liquid and gaseous hydrocarbons. However, the case of technologies using carbon-free or low-carbon fuels, such as hydrogen, ammonia, dimethyl ether, methanol, and other biofuels, raises an additional challenge. Most of the existing data correspond to pilot-scale projects or even laboratory-scale tests, which cannot always be considered as widely representative of a large-scale application. Therefore, assumptions on their performance are required for them to be considered within air pollution assessment models, which in turn generate a range of possible emissions factors. A starting point to build this range of values can be described in three categories of emissions factors: first, using existing emission limit values (ELV) for different combustion technologies as the upper limit to consider; secondly, as average values of collected emissions factors the expected value; and thirdly, best available techniques (BAT) as the lowest achievable value in the foreseeable future.

Fig. 2 presents an overview of the different metrics used to report emissions and the intermediate conversion steps between measurement and the final reported value. Goßrau et al. [12] divided these emission metrics into three main categories: relative, absolute and performance-based metrics. Relative metrics are equivalent to concentration-based metrics, considering values measured in volumetric terms. Absolute values refer to the total emissions or the emission rate of the process in mass basis. Finally, performance-based metrics encompass both input- and output-based emissions metrics, as previously introduced. The different conversion paths depicted in the figure are separated by data obtained from measurements on a wet basis (numbers 1 to 4) and on a dry basis (numbers 1' to 3'). The conversion factor C_{R1} (equation (1)) depicts the removal of water/humidity from the measurement (with $y_{(H_2O)_m}$ being the measured steam fraction in the product gases), while C_{R2} (equation (2)) represents the conditioning of the oxygen content (with $y_{(O_2)md}$ being the measured oxygen concentration on a dry basis) to a set level ($y_{(O_2)_x}$), according to the appropriate standard (see Table 3). The conversion factor C_{R3} is equal to the density of NO₂ ($\rho_{NO_2} = 2.054 \frac{kg}{m^3}$), following the logic that all NO is converted to NO₂ after being emitted [10]. Moreover, performance-based emission metrics are obtained from the ratio between the absolute emissions of the process to the fuel/energy used (input-based) or the unit of product (output-based).

$$C_{R1} = \frac{1}{1 - y_{(H_2O)_m}} \quad (1)$$

$$C_{R2} = \frac{0.21 - y_{(O_2)_x}}{0.21 - y_{(O_2)md}} \quad (2)$$

The discussion on the strengths and weaknesses of these emissions metrics has been previously approached by Baukal and Eleazer [13]. Their research focused on listing the different methods available for quantifying NO_x emissions from combustion processes, ranging from volume-based measurements to mass of NO_x normalized to net energy produced or units of product manufactured. Table 2 presents a summary of the comparative analysis of the advantages and disadvantages of different emission metrics.

An additional barrier is added by the sector-specific reporting conditions, where concentration-based emission metrics are usually presented on a dry basis at a process-specific reference O₂ concentration to mitigate the impact of air dilution on the reported concentrations. Table 3 lists existing reference concentrations currently in use by standards across the UK, EU, and USA for treating the environmental performance of combustion processes.

Currently, several authors have raised concerns about the

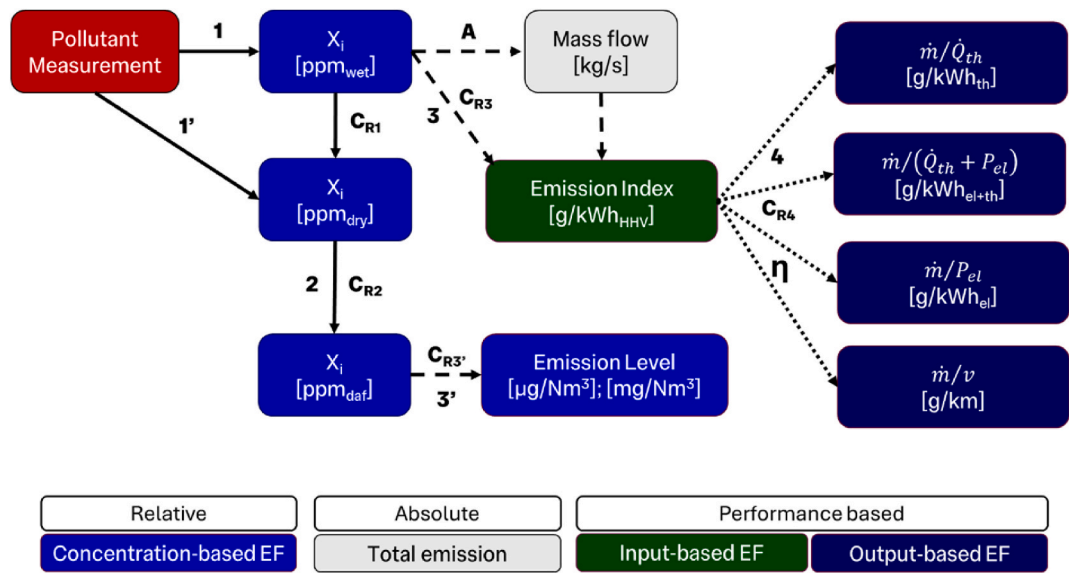


Fig. 2. Overview of different emission metrics and the intermediate conversion factors. Adapted from Ref. [12].

Table 2
Comparative analysis of existing emission metrics.

	Advantages	Disadvantages	Refs.
Concentration-based	- Easy to implement a CEMS to control compliance with regulations. - Does not require information on the input fuel consumption rate.	- Highly susceptible to fuel and oxidizer changes. - Dependent on measurement conditions (temperature and pressure). May induce errors in its conversion to performance-based metrics if not properly reported.	[9, 13]
Input-based	- Consistent method to compare specific emissions across different combustion systems where the effective use of heat is difficult to measure (e. g., Open flames, different burner designs). - Simplest emission metric for comparable emission factors in fuel-flexible systems.	- HHV or LHV can be used in different sectors, possibly causing confusion across climate and air pollution scientists using different datasets.	[45]
Output-based	- Provides incentives to improve performance of processes. - Clear definition of effective emissions per unit of energy, work or product produced.	- Requires constant measurements of both the emissions and the process performance. - Complex implementation.	[46]

Table 3
Reference concentration of O₂ (% v/v) for each sector considered.

Process	%O ₂	Ref
Gas burners, boilers, Oil and NG Facilities	3	[48,49]
Coal combustion	6	[48,49]
Waste Incineration (USA)	7	[50]
Waste Incineration (EU/UK)	11	[48]
Gas turbines, ICE	15	[48,49]

heterogeneity of emission metrics being used across combustion research using carbon-free or low-carbon fuels, with concentration-based emission metrics being the most challenging to use when seeking a fair comparison between different fuels and blends [8–12,15]. This challenge arises from the dependence of concentration-based emission metrics on both the thermodynamic (reactants' temperature and pressure) and operational conditions (equivalence ratio or adiabatic flame temperature) in which the reported combustion process occurred [14,47].

Depending on how pollutant measurements, as presented in Fig. 2, are reported, additional information is required to properly convert concentration-based emission metrics into performance-based emission metrics. Table 4 provides an overview of the usual requirements to perform the conversion of pollutant measurements into different emission metrics. Conversion parameters C_{R1} , C_{R2} , and $C_{R3'}$ were previously defined, and the parameters C_{R3} and C_{R4} are obtained from the different standards listed in Table 5 and presented in detail in Appendix A.

Regarding the difficulty in obtaining actionable emissions data from research conducted on the combustion of carbon-free or low-carbon fuels, existing standards (listed in Table 5) provide detailed procedures to properly report pollutant emissions from different stationary combustion sources, such as boilers, furnaces, gas burners [50–53], internal combustion engines (ICE) [54,55], and gas turbines (GT) [56]. A recommended flow diagram based on the PD CEN/TR 1404:2024 [52] standard is presented in the Appendix to be considered as a reference for the reporting of emissions from future experiments on the combustion of carbon-free and low-carbon fuels.

Douglas et al. have been producing a series of papers highlighting the necessity of migrating towards output-based emission levels to achieve a fair comparison between emissions from different fuels used for gas turbine applications [6–9]. An initial comparison on the dependence of reporting protocols on the fuel type being used was performed for NG and H₂ blends, where chemical equilibrium for various NG and H₂ blends at a set adiabatic flame temperature of 2000 K⁵ under atmospheric (1 bar and 300 K reactants temperature) and compressed (20 bar and 700 K reactants temperature) conditions were studied to highlight the dependence of volumetric emission levels on fuel composition [6]. An extension of this study, comparing also the effects of varying fuels on input- and output-based emission factors was performed for a set

⁵ Industrial combustors may operate in a range of 1000 K to 2500 K, but the ideal range of operation is between 1670–1900 K to minimize CO and NO_x emissions [70].

Table 4
Comparison of required parameters to convert pollutant measurements from combustion processes into different emission metrics.

	Wet basis	Dry basis	DAF basis ^a	Concentration based	Input-based ^b	Output-based ^b
Wet basis	–	C_{R1}	$C_{R1} \bullet C_{R2}$	$C_{R1} \bullet C_{R2} \bullet C_{R3'}$	C_{R3}	$C_{R3} \bullet C_{R4}$
Dry basis	$\frac{1}{C_{R1}}$	–	C_{R2}	$C_{R2} \bullet C_{R3'}$	$\frac{C_{R3}}{C_{R1}}$	$\frac{C_{R3} \bullet C_{R4}}{C_{R1}}$
DAF basis ^a	$\frac{1}{C_{R1} \bullet C_{R2}}$	$\frac{1}{C_{R2}}$	–	$C_{R3'}$	$\frac{C_{R3}}{C_{R1} \bullet C_{R2}}$	$\frac{C_{R3} \bullet C_{R4}}{C_{R1} \bullet C_{R2}}$
Concentration-based	$\frac{1}{C_{R1} \bullet C_{R2} \bullet C_{R3'}}$	$\frac{1}{C_{R2} \bullet C_{R3'}}$	$\frac{1}{C_{R3'}}$	–	$\frac{C_{R3}}{C_{R1} \bullet C_{R2} \bullet C_{R3'}}$	$\frac{C_{R3} \bullet C_{R4}}{C_{R1} \bullet C_{R2} \bullet C_{R3'}}$
Input-based ^b	$\frac{1}{C_{R3}}$	$\frac{C_{R1}}{C_{R3}}$	$\frac{C_{R1} \bullet C_{R2}}{C_{R3}}$	$\frac{C_{R1} \bullet C_{R2} \bullet C_{R3'}}{C_{R3}}$	$\frac{1}{C_{R4}}$	–
Output-based ^b	$\frac{1}{C_{R3} \bullet C_{R4}}$	$\frac{C_{R1}}{C_{R3} \bullet C_{R4}}$	$\frac{C_{R1} \bullet C_{R2}}{C_{R3} \bullet C_{R4}}$	$\frac{C_{R1} \bullet C_{R2} \bullet C_{R3'}}{C_{R3} \bullet C_{R4}}$		

^a Considering dry and air free basis as a range of set O₂ content from 0 % to any value listed in Table 3.
^b Conversion factors to input- and output-based emission metrics are listed in Appendix A.

Table 5
Comparison of different emissions reporting protocols from international standards and procedures for stationary combustion systems. CB: Concentration-based, IB: Input-based, OB: Output-based.

Standards	BS ISO 11042-1-1996 [56]	BS ISO 8178-4-2020 [55]	EPA Method 19 [50]	PAS 4444-2021 [53]	EN 676:2020 [51]	PD CEN/TR 1404:2024 [52]
Sector	Gas turbines	Internal combustion engines	Stationary combustion systems	Gas appliances using H ₂	Gas burners	Gas appliances
Pollutants considered	CO ₂ , CO, UHCs, VOCs, NH ₃ , NO _x , and SO ₂	CO ₂ , CO, UHCs, NO _x , PM, and SO ₂	NO _x , PM, and SO ₂	NO _x	NO _x and CO	NO _x and CO
Type of output	CB and OB	CB and OB	IB	IB	CB and IB	CB and IB
LHV	X	X		X	X	X
HHV			X		X ^a	
Conditions	wet and daf	wet and daf	daf	daf	daf	daf
Temperature	273.15 K and 288.15 K	298.15 K	70 °F (–299.26 K) ^b and 68 °F (298.15 K) ^c	288.15 K	288.15 K	273.15 K and 288.15 K
Pressure	101.3 kPa	101.325 kPa	760 mmHg (–101.325 kPa)	101.325 kPa	101.325 kPa	101.325 kPa

^a For class 5 boilers (installed after September 26, 2018).
^b For the determination of F-Factors [50].
^c For reporting of emissions [50].

adiabatic flame temperature of 1800 K under atmospheric (1 bar and 300 K reactants temperature) and compressed (17 bar and 700 K reactants temperature) conditions for NG and H₂ blends, pure propane and pure n-dodecane. This demonstrated that output-based emissions remained unaffected by fuel composition variations, and thus, were recommended as the best emission reporting measure to perform fair comparison between different fuels used in the same technology [9]. Parallel to these studies, Douglas et al. extended their analysis on reporting protocols to blends of hydrocarbons with ammonia (NH₃) and fully cracked ammonia (3H₂+N₂) [8], operating at equivalent conditions to the ones used in the previous study [9], which are representative of an F-class gas turbine. The indirect impacts of drying, dilution, thermodynamic properties, and performance effects were analyzed separately for each blend. Their main findings were that volumetric emissions had the least change when blending ammonia, being less than 3 % different from NG: but fully cracked ammonia emissions were overestimated by up to 20 % when reported on a volumetric basis, underscoring the relevance of using output-based emissions.

Garan et al. [11], understanding that the standards already use volumetric concentration emissions, proposed a generalised conversion method for fuel-flexible operation. Based on the previous works by Garg and Castaldini [57,58] on the effect of oxygen-enriched waste combustion in incinerators on concentration-based reporting methods, Garan et al. [11] proceeded to develop a generalised conversion method including the effects of dilution and heat content in the product gases. Incorporating measures to mitigate the effects of exhaust gas recirculation (EGR) schemes and oxygen enrichment on dilution of the pollutant’s concentration.

Schmitz et al. [10], provided a detailed analysis of the current EU regulatory framework and the applicable standards for air pollutants reporting, and presented an analysis of the impact of using NG from the

North Gas, H₂, and dimethyl ether (DME) on the current reporting methods of pollutants. Their study offered insights on the requirements and challenges of introducing performance-based emission metrics, highlighting the technical challenges posed by operational conditions in special cases such as the oxy-combustion of H₂, where H₂O is the main product, when subjected to existing reporting criteria of dry and air free conditions. The particular case of oxy-combustion of hydrocarbon fuels has been previously studied by Baukal et al. [13], suggesting that CO₂ concentrations acted as a reference proxy instead of O₂. However, since carbon-free fuels are not expected to contain relevant amounts of CO₂ in their product gases, new measuring approaches will be required to ensure accurate measurement of pollutants from the oxy-combustion of carbon-free fuels.

Goßrau et al. [12] presented an extension to the work done by Douglas et al. [9] producing a detailed analysis of the practical considerations for the case of using blends of NG and H₂ or NH₃ in energy conversion systems. Goßrau et al. [12] extended this analysis, following a similar approach to the procedure devised by Douglas et al. for blends of hydrocarbons with H₂ [9] or NH₃ [8], based on chemical equilibrium calculations, to account for the operation of non-premixed and premixed gas burners, and for large-scale gas turbines and combined heat and power plants. Combustion conditions within the GT were performed for a set outlet temperature and oxidizer mass flow under atmospheric (1 bar and 288.15 K reactants temperature) and compressed (25 bar and 721.7 K reactants temperature) turbine inlet conditions, representative of state-of-the-art turbine operation conditions. Additionally, the impact of common industry cycle adaptations such as exhaust gas recirculation and water and steam injection on emission metrics was comparatively assessed for using CH₄ and H₂ in the GT, observing a quantifiable impact of each cycle adaptation on the final reported measurement, and showcasing the relevance of incorporating all process conditions to

achieve a fair comparison between the emission intensity of fuels. These effects not only alter the reported emissions of NO_x but also those of other pollutants, while also having an impact of underreporting the savings in CO_2 emissions, a topic of interest for the carbon accounting of decarbonisation efforts.

Lastly, Lee and Cho [59] performed a numerical study based on chemical equilibrium analyses of CH_4 blended with four different carbon-free fuels, these being: pure H_2 , pure NH_3 , fully cracked NH_3 (N_2+3H_2), and partially cracked (60 %) NH_3 . They used an inlet temperature of 673 K and a pressure of 10 bar, setting an adiabatic flame temperature of 1800 K as reference condition to establish the equivalence ratios for different blends to ensure equivalent operation. They then computed the equilibrium composition of the gaseous products to analyse the differences between fuels. They also observed a discrepancy between the actual emissions and the reported emissions when using a concentration-based emission metric at a set O_2 concentration. One of their concluding remarks was the need for developing specific emissions standards for these fuels.

2.1. Overview of existing reporting methods and standards

There are industry-specific standards depending on the combustion process or device, which establish the appropriate emission measuring method for each pollutant and the corresponding reporting method, being either concentration-, input-, or output-based depending on the sector. Table 5 presents a non-exhaustive compilation of standards and methods for the standardized conversion of different pollutant emissions from a concentration-based (CB) emission to an input- (IB) or output-based (OB) emission rate from stationary combustion sources.

Each reporting protocol presents a different procedure to construct emission factors from available combustion data. Moreover, depending on the nature of the combustion process, different criteria and reference conditions may be considered. Equations and assumptions used in each of the presented standards are detailed in Appendix A.

As previously stated, to avoid dilution effects impairing a fair comparison between reported pollutants across different technologies, concentration-based reporting methods require all measurements to be presented on a dry-basis and a set O_2 content (see Table 3). However, for performance-based emission metrics there is a disagreement between the use of the lower (LHV) or higher heating value (HHV). European standards use LHV as the reference value to construct their emissions factors (being the case of new condensing gas boilers, class 6, the only exception), while US standards take HHV as a reference point. If not considered, this factor may induce variations of up to 17 % (for the case of ammonia combustion)⁶ in the implementation of pollutants emission factors.

From the standards presented in Table 5 there is a clear distinction between the different reporting conditions, where the reference temperature ranges from 273.15 K to 299.26 K, which needs to be taken into account when comparing concentration-based emissions. Fortunately, all standards agree on the reference pressure at 101.325 kPa, with a small difference for the BS ISO 11042-1-1996 which truncate this value to 101.3 kPa. Regarding the conditions considered, only the BS ISO 11042-1-1996 and BS ISO 8178-4-2020 provide a procedure to report on wet conditions at fixed O_2 contents, which, as presented by Douglas et al. [9] and Schmitz et al. [10], considerably mitigate the effect of using different fuels by reducing the dilution steps in the treatment of the raw measurements.

Only four standards from the table consider the reporting of emissions using concentration-based emission metrics, but all of them have procedures to produce performance-based emission metrics, either as an input-based or output-based emission factor. This observation is of

significant importance, as it underscores that there are existing standards capable of providing the tools to produce emission metrics to enable fair comparisons across the different fuels being considered in the global decarbonisation efforts.

3. Conversion of existing NO_x emission limit values (ELVs)

Using carbon-free and low-carbon fuels, with a special emphasis on H_2 , is a strategic pathway towards decarbonising existing processes and technologies; however, there are still many challenges to be addressed before achieving its widespread adoption. One of these challenges is providing early adopters with legal certainty to develop their business plans, while ensuring that sensible considerations towards the environment and public health are being taken into account.

A way forward is to implement sector-specific emission limit values (ELVs) for carbon-free and low-carbon fuel combustion. This should focus on NO_x emissions for the case of carbon-free fuels, as other pollutants are not expected to be part of the combustion products. Recently, the UK's Environment Agency published a guidance for setting ELVs for the combustion of pure H_2 and natural gas and H_2 blends. They proposed scaling the existing ELVs set for natural gas combustion on large and medium combustion plants by a fixed factor ranging from 1.00 to 1.37. Blends would be treated on a progressive scale from 1.00 for mixtures having up to 20 % H_2 and a factor of 1.37 would be used for the combustion of pure H_2 [60]. As previously mentioned, this correction factor is dependent on the combustion conditions, and on a set adiabatic flame temperature of 1800 K (usual operational target for industrial combustion) it has been shown, by chemical equilibrium calculations using different sets of reaction mechanisms, that it may vary from 1.36 to 1.40 for atmospheric (expected in a domestic boiler) to compressed (expected in gas turbines or internal combustion engines) inlet conditions of hydrogen and air mixtures. Changing the oxidant to oxygen-enriched air or pure oxygen [10], as well as performing cycle adaptations as EGR and water or steam injection [12], can further alter this conversion factor. The authors have found that the Environment Agency guidance has been a useful starting point as a reference, while more detailed and comprehensive evaluations are undertaken for each alternative fuel being considered in the decarbonisation efforts.

It has been reported that the challenges of using existing concentration-based metrics do not stop with H_2 combustion, as other sustainable fuels, such as cracked ammonia, dimethyl ether (DME), methanol and ammonia, require an adequate conversion factor when conventional methods of pollutant reporting are used. For the case of cracked ammonia (N_2+3H_2), the studies performed by Douglas et al. [7, 8] and Lee and Cho [59] showed that pollutant concentration on a dry basis were up to 21 % higher when compared to the equivalent mass-to-energy emission rate of CH_4 combustion, which is smaller than the up to 40 % difference reported for H_2 combustion [6–9,11,12,59], but still large enough to produce a significant impact in overestimating NO_x emissions from the process.

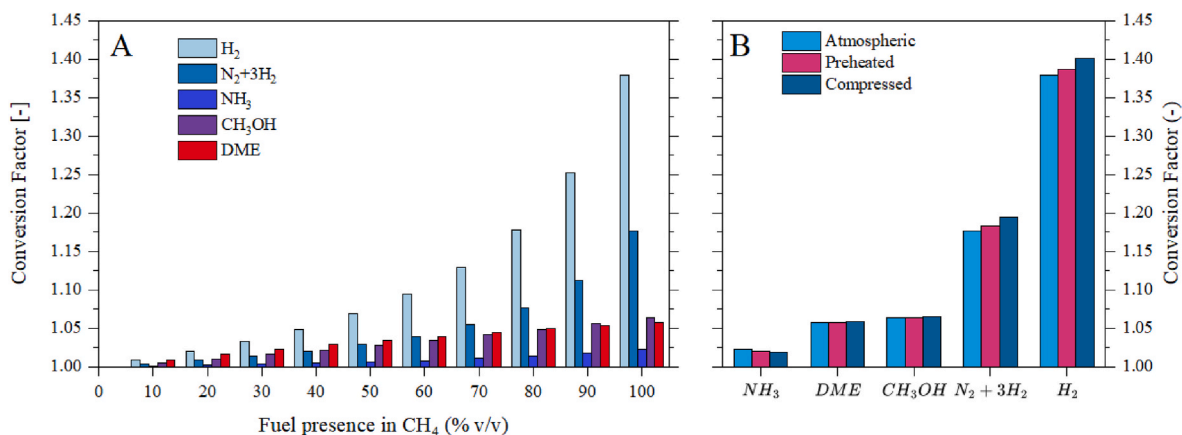
Moreover, inlet temperature and pressure of the fuel and oxidizer are process-dependent and range from ambient conditions (300 K and 1 bar) to high pressure and temperature (up to 700 K and 21 bar in modern gas turbines); therefore, conversion factors to adequate concentration-based emission metrics for different fuels should be also process specific. With this in consideration, Table 6 presents a list of conversion factors calculated for the ratio between the dilution factors (water and oxygen content) obtained for each fuel against methane (baseline) at three relevant process conditions (atmospheric, preheated, and compressed) found in free flames, furnaces and boilers, and gas turbines and internal combustion engines, which are also depicted in Fig. 3-B. These factors were obtained from zero-dimensional chemical equilibrium computations using a Python code running CANTERA and the GRI 3.0 chemical mechanism for methane, hydrogen, ammonia, cracked ammonia, and methanol combustion with air; and a specific chemical kinetic model presented by Pan et al. [61] was used for dimethyl ether (DME). All

⁶ Considering the ratio between the LHV and HHV of ammonia (1.00–18.6/22.5 = 17 %).

Table 6Conversion factors for ELVs from CH₄ to alternative fuels at an adiabatic flame temperature of 1800 K.

	Atmospheric ^a (300 K–1 bar)	Preheated ^b (423 K–1 bar)	Compressed ^c (700 K–17 bar)
Ammonia (NH ₃)	1.023	1.021	1.019
Dimethyl ether (CH ₃ OCH ₃)	1.057	1.057	1.058
Methanol (CH ₃ OH)	1.065	1.064	1.065
Cracked ammonia (N ₂ + 3H ₂)	1.176	1.183	1.194
Hydrogen (H ₂)	1.379	1.387	1.400

Conditions typically found in.

^a Domestic boilers, free flame burners, and medium scale combustion systems.^b Large combustion plants, such as furnaces, industrial ovens, and other high temperature applications.^c Gas turbines or Internal combustion engines.**Fig. 3.** Conversion factors for ELVs from CH₄ to alternative fuels under (A) different blends (in volume) of carbon-free and low-carbon fuels with CH₄ at atmospheric conditions, and (B) atmospheric, preheated and compressed conditions, for an adiabatic flame temperature of 1800 K.

calculations were performed for a set adiabatic flame temperature of 1800 K to compare the dilution effect for similar operation conditions across all fuels. This assumption serves the purpose of providing comparable operation conditions expected to be found in any real application of these fuels in the different combustion technologies available. Process conditions and fuels considered were selected to replicate the conversion factors obtained by Douglas et al. [6–9], Goßrau et al. [12], Garan et al. [11], Lee and Cho [59], and Schmitz et al. [10].

Fig. 3-A presents the evolution of the conversion factors magnitude for the combustion, in atmospheric conditions (300 K and 1 bar), of CH₄ blends with different carbon-free and low-carbon fuels ranging from 0 % to 100 % alternative fuel in the blend. At low blend ratios (up to 20 % v/v) the conversion factor is almost negligible (lower than 1.02) with H₂ and DME having the highest values (1.019 and 1.016, respectively). Therefore, it would be expected that there would be a low impact of using concentration-based emission metrics for air pollutants reporting on blends of carbon-free or low-carbon fuels with natural gas.

Furthermore, an overview of Fig. 3-A and Fig. 3-B showcases that the fuels most susceptible to having their emissions overestimated, when concentration-based emission metrics are used, are pure hydrogen and cracked ammonia, both requiring conversion factors in the range of 1.176–1.194 and 1.379–1.400, respectively, for the different expected operation conditions considered when combusted as a pure fuel. Other fuels presented an almost steady behavior across all tested conditions, with methanol and DME displaying a similar conversion factor around 1.06. Lastly, the dilution effects from oxygen and water correction on ammonia, the fuel producing the highest amount of water per unit of energy released, effectively cancel themselves, resulting in the smallest conversion factor of the group.

All presented values are in accordance with the magnitudes and trends of conversion factors published in the referred studies and showcase the need of performing adequate conversion steps in the reporting of emissions from new fuel being considered in the

decarbonisation efforts to ensure that a fair assessment is conducted on the environmental merits of each alternative. However, the observed variation between the three operation modes presented (atmospheric, preheated, and compressed) proved to be insignificant⁷ (<0.5 %) for NH₃, DME and CH₃OH, and small⁸ for cracked ammonia and H₂ (~1.5 %). Therefore, for the sake of simplicity, it would be advisable that sectors forced to use concentration-based emission metrics should consider the use of conversion factors only for the case of using cracked ammonia and hydrogen as a fuel. This recommendation is based on the fact that both fuels exhibit a greater sensitivity to the dilution factors (drying and oxygen correction) used in current reporting protocols, resulting in an overestimation of their emissions well over the expected threshold for the accuracy of existing emissions measuring systems [54, 56].

3.1. Maximum ELVs for carbon-free and low-carbon fuels use in medium combustion systems as a single fuel

Building upon the conversion factors presented in the previous section, and the guidance published by the UK's Environment Agency on emissions from H₂ combustion [60], current ELVs from EU Directive 10/75 for industrial emissions [48] were converted using the conversion factors from Table 6 and collected in Table 7 and Table 8. Here, the converted NO_x ELVs for the combustion of carbon-free and low-carbon fuels from existing and new plants were set, respectively, by plant and thermal input. Reference conditions for these ELVs are 273.15K, 101.3 kPa, dry, 3 % oxygen for boilers and 15 % oxygen for gas turbines and engines. A conversion of NO_x ELVs from mg/Nm³ to mg/kWh was made

⁷ The required resolution of the instruments used to detect CO, NO_x and SO_x in combustion products is usually 0.5 % or 1.0 % of the full scale of the measuring device [54,56].

⁸ The measuring stability requirement for flue gases is usually 2 % [54,56].

Table 7NO_x ELVs for existing plant⁹ using 100 % carbon-free or low-carbon fuel, scaled from existing ELVs for NG.

Plant type and thermal input (MW _{th})		Natural Gas	Cracked Ammonia	Ammonia	Methanol	DME	Hydrogen ^a	
		(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/kWh)
GT	≥50	50	59.7	51.0	53.3	52.9	68.5	150
Boiler		100	118.3	102.1	106.4	105.7	137.0	100
ICE		100	119.4	101.9	106.5	105.8	137.0	300
GT	>5	150	179.1	152.9	159.8	158.7	205.5	450
Boiler	<50	200	236.6	204.2	212.8	211.4	274.0	200
ICE		190	226.9	193.6	202.4	201.0	260.3	570
GT	≥1	150	179.1	152.9	159.8	158.7	205.5	450
Boiler	≤5	250	295.8	255.3	266.0	264.3	342.5	250
ICE		190	226.9	193.6	202.4	201.0	260.3	570

^a A fixed conversion factor of 1.37 was used for H₂ in line with current guidance [60].⁹ For LCP, an existing plant means a plant with a permit for combustion of a conventional fuel operating since before 08-Jan-2014. For MCP the operation date is before 20-Dec-2018.**Table 8**ELVs for new plant¹⁰ using 100 % of carbon-free or low-carbon fuel, scaled from existing ELVs for NG.

Plant type and thermal input (MW _{th})		Natural Gas	Cracked Ammonia	Ammonia	Methanol	DME	Hydrogen ^a	
		(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/Nm ³)	(mg/kWh)
GT	≥50	50	59.7	51.0	53.3	52.9	68.5	150
Boiler		100	118.3	102.1	106.4	105.7	137.0	100
ICE		75	89.6	76.4	79.9	79.4	102.8	225
GT	>5	50	59.7	51.0	53.3	52.9	68.5	150
Boiler	<50	100	118.3	102.1	106.4	105.7	137.0	100
ICE		95	113.4	96.8	101.2	100.5	130.2	285
GT	≥1	50	59.7	51.0	53.3	52.9	68.5	150
Boiler	≤5	100	118.3	102.1	106.4	105.7	137.0	100
ICE		95	113.4	96.8	101.2	100.5	130.2	285

^a A fixed conversion factor of 1.37 was used for H₂ in line with existing guidance [60].¹⁰ For LCP, a new plant means a plant with a permit for combustion of a conventional fuel operating after 08-Jan-2014 but before 01-Jan-2025. For MCP the operation date is after 20-Dec-2018 but before 01-Jan-2025.

for hydrogen following the procedure described in [Appendix A](#).

The presented values may be considered as reference information to perform fair assessments of alternative fuels across the different existing combustion technologies found in energy-intensive industries, as well as to indicate a possible ceiling for emission factors values of different combustion technologies to consider when performing air quality or environmental assessments of either retrofitting alternative fuels to existing or “new” combustion plants or implementing new combustion technologies running on carbon-free or low-carbon fuels.

Even though new technologies are expected to have a better environmental performance than the existing ELVs, which were developed considering the BAT at the time of the last BREF document published on Large Combustion Plants during 2017 [62], this could be enough to make a case for continuing to use the existing ELVs for NG, without conversion, across the different alternative fuels being considered, in order to indirectly force new technologies to have a better emissions performance than existing combustion systems burning natural gas.

3.2. Case study: NO_x emissions from gas appliances

The latest UK Housing Survey reported that there are almost 25 million houses connected to the gas grid, with a gas boiler population of

over 22.5 million in 2022, from which almost 90 % correspond to high-efficiency condensing boilers [63]. Among the decarbonisation efforts being considered, domestic gas appliances may have to run with blends of H₂ and natural gas [1]. A previous study by Wright and Lewis [15] considered the possible impact of blending H₂ in the UK’s NG pipeline on NO_x emissions from space heating boilers. Within the limitation of their assumptions was the lack of homogeneity among the sparse dataset of NO_x emission data from the combustion of hydrogen blends, as well as the fact that most of these studies did not account for the difference in dry stoichiometric combustion products per unit of energy seen in the combustion of carbon-free and low-carbon fuels. Moreover, recently, Lebel et al. [64] raised concerns about the effects of gas appliances emissions on indoor air quality, identifying an average NO_x emission factor of 78.1 mg/kWh for residential gas cookers operating with natural gas, an emission intensity high enough to cause undesired NO_x exposure in dwellings with small kitchens and poor ventilation.

Therefore, to highlight the relevance of the use of adequate emission metrics to fairly assess the emission performance of fuel-flexible combustion systems in a relevant sector such as residential gas appliances, two different gas appliances groups running with different blends of H₂ and NG were considered. [Fig. 4](#) depicts the NO_x emission level (ppmvd) and NO_x emission factor of two groups of gas appliances tested in the EU

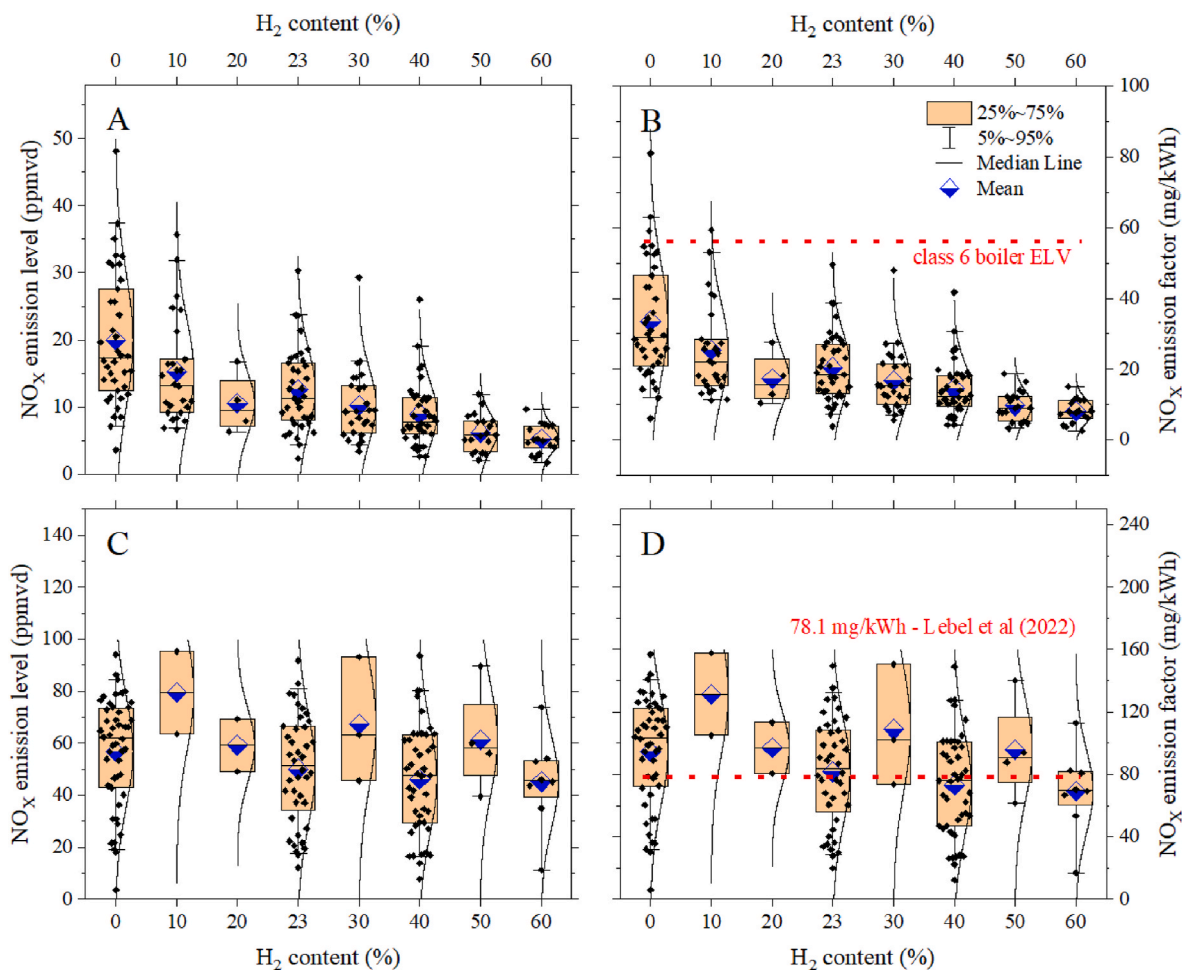


Fig. 4. NO_x emission levels at different H₂ content (% v/v) for NG combustion in: (A) Premixed condensing boilers (ppmvd) and (C) atmospheric gas cookers (ppmvd) [65]; and converted NO_x emission factors for (B) Premixed condensing boilers (mg/kWh) and (D) atmospheric gas cookers (mg/kWh). Black scattered diamonds represent the number of tests performed at each H₂ concentration.

project “Testing Hydrogen admixture for Gas Applications” (THyGA¹¹) [65–67]. This project evaluated 102 different gas appliances, with blends of up to 60 % (v/v) H₂ and natural gas, from which atmospheric gas cookers and fully premixed gas boilers were the most tested gas appliances with 31 and 20 different units tested, respectively. Detailed information on the dataset can be found in Ref. [65].

Fig. 4-A presents the concentration of NO_x in ppm in a dry and air free basis (ppmvd) for the combustion of H₂ blends in fully premixed condensing boilers, with an average NO_x concentration of 19.9 (ppmvd) and 5.3 (ppmvd) for 0 % and 60 % H₂ content, respectively. From this dataset one could infer that the effective reduction of NO_x emissions by blending H₂ into the NG would be 73.6 %. However, this treatment does not consider the difference in dry stoichiometric combustion products per unit of energy from using H₂, which for a 60 % would amount to almost 9 % (see Fig. 3-A). Performing the same procedure to the input-based emission metrics presented in Fig. 4-B provides an average effective reduction of 76.3 % of NO_x emissions when operating at 60 % H₂ content, thus the concentration-based metric was underestimating the positive effect on NO_x emissions observed from the combustion of H₂.

For the case of the dataset of NO_x concentrations from gas cookers, Fig. 4-C presents a trend that is not as obvious as with the fully premixed

condensing boilers. Since the most populated data points for these experiments are 0 %, 23 % and 40 %, comparing their mean values is considered to provide the most reliable point of comparison for this gas appliance group. The mean NO_x concentration at 0 % and 40 % of H₂ was 56.8 (ppmvd) and 46 (ppmvd), respectively; therefore, the reduction of NO_x emissions corresponds to 19 %. However, when input-based emission metrics are considered (Fig. 4-D), the mean emission factors for 0 % and 40 % H₂ content are 95.6 (mg/kWh) and 73.8 (mg/kWh), respectively, representing a mean effective reduction of NO_x emissions of 22.8 % (with the corresponding conversion factor of ~1.05, see Fig. 3-A).

4. Final remarks and outlook

Existing GHG and pollutant reporting protocols vary from sector to sector and between countries, and while concentration-based emission metrics are widely implemented in sectors where a Continuous Emission Measuring System (CEMS) is in place (i.e., large stationary sources), performance-based metrics are mostly used on small to medium stationary sources and all mobile sources. Therefore, developing a unique solution to cover the impact of using carbon-free and low-carbon fuels on the reporting protocols used in all sectors is not a straightforward task. However, the present document reviewed several sound and replicable approaches that could enable an update to existing methods to achieve a fair comparison between pollutants emissions metrics of different fuels.

¹¹ <https://thyga-project.eu/wp-content/uploads/THYGA-OVERVIEW-WP3-test-results.xlsx>.

In particular, this study has reviewed existing challenges and appropriate modifications to reporting protocols. While presenting an overview for the different NO_x emissions from the combustion of carbon-free and low-carbon fuels across the different possible industrial and residential applications, with a focus on their method of reporting and the requirements of air pollution scientist as final users, providing conversion factors for blends containing, or pure combustion of, hydrogen, dimethyl ether, methanol, ammonia, and cracked ammonia.

In the case of sectors where concentration-based metrics are a standard, the use of the generalised emission conversion factor presented by Garan et al. [11] is considered to be the best approach to account for the changes in the heat released per unit of volume of combustion products of a wide range of fuels. However, other approaches, such as the guidance published by the Environment Agency on emissions from H₂ combustion [60], provide an alternative method to make fair assessments of the air quality and environmental merits of fossil fuel replacement by low-carbon or carbon-free fuels.

Where sectors are already using performance-based emission metrics, it has been shown that values computed from a wet-basis measurement are comparable across different fuels. This enables a fair assessment of the environmental impacts of deploying different technologies. Sectors already prepared to benefit from these emission metrics are stationary gas turbines and internal combustion engines following both the US EPA 40 CFR part 60 standard [50] or the ISO 11042-1-1996 [56] and the ISO 8178-4-2020 [55] standards, all providing detailed procedures to present output-based pollutants emission metrics.

Furthermore, across this study, the relevance of properly accounting emissions was highlighted, where use of concentration-based emission metrics to assess the emission performance of adding carbon-free fuels to combustion process may result in the overestimation of NO_x emissions and the underestimation of CO₂ savings, thus incorrectly attributing the benefits obtained from their incorporation.

Finally, output-based performance metrics have been gaining relevance across international standards [45,46] and are highly recommended as a near-future replacement for conventional concentration-based emission metrics to ensure robust emission metrics capable of being compared across fuels. They are useful for both the fair environmental assessment of air pollutants being emitted by alternative carbon-free fuels, such as NO_x, and for the correct accounting of the savings of carbon emissions achieved by blending fossil fuels with H₂ or ammonia.

CRedit authorship contribution statement

Nicolás Ripoll Kameid: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization. **Helen ApSimon:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2025.03.295>.

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Glossary

BAT: Best available techniques
 BREF: BAT reference document
 BS: British Standard
 CB: Concentration-based
 CEMS: Continuous emissions monitoring system
 CEN: Comité Européen de Normalisation, English: European Committee for Standardization
 daf: Dry and air free
 DME: Dimethyl ether
 EA: Environment Agency
 ECS: Emission control system
 EGR: Exhaust gas recirculation
 ELV: Emission limit value
 GAINS: Greenhouse gas - Air pollution Interactions and Synergies
 GHG: Greenhouse gas
 GT: Gas turbine
 HHV: Higher heating value
 IB: Input-based
 ICE: Internal combustion engine
 IIASA: International Institute for Applied Systems Analysis
 ISO: International Organization for Standardization
 LHV: Lower heating value
 LCP: Large combustion plant
 MCP: Medium combustion plant
 NG: Natural gas
 OB: Output-based
 PM: Particulate matter
 scm: Standard cubic meter
 SI: Steam injection
 UHCs: Unburnt hydrocarbons
 UKIAM: United Kingdom integrated assessment model
 VOCs: Volatile organic compounds
 WI: Water injection