

Bulk hydrogen production and the impact on turbomachinery lifing

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Abstract. The EU has made the commitment to reduce pollutant gases emissions by 2030 and achieve climate neutrality by 2050. To achieve these targets the power generation sector must engage. Gas turbines will play a part through the use of alternative fuels such as H₂. However the adoption of H₂ as a fuel presents multiple engineering challenges, from flame stability, to NO_x emissions, to materials' degradation. The latter is inherently linked to the technologies used to produce hydrogen in the bulk quantities required. Different technologies will generate H₂ with differing quantities and types of contaminants (i.e., Cl-based for seawater electrolysis, S-based from steam methane reforming). This is important as, upon combustion, these contaminants can form harmful species in the exhaust stream, linked to mechanisms causing materials degradation. It is therefore crucial to understand the types of contaminants that are present in bulk H₂ and so in the combusted gases. This work links together fuel and ingested air chemistry in the gas turbines to the chemical composition of the combusted gases, to the degradation mechanism that might arise in blading materials, and finally their impact on the gas turbine life. Exhaust gas composition has been predicted via thermodynamic modelling, and the condensation of harmful species that will ultimately dictate the corrosion mechanisms (e.g., alkali vapour) calculated.

1 Introduction

The European Union has set a target (Renewable Energy Directive – RED III) for the industrial sector to increase the use of non-biogenic renewable fuels to 42% by 2030 and to 60% by 2035 [1], [2]. Some European countries, such as Germany, Netherlands and France, to name a few, have published strategies and set ambitious targets for hydrogen use in the near future [3]. Hydrogen is identified as one of the fuels that could help the transition. The use of hydrogen as a fuel for gas turbines (GTs) comes with a variety of engineering challenges which need to be addressed. These include flame stability, combustion dynamics and NO_x emissions [4], [5], as well as corrosion due to impurities present in the fuel. Turbine original equipment manufacturing (OEMs) are working to address these issues to maintain their competitive edge. These challenges come from the different properties of hydrogen in respect to natural gas (for which GTs we designed); while natural gas has 312% the calorific value of hydrogen per unit volume, it has only 43% calorific value per unit mass [4]. This poses problems for the blending of hydrogen with natural gas. In fact, to maintain the power output, the volumetric flow of the fuel combusted in GTs needs to increase.

The fuel and air are mixed and ignited in the combustion chamber, producing a high temperature and high

velocity exhaust gases (1200–1400°C) [6]. These gases are directed by the vanes and blades as they pass through the turbine. As the hot gases pass through the turbine stages, they expand rapidly, and their temperature and pressure decrease, eventually exhausting at approximately 555°C for Open Cycle Gas Turbine (OCGT) applications and ambient pressure. GTs blades are designed with internal and film cooling to keep the metal surface temperature down, below the exhaust gas temperature. Fuel and air can contain impurities, such as sodium, water vapour, and dust (from the air) and sulphur, water vapour, and chlorine (from the fuel) [5], [6], [7]. These contaminants can react during combustion and form corrosive species, such as alkali vapours [5], [7], [8], [9]. These vapours enter the turbine section at temperature above 1000°C and when encountering a cooler surface, they can condense on blading materials, causing hot corrosion [5], [7], [8], [9]. Hydrogen can be produced in several ways and depending on how it is produced and what level of filtration has been used, it can result in a wide range of corrosive species in the exhaust gas. Water electrolysis is one of hydrogen production methods. If the hydrogen is produced using electricity from renewable sources, such as solar or wind, the resulting hydrogen is defined as "green". Green hydrogen has the potential for helping decarbonising the energy sector. Furthermore, the hydrogen produced by electrolysis is usually considered

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clean hydrogen, unlike the hydrogen produced from different sources such steam-methane reforming. Nevertheless, the hydrogen produced by electrolysis could contains impurities such as oxygen, water vapour and chlorine [10], [11], [12]. These species once combusted could potentially affect the remaining life of blading materials. This study makes use of an OCGT plant located on the coast of Ireland as a case study. This is equipped with a Siemens-Energy SGT-400. This model of turbine has been used for HYFLEXPOWER project and operated on 100% hydrogen [13]. For the purpose of the study the hydrogen used would be produced by electrolysis using wind power. Natural gas is piped in from the high-pressure transmission network. The study analyses 5 different cases, from 100% NG to 100% H₂.

2 Methodology

Five scenarios were analysed in the work, and the definition for them is given in Table 1. The power output was kept constant for five scenarios, for this reason the fuel flow was adjusted. For each scenarios the chemical composition of the air and fuel was kept constant. The chemical composition for the H₂ is given in Table 2, the chemical composition of the air is taken as in [14], and the chemical composition of the fuel is given in Table 3. The composition of the fuel post-NG/H₂ mixing has been calculated using local pipeline quality gas composition and H₂ electrolyser product composition information from the literature.

Table 1 Different scenario analysed.

Scenario	Natural Gas (%)	Hydrogen (%)	Fuel Flow (kg/s)	Exhaust Flow (kg/s)
1	100	0	0.754	38.73
2	70	30	0.703	38.86
3	50	50	0.64*	38.98*
4	30	70	0.55*	39.10*
5	0	100	0.30*	39.23*

* Denotes calculated values.

Table 2 Composition of Electrolyser product fuel [10], [11], [12].

Composition	Symbol	Molar Mass (g/mol)	Hydrogen Molar Fraction (%)
Hydrogen	H ₂	2.02	99.955%
Oxygen	O ₂	32	0.010%
Carbon Monoxide	CO	28.01	0.005%
Carbon Dioxide	CO ₂	44.01	0.005%
Nitrogen	N ₂	28.02	0.005%
Argon	Ar	39.95	0.005%

Water Vapor	H ₂ O	18.02	0.010%
Chlorine	Cl	35.45	0.005%

The mass flow of the fuel and the exhaust was only provided for scenarios 1 and 2, so the first step in predicting the air and fuel blend compositions is to extrapolate these for each scenario based on the known calorific values of both fuels and the mass flow for the 100% NG case. To do this, the power and efficiency were assumed to be constant across the scenarios and the calorific values (Table 4) were used along with the volume fractions for each fuel in the blend to predict a realistic fuel mass flow $\dot{m}_{fuel}$ for each scenario.

Table 3 Pipeline gas composition.

Composition	Symbol	Molar Mass (g/mol)	Nat Gas Molar Fraction (%)
Methane	CH ₄	16.04	94.08%
Ethane	C ₂ H ₆	30.07	3.20%
Propane	C ₃ H ₈	44.1	0.60%
Iso-Butane	i-C ₄ H ₁₀	58.12	0.10%
n-Butane	n-C ₄ H ₁₀	58.12	0.10%
Iso-Pentane	i-C ₅ H ₁₂	72.15	0.10%
Carbon Dioxide	CO ₂	44.01	0.50%
Nitrogen	N ₂	28.02	1.20%
Hydrogen Sulphide	H ₂ S	34.08	0.12%

$$\dot{m}_{fuel} = \frac{Power}{Efficiency \times Calorific Value} \quad (1)$$

$$CV_{mass} = \frac{CV_{volume}}{\rho} \quad (2)$$

After the mass flow for each scenario was calculated, the fuel blending composition was established using a method similar to the intake air. The volume fraction Φ for each component in the stream was calculated based on the initial molar fraction x for each fuel multiplied by the volume fraction for that fuel at each scenario using (4).

$$\Phi_{ij} = \frac{n_{ij}}{n_i} \quad (3)$$

$$\Phi_{ij} = (x_{ij,NG})(\Phi_{ij,NG}) + (x_{ij,H_2})(\Phi_{ij,H_2}) \quad (4)$$

The molar mass was then calculated for each component in the stream. The j th component molar mass M_{ij} in stream i was calculated using (5) by multiplying the molar mass of j th component M_j from literature [1] by the volume fraction of component j in stream i Φ_{ij}

$$M_{ij} = M_j \Phi_{ij} \quad (5)$$

The total molar mass in stream i M_i was then calculated by the sum of all the molar masses of each component using (6). Mass flow was then calculated for each component using (7)

$$M_i = \sum M_j \Phi_{ij} \quad (6)$$

$$\omega_{ij} = \frac{\Phi_{ij} \times M_{ij}}{M_i} \quad (7)$$

To calculate the chemical composition after combustion in each of the different scenario, the compositions of air and fuel were used as input for a thermodynamic software, MTDATA. The software minimises the Gibbs free energy of the system and the resulting chemical compositions. The software was also used to predict the Gibbs free energy of Na_2SO_4 species when evaporating. Na_2SO_4 was used in this study as it was found present in both natural gas and hydrogen post-combustion exhaust gas, making the comparison easier, furthermore, sodium sulphate is known to induce hot corrosion. This was then used to complete the deposition model as in [2] and condensation rates for the different blading materials in the different stages. The procedure for the calculation of the deposition rates is detailed elsewhere [2].

Table 4 NG and H_2 Calorific values and density [3].

Scenario	Unit	NG	H_2
CV_{volume}	MJ/m^3	37.8	12.1
ρ	kg/m^3	0.656	0.090
CV_{mass}	MJ/kg	57.53	134.62

The values in Table 4 were calculated using equation (2). It highlights the difference between the calorific values by volume and mass for both natural gas and hydrogen. For the calculation, it was assumed the hydrogen pure, as the hydrogen used for the study was 99.955% pure. While the scenarios had a near linear increase in volume fraction, the difference in CVs shown in Table 4 resulted in the mass fractions not being linear and having a significant step change in mass fraction between scenarios 4 and 5. This increase in hydrogen's calorific value resulted in an overall 60% reduction in fuel mass flow from scenarios 1 to 5 but also equated to a 3.3 fold increase of the volume flow between scenario 1 and 3. Equation (1) gave the following results for 100% NG and 100% H_2 with constant power and efficiency. Based on that, the values for scenarios 2, 3, and 4 were extrapolated from these.

3 Results

This section presents the results obtained from the deposition modelling and the minimisation of the Gibbs free energy for the different scenarios. Figure 1 shows the results obtained for the amount of flow in the exhaust section compared to the amount of fuel flow. As it can be seen, the higher hydrogen's calorific value resulted in an overall 60% reduction in fuel mass flow from scenarios 1 to 5 but also equated to a 3.3 fold increase of the volume flow between scenario 1 and 3, Table 1 and Figure 1. The calculations assumed constant power and efficiency for 100% NG and 100% H_2 . This has the follow-on consequence of increasing the total amount of contaminants present in the section, but not their concentration.

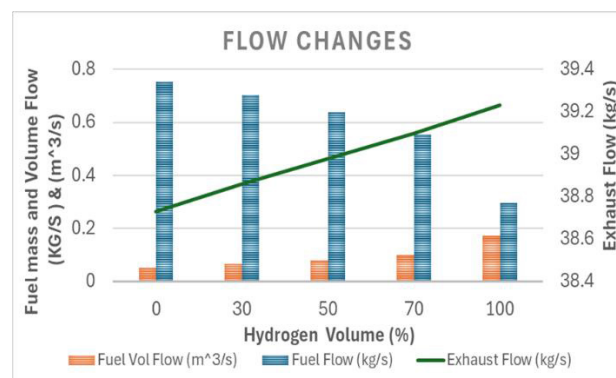


Figure 1 Mass and Volume flow of fuel and air for increasing content of H_2 .

The resulting mass fractions of contaminants post-filtration are shown in Table 8. Further reductions to these mass fraction would be possible by upgrading the filtrations system which may be a necessary step to combat the increased mass flow of air and contaminants through the machine. The filtration procedure is in line with the procedure explained in [2]. The data in Table 5 were arrived at using the seasonal mean concentrations of measured components at five sites in Ireland as per the below. Values were converted to ppm. The maximum seasonal figures were then reduced based on intake filtration removing 100% of coarse contamination and a 70% reduction in the fines [4].

Table 5 Post-filtration air contaminants' molar fraction results for all scenarios.

Component	Symbol	Mass Fraction ω_{ij}
Chloride	Cl	0.022%
Sodium	Na	0.027%
Magnesium	Mg	0.004%
Potassium	K	0.002%
Calcium	Ca	0.020%
Ammonium	NH_4	0.068%
Sulphate	SO_4	0.016%
Nitrate	NO_3	0.026%

The molar fraction of Na_2SO_4 in the flue gas resulting from the MTDATA predictions show a sharp rise between 1400K and 1600K, peaking between 1600K and 1650K before reducing rapidly again. This increases starts soon after the components melting point of 1161K [18] due to the increased vaporisation of the liquid Na_2SO_4 and peaks before the components boiling point of 1702K [18]. With a turbine inlet temperature of 1529.15K from [16], [17] the concentration of Na_2SO_4 is near its peak at this point, and increasing the temperature in this zone would likely result in a further increase in deposition. Scenario 3 is seen to have a significantly higher peak than the others.

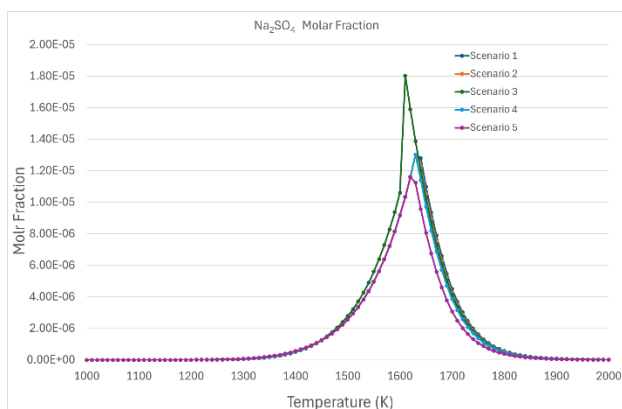


Figure 2 Molar fraction of Na_2SO_4 in the flue gas for each scenario.

The molar fraction of H_2O in the flue gas resulting from the MTDATA predictions for each scenario showed that the increase in hydrogen content has a significant impact on the levels of water vapour in the exhaust stream.

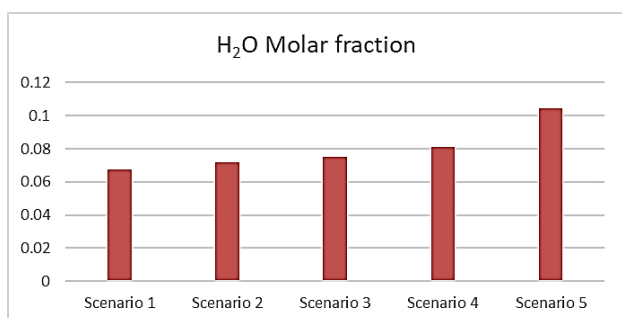


Figure 3 Water vapour molar fraction per scenario.

The blending of hydrogen into natural gas greatly modifies the combustion chemistry occurring within the turbine. The results demonstrate that elevation of hydrogen concentration results in alterations in the molar proportions of different combustion products, namely water vapour H_2O and sodium sulphate Na_2SO_4 [5], [6]. The combustion of hydrogen produces a higher water vapour content in comparison to natural gas.

Figure 4 and Figure 5 reports the condensation found for the different scenarios. Figure 5 shows the condensations flux for the compressor turbine stage 1 (CT1) blades versus metal temperature. As it can be seen from the graph, there is no clear variation for the dew point for the different scenarios, but on the other hand the flux rate is different for all the different scenarios, with a peak for scenario 3 (50% blend). This is in line to the thermodynamic modelling showing an increase in Na_2SO_4 molar fraction. This has implications for the GTs maintenance and service. From the calculations it seems that the same level of deposits, and therefore potential high temperature corrosion, would be similar to what is experienced currently for natural gas-powered gas turbines. This is also confirmed by the findings reported in Figure 4, which are comparing the depositions on different stages of the GTs. From the findings it can be seen how the main factor affecting the depositions rates are related to the position (and therefore the local gas conditions) within the GTs. This can be observed in both scenarios 1 and 5, where the highest deposition rates are calculated for CT-1 and

nozzle guide vane (NGV) -1, while CT-2 and NGV-2 could experience a lower deposition rate. The final rate would also depend on the local temperature on the different blading materials. Some temperature variation is to be expected within the same blade [7], [8], [9]. The expected variation could be more than 100°C [9], which could result in non-uniform deposition of alkali vapours and localised corroded areas.

The results show that the metal temperature of the blade and vanes has a significant impact on the level of deposition. One way of reducing the deposition could be to increase the metal temperature, so that the entire blade would be above the dew point of the Na_2SO_4 . This could be done with materials' advancements, such as thermal barrier coatings. Furthermore, higher H_2 content leads to an increase in both the total gas velocity and mass flow through the turbine, which would affect deposition and evaporation rates.

Generalising the results, the expectation would be that the results would change unit by unit, OEM by OEM and site by site. Sites on the coastal areas will be more affected than those inland. In the same way units with higher firing temperatures are also likely to show higher condensation. On the other hand, some larger GTs would operate at higher pressure and cooler compressor bleeds which could, in turn, improve results.

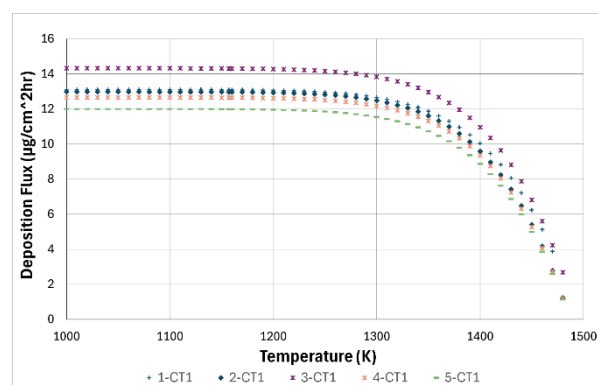
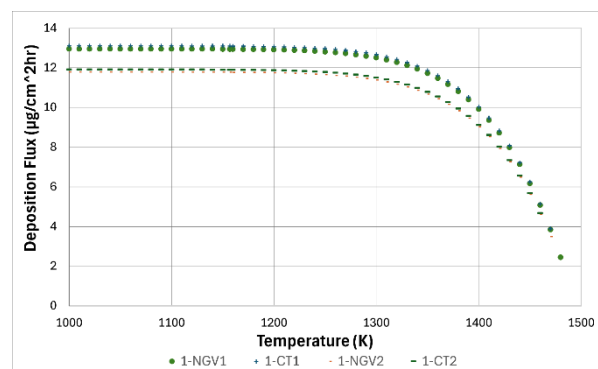


Figure 4 Flux of condensation, for scenario 1 to 5 of Na_2SO_4 of the compressor turbine stage 1 blades versus metal temperature.



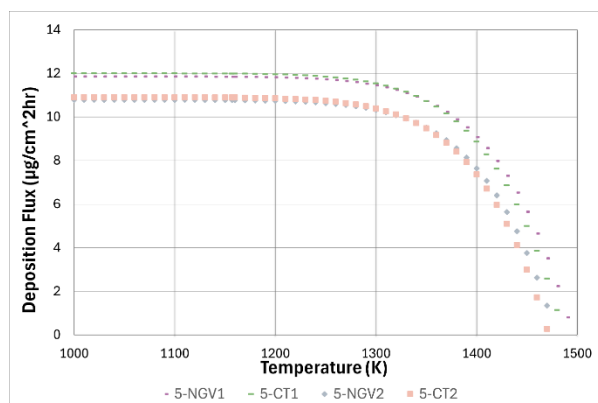


Figure 5 Flux of condensation, for scenario 1 and 5 of Na_2SO_4 across all blade and vanes in the compressor turbine versus metal temperature.

4 Conclusion

This work focused on calculating the deposition rates that could be experienced by GTs using H_2 as a fuel at different blending level (0% to 100%). The findings indicate that changing the hydrogen content in the fuel blend has a fundamental impact, resulting in higher water vapour in the exhaust emissions, and the amount of alkali vapours. These vapours are the ones responsible for high temperature corrosion of blading materials.

Furthermore, the work emphasises the need of sophisticated thermodynamic modelling methods, such as MTDATA, in forecasting phase behaviour and chemical reactions in the turbine environment. The MTDATA software predicted the presence of many condensed components that could lead to hot corrosion of the GTs blades and vanes. It was found the fluxes were highest on the NGV-1 and CT-1 components than the following stages NGV-2 and CT2. It was also found that the level of deposition was far higher for scenario 3 versus all other scenarios due to the criticality of this specific mix.

Ultimately, with the growing use of hydrogen-rich fuels in gas turbine operation, there is an urgent requirement for more accurate modelling and monitoring of combustion processes, namely in relation to the control of pollutants such as Na_2SO_4 . The results of this evaluation will contribute to the enhancement of design and operational approaches, therefore guaranteeing the efficient and dependable running of turbines while achieving rigorous emissions objectives. Subsequent investigations should prioritise the enhancement of the assumptions employed in modelling and the examination of the consequences of various cooling techniques and material selections to further alleviate the hazards linked to hydrogen mixing in gas turbines. The Acknowledgements, Fundings, Data availability statement, Author contribution statement, should be typed in 9-point Times, without title.

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2025-11-13

EDP Sciences

<https://doi.org/10.1051/e3sconf/202566301010>

White R, Potter A, Sumner J, Mori S. (2025) Bulk hydrogen production and the impact on turbomachinery lifing. In: E3S Web of Conferences, Volume 663, Article number 01010. 12th International Gas Turbine Conference: Advancing Turbomachinery Innovations and Strategies for Net-Zero Pathways (IGTC 2025), 14-15 October 2025, Brussels, Belgium