GT2014-25470

EVALUATION OF GASEOUS EMISSIONS FROM HYDROGEN COMBUSTION AIRCRAFT ENGINES

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ABSTRACT

From an engineering point of view, hydrogen is an interesting aircraft fuel. Compared to hydrocarbon fuels, the number of emission species that may occur is reduced, if pure hydrogen is considered as fuel. All emissions containing carbon atoms might be neglected. Thus, the well known relationships for emission indices, combustion efficiency as well as the dry air–fuel–ratio, especially the presented analytic equations, are no longer applicable. Hence, a new set of equations for hydrogen air combustion is derived in this paper, which has not yet been done according to the author's knowledge. This derivation is based on the basic definitions and assumptions from ARP1533B. Thus, the analysis strategy is very similar. As modern computational power is large enough to invert a small matrix in real time, the matrix method already described was chosen. This also has the advantage of incorporating interference effects easily. The emission analysis algorithm is validated by means of a generic test case. Furthermore, a statistically non–linear sensitivity analysis of the input parameters was carried out in order to quantify their measurement uncertainty as a propagated error on the output parameters. Additionally, some small mistakes and improvements, which attracted attention in ARP1533B, will also be mentioned within this paper.

NOMENCLATURE

AFR   Dry air–fuel–ratio, the ratio of the mass flows of dry air to fuel

EI Emission index, g emission/kg fuel

h Number of moles of water vapour per moles of dry air

h_{sd} Water vapour mole fraction, Number of moles of water vapour per number of moles in the semidry exhaust sample

M_{Air} Molar mass of dry air (default value = 28.965 g/mol)

M_H Atomic mass of hydrogen (default value = 1.008 g/mol)

M_{H_2O} Molar mass of water (default value = 18.0154 g/mol)

M_{NO_2} Molar mass of nitrogen dioxide (default value = 46.0055 g/mol)

M_{NO} Molar mass of nitric oxide (default value = 30.0061 g/mol)

n Number of moles

p Thermodynamic pressure

P_1 Number of moles of carbon dioxide in the exhaust sample per mole of fuel

P_2 Number of moles of nitrogen in the exhaust sample per mole of fuel

P_3 Number of moles of oxygen in the exhaust sample per mole of fuel

P_4 Number of moles of water vapour in the exhaust sample per mole of fuel

P_6	Number of moles of unburned hydrogen in the exhaust sample per mole of fuel
P_7	Number of moles of nitrogen dioxide in the exhaust sample per mole of fuel
P_8	Number of moles of nitric oxide in the exhaust sample per mole of fuel
P_T	Number of moles in the exhaust sample per mole of fuel
R	Mole fraction of oxygen in dry inlet air (default value = 0.20948)
S	Mole fraction of nitrogen (default value = 0.78084) plus mole fraction of argon (default value = 0.00934) in dry inlet air (default value = 0.79018)
T	Mole fraction of carbon dioxide in dry inlet air (default value = 0.00034)
X	Number of moles of dry air / one mole of fuel
$\mathcal{X}_{H_2O}$	Mole fraction of water vapour
Y_{H_2O}	Mass fraction of water vapour
y	Number of H atoms in the characteristic fuel molecule (default value = 2)
$[CO_2]$	Mole fraction of carbon dioxide in the exhaust sample
$[N_2]$	Mole fraction of nitrogen in the exhaust sample
$[O_2]$	Mole fraction of oxygen in the exhaust sample
$[H_2O]$	Mole fraction of water vapour in the exhaust sample
$[H_2]$	Mole fraction of unburned hydrogen in the exhaust sample
$[NO_2]$	Mole fraction of nitrogen dioxide in the exhaust sample
$[NO_x]$	Mole fraction of oxides of nitrogen in the exhaust sample
$[NO]$	Mole fraction of nitric oxide in the exhaust sample
L'	Interference coefficient effect of CO_2 on the measurement of NO and NO_x (concentration factor effect)
L''	Interference coefficient effect of CO_2 on the measurement of O_2 (zero shift)
M'	Interference coefficient effect of H_2O on the measurement of NO and NO_x (concentration factor effect)
M''	Interference coefficient effect of H_2O on the measurement of O_2 (zero shift)
N'	Interference coefficient effect of NO on the measurement of O_2 (zero shift)
N''	Interference coefficient effect of NO_2 on the measurement of O_2 (zero shift)
$\eta_{NO_x,Conv.}$	Efficiency of NO_2/NO converter
η_b	Combustion efficiency
μ	Measured mean value
σ	Standard deviation, as the percental full scale uncertainty times the used full scale

Indices

w	Wet concentrations, with the complete number of water vapour moles
sd	Semidry concentrations, where a part of the water vapour was removed from the exhaust sample
dry	Dry concentrations, where the complete water vapour was removed from the exhaust sample
dp	Dew point
0	Inlet conditions
i	Species i
abs	Absolute number of moles in a sample
$fuel$	Fuel species
ref	Reference value

INTRODUCTION

Up to now, pure hydrogen is not yet intended to serve as aircraft engine fuel by the ICAO. Thus, an aircraft engine certification with hydrogen as fuel would not be possible under the current ICAO rules. The required procedures of sampling and measurement as well as analysis and evaluation of gaseous emissions from aircraft engines are well defined in ARP1256D [1] and ARP1533B [2] respectively, which eventually emerge into the ICAO Annex 16 Volume II [3] rules for the certification of aircraft engines. However, the derived relationships to compute emission indices, combustion efficiency as well as the dry air–fuel–ratio, especially the analytic equations presented, apply only to hydrocarbon fuels. The number of emission species, which may occur, is reduced, if pure hydrogen is considered as aircraft engine fuel. All emissions containing carbon atoms can be neglected. Thereby, the solution matrix of hydrocarbon fuels becomes singular for pure hydrogen and can no longer be inverted. Therefore, a new set of equations is derived in this paper for hydrogen air combustion. This derivation is based on the basic definitions and assumptions from ARP1533B. Hence, the analysis strategy is very similar. Nevertheless, the analysis algorithm is based on other measured emissions, like O_2 and H_2 but also on NO and NO_x concentrations. Additionally, two different water vapour mole fractions, h and h_{sd}, are needed, exactly as in ARP1533B. Analytical equations for the emission parameters, which may need further assumptions, were not derived. Instead, the solution matrix is inverted directly each time. This is no longer a problem nowadays, as this can be done in real time because of sufficiently large computational power. Emission indices are widely used to characterise aircraft engine emissions, whereas for heavy duty gas turbines, mainly emission mole fractions on a dry basis are used, which are further corrected to a reference oxygen concentration. It is also possible to compute such corrected emissions with the solution vector of the matrix, which is provided by the

proposed analysis. Additionally, a connection between the emission indices and the corrected emission values at dry conditions is also depicted.

MEASUREMENT EQUIPMENT

In order to determine of the exhaust gas emissions of hydrogen burning aircraft engines, the following measurement equipment is suggested.

Oxides of nitrogen

The requirements for the oxides of nitrogen analyser are already described in [1, Chap. 5.3] for hydrocarbon fuels. This system is based on a chemiluminescent detector (CLD) and can also be used without any further limitations for hydrogen fuel. In order to also detect nitrogen dioxide (NO_2) by means of the CLD method, the NO_2 has to be first reduced to nitric oxide (NO). The efficiency of this converter affects the emission values. Thus, the determination of the NO_x converter efficiency is described in [1, Chap. 6.2.5]. The described equipment is rather complex and there is some uncertainty on how the variable ozone generation affects the converter efficiency. Hence, it is suggested to use certified nitrogen dioxide calibration gas similar to the nitric oxide calibration gas, which is used for the daily calibration of the CLD. The converter efficiency can then be calculated with the following equation:

$$\eta_{NO_x,Conv.} = \frac{[NO_{x,Meas.}]}{[NO_{2,Cal.}]} 100 \ \% \qquad (1)$$

If the NO_2 calibration gas is free of NO only the NO_x channel of the CLD should detect any emission, whereas the corresponding NO channel should not detect anything. The drawback of this approach is that another bottle of calibration gas has to be acquired.

Water vapour

An optical dew point hygrometer is used to determine the dew point temperature in the inlet as well as after a possible sample drying of the exhaust gases as described in [1, Chap. 5.4]. Additionally to the dew point temperature measurement, the absolute pressure has to be measured in both cases at the same position. This can be accomplished with any standard pressure transducer.

Oxygen

Oxygen has a high paramagnetic susceptibility at temperatures below 300°C. This effect could be used for determining the oxygen concentration. The exhaust gas flows through a dumb bell in a magnetic field. Due to the paramagnetic susceptibility of oxygen, the dumb bell is deviated. This deviation is proportional to the oxygen volume concentration and can be measured with a magnetic torsion balance.
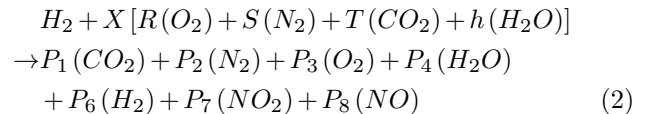
Hydrogen

The hydrogen concentration measurement is based on the Electron Impact Ionisation Mass Spectroscopy (EIMS) principle. By using the electron ion source, the gas sample ions are energised, focused and separated further on in a magnetic field, in order to detect hydrogen. The analysis is performed on a cold and dry exhaust gas. The typical measurement uncertainty of such a system is no more than 2 % of the measured value. The water vapour interference effect of 20 Vol.% H_2O is in general smaller than the zero drift (0.5 ppm) and the detection limit (1 ppm).

MATHEMATICAL DESCRIPTION
Chemical equation

The overall chemical reaction for one mole of hydrogen with air is defined as:

$$H_2 + X\left[R\left(O_2\right) + S\left(N_2\right) + T\left(CO_2\right) + h\left(H_2O\right)\right]$$
$$\rightarrow P_1\left(CO_2\right) + P_2\left(N_2\right) + P_3\left(O_2\right) + P_4\left(H_2O\right)$$
$$+ P_6\left(H_2\right) + P_7\left(NO_2\right) + P_8\left(NO\right) \qquad (2)$$

where $P_1 - P_4$ and $P_6 - P_8$ are the mole fractions of each exhaust gas constituent per one mole of fuel. Exhaust gas constituents other than N_2, O_2, H_2O, H_2, CO_2, NO_2, and NO are neglected. This includes carbon monoxide as well as sulphur dioxide, because CO_2 is considered as an inert species and SO_2 can only arise from fuels containing sulphur, which is not given in this case. In order to have the same numbering for the mole fractions P_i than in [2], the corresponding $P_5\left(CO\right)$ and $P_9\left(SO_2\right)$ mole fractions are omitted. Noble gases are not participating during the reaction. Thus, this overall reaction adds all noble gases to the nitrogen content of 79.018 Vol.% for dry inlet air.

Basic Equations

Eight independent relations are needed in order to solve for the eight unknowns, X, $P_1 - P_4$ and $P_6 - P_8$, in Eqn. (2). For the sake of simplicity, the assignment of the constituents to the per fuel mole fractions is neglected hereafter in this paper. Furthermore, the total mole fraction as total number

of moles of product per mole fuel is defined as:

$$P_T = P_1 + P_2 + P_3 + P_4 + P_6 + P_7 + P_8 \qquad (3)$$

Based on the definition of the mole fractions P_i and P_T, the following relationships for wet concentrations of exhaust gas constituents can be obtained with the number of moles for each species:

$$[\chi_i] = \frac{n_i}{n_{abs}} = \frac{n_i}{n_{fuel}} \frac{n_{fuel}}{n_{abs}} = \frac{n_i}{n_{fuel}} \frac{1}{\frac{n_{abs}}{n_{fuel}}} = \frac{P_i}{P_T} \qquad (4)$$

Moles of carbon dioxide:

$$P_1 = P_T [CO_2]_w \qquad (5)$$

Moles of oxygen:

$$P_3 = P_T [O_2]_w \qquad (6)$$

Moles of water:

$$P_4 = P_T [H_2O]_w \qquad (7)$$

Moles of hydrogen:

$$P_6 = P_T [H_2]_w \qquad (8)$$

Moles of the oxides of nitrogen:

$$P_7 + P_8 = P_T [NO_x]_w \qquad (9)$$

Moles of nitric oxide:

$$P_8 = P_T [NO]_w \qquad (10)$$

Additionally the balances for the four different atoms are used:
Carbon balance:

$$TX = P_1 \qquad (11)$$

Hydrogen balance:

$$2 + 2hX = 2P_4 + 2P_6 \qquad (12)$$

Oxygen balance:

$$(2R + 2T + h)X = 2P_1 + 2P_3 + P_4 + 2P_7 + P_8 \qquad (13)$$

Nitrogen balance:

$$2SX = 2P_2 + P_7 + P_8 \qquad (14)$$

Sample Drying

The measurement of some exhaust constituents has to be performed under semidry conditions. In the case of hydrogen air combustion this is the measurement of hydrogen and oxygen, but also CO_2 and CO are commonly measured semidry. According to ARP1533B [2, Chap. 5.2.3], it is assumed that only pure water is removed from the exhaust gas during the cooling in the dryer before entering the analysers. Thus, the massflow of all other gas constituents remains constant, except for water. But as the total mole number is changing due to water removal, the mole fractions, and thus the concentrations, are also changing. The washing out of other constituents, such as oxides of nitrogen or unburned hydrocarbon, is neglected during the computation of semidry concentrations. Thus, the semidry total mole fraction $P_{T,sd}$ is defined as follows:

$$\begin{aligned} P_{T,sd} &= P_1 + P_2 + P_3 + P_{4,sd} + P_6 + P_7 + P_8 \\ &= P_T - P_4 + P_{4,sd} \end{aligned} \qquad (15)$$

The water content of the sample after the dryer is defined as water concentration according to the ARP1533B [2, Eq. 26]

$$h_{sd} = [H_2O]_{sd} = \frac{P_{4,sd}}{P_T - P_4 + P_{4,sd}} = \frac{P_{4,sd}}{P_{T,sd}} \qquad (16)$$

Without assuming that $P_{4,sd}$ is small, the following mathematical correct derivation can be made from Eqn. (16):

$$\begin{aligned} P_{4,sd} &= h_{sd} \left(P_T - P_4 + P_{4,sd} \right) \\ P_{4,sd}(1 - h_{sd}) &= h_{sd} \left(P_T - P_4 \right) \\ P_{4,sd} &= (P_T - P_4) \frac{h_{sd}}{1 - h_{sd}} \end{aligned} \qquad (17)$$

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Inserting Eqn. (17) into Eqn. (15) gives the following relationship:

$$P_{T,sd} = P_T - P_4 + P_{4,sd} = (P_T - P_4) + (P_T - P_4) \frac{h_{sd}}{1 - h_{sd}}$$

$$= (P_T - P_4) \left(1 + \frac{h_{sd}}{1 - h_{sd}}\right)$$

$$= (P_T - P_4) \left(\frac{1 - h_{sd}}{1 - h_{sd}} + \frac{h_{sd}}{1 - h_{sd}}\right)$$

$$= (P_T - P_4) \frac{1}{1 - h_{sd}} \qquad (18)$$

This approach might also be used in ARP1533B for the evaluation of hydrocarbon emissions. With Eqn. (18) the mole fractions of the gas constituents on a semidry basis are defined in the same way as for the wet concentrations in Eqn. (4). This gives for carbon dioxide:

$$[CO_2]_{sd} = \frac{P_1}{P_{T,sd}} = \frac{P_1}{P_T - P_4 + P_{4,sd}} = \frac{P_1}{P_T - P_4} (1 - h_{sd}) \qquad (19)$$

This is the corresponding definition to [2, Eq. 28], but mathematically correct. Additionally, it gives the correct linear behaviour if removing water from the sample. It can also be used instead of the one given in ARP1533B, even if the difference between the two definitions is for very small h_{sd} values also small. The semidry oxygen concentration is:

$$[O_2]_{sd} = \frac{P_3}{P_{T,sd}} = \frac{P_3}{P_T - P_4} (1 - h_{sd}) \qquad (20)$$

The semidry hydrogen concentration is given as:

$$[H_2]_{sd} = \frac{P_6}{P_{T,sd}} = \frac{P_6}{P_T - P_4} (1 - h_{sd}) \qquad (21)$$

Additionally, the NO and NO_x concentrations may also be defined on a semidry basis in the same mathematically correct manner.

$$[NO]_{sd} = \frac{P_8}{P_{T,sd}} = \frac{P_8}{P_T - P_4} (1 - h_{sd}) \qquad (22)$$

$$[NO_x]_{sd} = \frac{P_7 + P_8}{P_{T,sd}} = \frac{P_7 + P_8}{P_T - P_4} (1 - h_{sd}) \qquad (23)$$

Furthermore, if h_{sd} is equal to zero, Eqn. (19) to Eqn. (23) recover the definition of dry concentrations as in [2, Eq. 39,

41, 43, 44, 45]. With Eqn. (4) the definition of h_{sd} from Eqn. (16) can be rewritten as an ordinary mole fraction. This mole fraction is further related to the partial pressure in the case of ideal gas behaviour according to Dalton's law in the following way:

$$h_{sd} = \frac{P_{4,sd}}{P_{T,sd}} = \frac{n_{H_2O}}{n_{abs}} = \frac{p_{H_2O}}{p_{abs}} \qquad (24)$$

Contrary to the definition of the water content of the semidry sample gas in Eqn. (24), the water content of the inlet air ("humidity"), h, is specified as number of moles water vapour per number of moles dry air, as X is also defined as number of moles dry air per mole fuel. Again with Dalton's law, this results in the following definition with the partial water pressure:

$$h = \frac{n_{H_2O}}{n_{abs} - n_{H_2O}} = \frac{p_{H_2O}}{p_{abs} - p_{H_2O}} \qquad (25)$$

The same definition is also expressed in [2, Eq. B7], but in ppm. As h_{sd} is a mole fraction expressed with the total mole number, the correct definition from Eqn. (24) should be used instead of [2, Eq. B7]. Nevertheless the partial water pressure might be computed from the dew point temperature and the saturation pressure, with all the assumptions as described in the original publication of Hardy [4], as explained in [2, App. B] or [4] for both definitions of "humidity". Additionally, just a remark, the factor $g6$ in the first table of [2, App. B] has a wrong prefix according to the original publication of Hardy [4].

Interference effects

ARP1533B made a distinction between the "zero shift" and "concentration factor" interference effect. For the EIMS system there is only one negligible interference effect for water steam, as already described above. In general, the paramagnetic oxygen sensor has a zero shift effect to different gas components. L'', M'', N', and N'' are the interference coefficients for the paramagnetic oxygen sensor. The given numbers are only indicative and may not be representative for present systems:

$L'' = -0.0028$, mole O_2 per mole CO_2
$M'' = -0.0005$, mole O_2 per mole H_2O
$N' = +0.43$, mole O_2 per mole NO
$N'' = +0.19$, mole O_2 per mole NO_2

It is obvious that especially the oxides of nitrogen can cause a significant zero shift to the measured oxygen value. As carbon monoxide was already neglected in Eqn. (2), it will also be omitted for the interference effects in the case of

hydrogen combustion. In order to correct the O_2 measurement, the interference coefficients are incorporated into Eqn. (6):

$$P_3 = P_T [O_2]_w + L'' P_1 + M'' P_4 + N'' P_7 + N' P_8 \qquad (26)$$

The corrections have to be made with the concentrations which are present during the measurement of the exhaust gas emission. That means if the oxygen is measured at semidry conditions, also the semidry water concentration has to be used in order to correct the oxygen concentration. Furthermore, the same assumption applies during sample drying, which means that only pure water is removed during the cooling of the sample gas, and the massflow of the oxides of nitrogen as well as the unburned hydrogen remain constant. For a semidry oxygen measurement, the interference coefficients are incorporated into Eqn. (20). Additionally, Eqn. (17) is used in order to eliminate $P_{4,sd}$, which results in:

$$
\begin{aligned}
P_3 &= [O_2]_{sd}(P_T - P_4)\frac{1}{(1 - h_{sd})} + L'' P_1 + M'' P_{4,sd} \\
&\quad + N'' P_7 + N' P_8 \\
&= [O_2]_{sd}(P_T - P_4)\frac{1}{(1 - h_{sd})} + M''(P_T - P_4)\frac{h_{sd}}{1 - h_{sd}} \\
&\quad + L'' P_1 + N'' P_7 + N' P_8 \\
&= \left([O_2]_{sd} + M'' h_{sd}\right)\frac{(P_T - P_4)}{(1 - h_{sd})} + L'' P_1 + N'' P_7 + N' P_8 \;(27)
\end{aligned}
$$

The derivation of the interference effects of the NO_x and NO measurements was already done in ARP1533B [2, Eq. 25, 20] and are given here just for the sake of completeness. Furthermore, the efficiency of the NO_2 converter is already incorporated into the NO_x equation, which results in:

$$[NO_x]_w P_T + L'[NO_x]_w P_1 + M'[NO_x]_w P_4 - \eta P_7 - P_8 = 0 \qquad (28)$$

The NO equation corresponds to:

$$[NO]_w P_T + L'[NO]_w P_1 + M'[NO]_w P_4 - P_8 = 0 \qquad (29)$$

As the oxides of nitrogen are measured on a hot and wet basis, the derivation of the mathematically correct semidry formulation is omitted here. Nevertheless, this can be achieved with the help of Eqn. (22) and Eqn. (23) in the same way as with the derivation of the oxygen formulation. The interference coefficients are also taken from ARP1533B

as:
$L' = 0.14$, percent of reading of NO per percent CO_2 (concentration factor effect)
$M' = 0.28$, percent of reading of NO per percent H_2O (concentration factor effect)

Matrix Solution

In order to solve for the unknowns, the nine linear independent equations are written in matrix form. It is assumed that the oxygen concentration is measured as semidry, while the NO and NO_x concentrations are available on a wet basis. Furthermore, the dew point temperature as well as the absolute pressure at the inlet and after the exhaust gas cooler are measured. Thus, the following equations are used, in order to set up the matrix: Eqn. (11)-Eqn. (14), Eqn. (27), Eqn. (21), Eqn. (28), Eqn. (29) and Eqn. (3). The first six equations are rearranged for a better overview:

$$P_1 - TX = 0 \qquad (30)$$

$$2P_4 + 2P_6 - 2hX = 2 \qquad (31)$$

$$2P_1 + 2P_3 + P_4 + 2P_7 + P_8 - (2R + 2T + h)X = 0 \qquad (32)$$

$$2P_2 + P_7 + P_8 - 2SX = 0 \qquad (33)$$

$$
\begin{aligned}
&\left([O_2]_{sd} + M'' h_{sd}\right) P_T + L''(1 - h_{sd}) P_1 - (1 - h_{sd}) P_3 \\
&- \left([O_2]_{sd} + M'' h_{sd}\right) P_4 + N''(1 - h_{sd}) P_7 \\
&+ N'(1 - h_{sd}) P_8 = 0 \qquad (34)
\end{aligned}
$$

$$[H_2]_{sd} P_T - [H_2]_{sd} P_4 - (1 - h_{sd}) P_6 = 0 \qquad (35)$$

If all coefficients can be written into a matrix, as shown in Tab. 1, the matrix can be solved numerically with every common linear algebra package. Within this work, the linear algebra module, which is shipped with the *numpy* python package, was used.

In case, the NO and NO_x concentrations were also measured on a semidry basis, Eqn. (22) and Eqn. (23) have

TABLE 1. Matrix

Eq.	P_T	P_1	P_2	P_3	P_4	P_6	P_7	P_8	X	b
30	0	1	0	0	0	0	0	0	$-T$	0
31	0	0	0	0	2	2	0	0	$-2h$	2
32	0	2	0	2	1	0	2	1	$-(2R+2T+h)$	0
33	0	0	2	0	0	0	1	1	$-2S$	0
34	$\left([O_2]_{sd}+M''h_{sd}\right)$	$L''(1-h_{sd})$	0	$-(1-h_{sd})$	$-\left([O_2]_{sd}+M''h_{sd}\right)$	0	$N''(1-h_{sd})$	$N'(1-h_{sd})$	0	0
35	$[H_2]_{sd}$	0	0	0	$-[H_2]_{sd}$	$-(1-h_{sd})$	0	0	0	0
28	$[NO_x]_w$	$L'[NO_x]_w$	0	0	$M'[NO_x]_w$	0	$-\eta$	-1	0	0
29	$[NO]_w$	$L'[NO]_w$	0	0	$M'[NO]_w$	0	0	-1	0	0
3	-1	1	1	1	1	1	1	1	0	0

to be used instead of Eqn. (28) and Eqn. (29). Depending on the measurement system, additional interference factors might also be further applied to Eqn. (22) and Eqn. (23). On the contrary, if all concentrations are known on a wet basis like within CFD results, Eqn. (6), Eqn. (8), Eqn. (9) and Eqn. (10) can be used directly for the matrix preparation without any further assumptions or interference corrections. As the solution of that matrix also includes the water concentration, this might be an additional verification value beside the AFR for CFD results.

Emission Parameters

Once the P vector is computed, other emission parameters can be obtained in the same way as for hydrocarbon fuels. The dry Air–Fuel–Ratio might be computed in the same way as in ARP1533B [2, Eq. 46], but with zero carbon atoms

$$AFR = \frac{X M_{Air}}{2 M_H} \qquad (36)$$

The emission indices for NO and NO_x are defined in the same manner as in ARP1533B [2, Eq. 49, 50]. Thus, the NO_x emission index for hydrogen as fuel reduces to

$$EI_{NO_x} = \frac{(P_7 + P_8) M_{NO_2} 10^3}{2 M_H} \qquad (37)$$

and the NO emission index for hydrogen fuel is

$$EI_{NO} = \frac{P_8 M_{NO} 10^3}{2 M_H} \qquad (38)$$

The emission index for hydrogen can be derived from the definition of the unburned hydrocarbon EI, but again with zero carbon atoms

$$EI_{H_2} = \frac{P_6 M_{H_y} 10^3}{y M_H} \overset{y=2}{=} \frac{P_6 M_{H_2} 10^3}{2 M_H} = P_6 10^3 \qquad (39)$$

In ARP1533B the combustion efficiency is calculated on an enthalpy basis. The inefficiencies due to unburned hydrocarbon and carbon monoxide are subtracted from 100 %. Thus, negative effects from NO_x, H_2 and dissociation of combustion products are neglected. In the case of purely hydrogen combustion, this would lead to a combustion efficiency of 100 % per definition. Therefore, the combustion efficiency can be computed based solely on hydrogen concentrations with the emission index from Eqn. (39) as follows

$$\eta_b = 100 - 0.1 EI_{H_2} = 100 - 100 P_6 = (1 - P_6) 100 \qquad (40)$$

Alternatively to the NO_x emission indices, the NO_x emission might also be corrected to a reference oxygen concentration $O_{2,ref}$ under dry conditions. As already mentioned, if h_{sd} is equal to zero, dry concentrations of O_2 and NO_x can be obtained with Eqn. (20) and Eqn. (23) respectively. Thus, the corrected oxides of nitrogen emissions can be computed

$$NO_{x,c} = NO_{x,dry} \frac{20.948 - O_{2,ref}}{20.948 - O_{2,dry}} \qquad (41)$$

If EI_{NO_x} from Eqn. (37) is used for the computation of the dry NO_x emissions in Eqn. (23), the corrected $NO_{x,c}$ concentration might be directly linked to the emission index. But it is important to note that the conversion depends on the water as well as the oxygen concentrations in the exhaust gas. As these two concentrations depend mainly on the excess air ratio, the conversion factor is not constant. Consequently, the conversion from emission index to corrected emission concentrations is not linear.

Sensitivity Analysis

In order to solve the matrix in Tab. 1 eight values have to be measured. These include the concentrations of NO, NO_x, O_2 and H_2. Furthermore, to be able to compute the water vapour mole fractions h and h_{sd} the corresponding dew point temperatures $T_{dp,0}$, $T_{dp,sd}$ and absolute pressures p_0, p_{sd} are needed.

All eight measurement values are afflicted with some uncertainties. In order to quantify the propagated error of these uncertainties to the emission parameters (EI, AFR, etc.), Heneghan et al. proposed a statistical sensitivity analysis. This method, which also takes non–linear effects into account, contrary to the first order differentiation of analytical emission equations, is described in detail elsewhere [5]. Within this paper, just a short summary is given. The measured value is added with some "noise". This "noisy" variable is computed with the following equation

$$\phi = \text{norminv}\left(\text{RAND}\left(\right), \mu, \sigma\right) \tag{42}$$

For the norminv function, the implementation from [6] was used in this paper. Additionally, RAND() is a random number between zero and one and μ is the measured mean value. Whereas the standard deviation σ is computed as the percental full scale uncertainty times the used full scale. A set of N "noisy" emission parameters is computed based on N "noisy" input parameters from Eqn. (42). The propagated error due to the measurement uncertainties is determined as the normalised standard deviation from the vector of N computed emission parameters.

GENERIC TEST CASE

In order to validate the proposed emission analysis, a comprehensible chemical equilibrium computation of a hydrogen air combustion was done with the GRI3.0 mechanism in Cantera [7]. The chemical equilibrium is the thermodynamic limit, which is only reached if the residence time of the gas mixture within the thermodynamic system approaches infinity. The NO_x emissions will reach their maximum at chemical equilibrium and will thus be much higher when compared to actual combustion chambers with a finite residence time. The initial conditions are an excess air ratio of two, inlet temperature of 400 K and inlet pressure of 219000 Pa. The mass specific inlet water concentration is $h_m = 0.00634 \frac{kg_{H_2O}}{kg_{\text{dry air}}}$ as specified by the ICAO standard [3, p. III-2-2]. This mass fraction has to be converted into a mole fraction:

$$Y_{H_2O} = \frac{\dot{m}_{H_2O}}{\dot{m}_{abs}} = \frac{h_m}{1 - h_m} = 0.0063805 \tag{43}$$

$$M_{Air,w} = \frac{1}{\frac{Y_{H_2O}}{M_{H_2O}} + \frac{1 - Y_{H_2O}}{M_{Air}}} = 28.855 \frac{g}{mol} \tag{44}$$

$$\mathcal{X}_{H_2O} = Y_{H_2O} \frac{M_{Air,w}}{M_{H2O}} = 0.010219 \tag{45}$$

$$h = \frac{\mathcal{X}_{H_2O}}{1 - \mathcal{X}_{H_2O}} = 0.010325 \frac{\text{moles water vapour}}{\text{moles dry air}} \tag{46}$$

All concentrations of this chemical equilibrium computation are on a wet basis. The semidry concentrations are calculated based on the wet concentrations with Eqn. (20) and Eqn. (21). Therefore, the semidry water vapour concentration h_{sd} is calculated with the assumed semidry dew point temperature ($T_{dp,sd} = 278.15$ K) and corresponding absolute pressure ($p_{sd} = 97600$ Pa), which results in the semidry water vapour mole fraction as defined in Eqn. (16). With that conversion, the mole fractions used for the test case are:

$$NO_w = 2022 \text{ ppm}$$
$$NO_{x,w} = 2028 \text{ ppm}$$
$$h_{sd} = 8973 \text{ ppm}$$
$$O_{2,sd} = 11.485 \text{ \%}$$
$$H_{2,sd} = 13.59 \text{ ppm}$$
$$H_2O_w = 19.1415 \text{ \%}$$

The emission matrix as shown in Tab. 1 was solved in order to compute the output emission parameters. The NO_x converter efficiency was assumed to be 100 %. Additionally, as the hydrogen concentration is very small, their influence on the emission parameters was evaluated. Therefore, the hydrogen concentration was set to zero in a second run. The emission results are presented in Tab. 2.

TABLE 2. Emission Results

	$H_2 = H_{2,sd}$	$H_2 = 0$
AFR	69.168	69.171
$EI_{NO_x} \left[\frac{g}{kg_{fuel}}\right]$	261.836	261.845
$NO_{x,dry}$ @ 15% O_2 [ppm]	1696.942	1696.954
$EI_{H_2} \left[\frac{g}{kg_{fuel}}\right]$	0.059157	0
η_b [%]	99.994	100

The hydrogen concentration mainly affects the combustion efficiency as well as the EI_{H_2}. As the hydrogen in the exhaust is usually very low, the combustion efficiency is nearly 100 %. This has been already reported by Marek et al. [8]. Furthermore, the unburned hydrogen emissions have almost no effect on NO_x emissions. Hence, the measurement of unburned hydrogen might be neglected. A hydrogen air mixture with an excess air ratio of two has an AFR=68.4. The deviation of the emission analysis to that value is in the order of 1 %. The calculated AFR is a good value to verify the analysis if air and fuel massflows are known from additional measurements. As the input emissions are treated as measured values, the interference effects were also taken into account. Thus, the output emissions from the P vector are not able to capture the wet input emissions.

Dew point temperature and pressure uncertainties

In order to quantify the measurement uncertainty of the dew point temperature and the related absolute pressure, a sensitivity study as described above is examined. The relative error for the dew point temperature and the absolute pressure is set to $\Delta T_{dp} = 0.4\ K$ and $\Delta p = 5000\ Pa$ respectively. For each of the four measured values, 10000 individual samples were computed and the propagated errors to the emission parameters evaluated. Furthermore, the influence of the hydrogen measurement was determined again with a second set of variations, whereas hydrogen emissions were set again to zero. For these two cases, the propagated error for EI_{NO_x} is shown in Fig. 1. The uncertainties computed with the same relative error have a larger effect on the EI_{NO_x} error at the inlet than the semidry uncertainties. Nevertheless, both propagated errors due to the dew
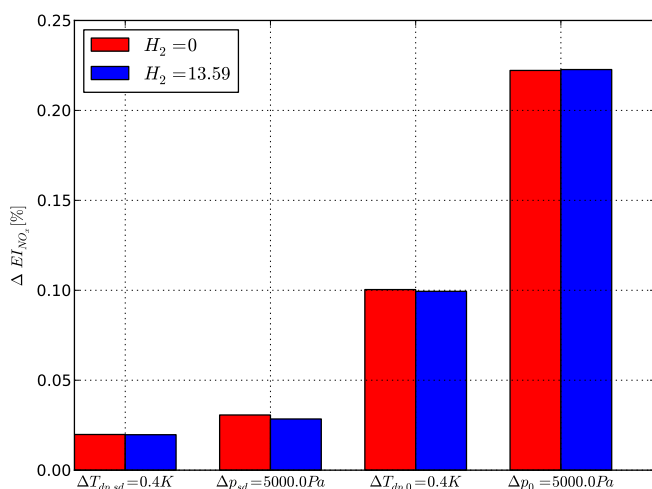

FIGURE 1. Propagated Error EI_{NO_x}

point measurements are small. The uncertainty caused by the semidry water concentration to the EI_{NO_x} is only due to the water vapour interference effect of the CLD analyser. In Fig. 2 the propagated errors of the AFR are shown. The
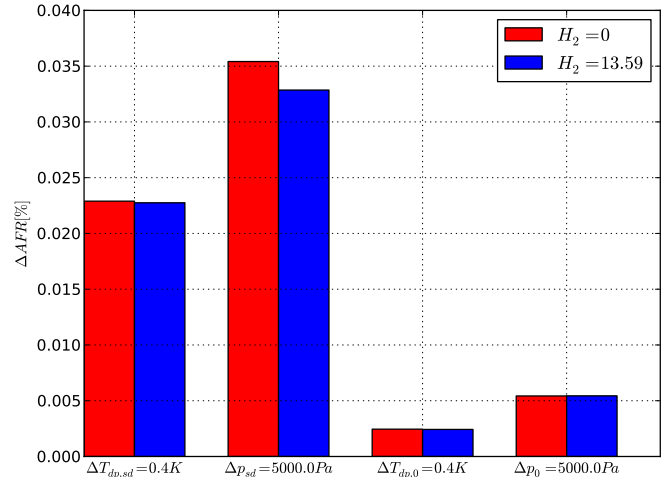

FIGURE 2. Propagated Error AFR

influence of the dew point measurements on the AFR are contrary to that of the EI_{NO_x}. In the case of the AFR, the semidry uncertainties are more pronounced. This might be due to the fact that the AFR is mainly based on the O_2 measurement, which is done with semidry exhaust gas. Nevertheless, the absolute propagated error of the AFR is even an order smaller than the EI_{NO_x} error. In both cases, EI_{NO_x} and AFR, the hydrogen content has only had a negligible effect on the propagated error. Furthermore, the influence on the combustion efficiency is almost not measurable and below $\Delta \eta_b = 4E-6$ %. Whereas the influence on the EI_{H_2} is also very small and roughly $\Delta EI_{H_2} = 0.06$ %.

**Extremum dew point water vapour concentrations**

As already shown, the propagated error due to the semidry dew point measurement was below 0.035 % for all emission parameters. This might be due to the fact that the water mole fraction rises exponentially with the dew point temperature as shown in Fig. 3. For dew point temperatures below 10°C, the water concentration for ambient conditions is very small, thus an even smaller variation of the measured value might not lead to an larger propagated error.

Thus, the maximum possible error is evaluated for two cases. In the first case the difference between the corresponding $h_{sd} = 8973$ ppm and the extreme case of perfectly dry exhaust gas with $h_{sd} = 0$ ppm is evaluated. This case

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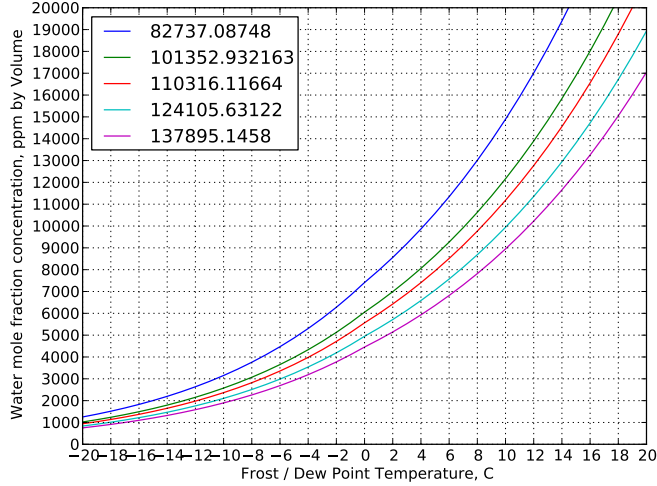
FIGURE 3. Water mole fraction versus dew point temperature with absolute pressure in Pascal as an additional parameter

might occur if the flue gas is extremely diluted in such a way that there is no water condensation within the gas cooler. Hence, the temperature of the gas cooler is no longer equivalent to the dew point temperature. In the second case, the upper limit of the water mole concentration was assumed to be $h_{sd} = 10000$ ppm. This effect may occur if the exhaust gas massflow through the gas cooler or the inlet temperature of the gas cooler are too high. Again, the influence of the hydrogen measurement was also considered. In that case the influence of the extremum water concentrations are almost the same for EI_{NO_x} and AFR, in terms of relative behaviour as well as absolute values. Thus, only the results for EI_{NO_x} are presented in Fig. 4.
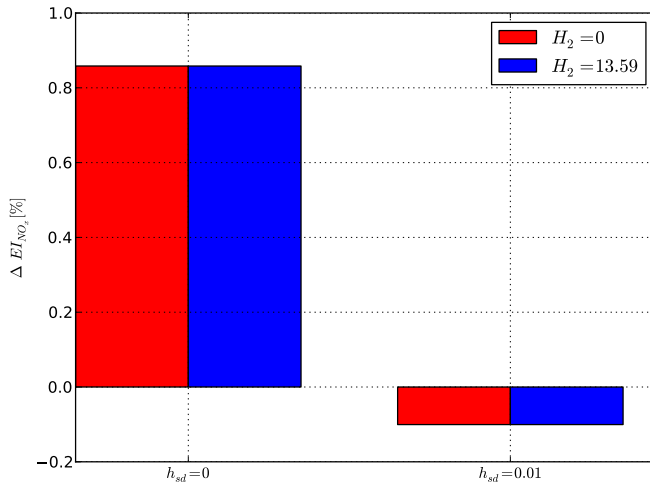
FIGURE 4. Extremum difference EI_{NO_x}

Even in the solely theoretical event that the exhaust gas would be perfectly dry, the maximum error is below 1 % for both EI_{NO_x} and AFR. Moreover, if the semidry water concentration is larger, the error norm is in both cases lower than 0.1 %. And again the hydrogen measurement has an negligible effect on the EI_{NO_x} and AFR errors. The influence on combustion efficiency is almost not measurable and below 1.2E-4 %. If the unburned hydrogen is measured, the EI_{H_2} error due to the h_{sd} discrepancy is roughly 2.0 %.

Oxygen concentration uncertainty

The propagated error due to the uncertainty at the oxygen measurement is evaluated using the sensitivity analysis. Again, 10000 individual samples were considered, in order to be statistically independent. For the O_2 measurement a 3 % relative error on a full scale of 25 Vol.% was assumed. This gives a standard deviation of 0.75 Vol.% O_2. Also, the influence of the hydrogen measurement was taken into account again. The results of the propagated errors are summarised in Tab. 3.

TABLE 3. Oxygen concentration uncertainties

	$H_2 = H_{2,sd}$	$H_2 = 0$
ΔAFR [%]	7.56	7.47
ΔEI_{NO_x} [%]	6.56	6.48
$\Delta NO_{x,dry}$ @ 15% O_2 [%]	6.50	6.42
ΔEI_{H_2} [%]	8.43	-
$\Delta \eta_b$ [%]	4.94	-

The propagated error due to the uncertainty at the oxygen measurement is very high for all emission parameters. For that test case, the variation is between 4.94 % and 8.43 %. The influence of the hydrogen measurement is again negligible. Thus, the measurement accuracy of the oxygen concentrations are the most crucial point for the analysis of hydrogen exhaust gases, due to their larger influence on the emission parameters compared to other measured values.

Oxides of nitrogen and carbon dioxide concentration uncertainty

For the nitric oxide as well as the oxides of nitrogen concentration, a relative error of 1 % of the measured value was assumed. In order to avoid unphysical behaviour, randomly generated NO values larger than the fixed NO_x value or vice versa, and randomly generated NO_x values smaller than the fixed NO value, are neglected during this call of

the sensitivity study, and a new value for either nitric oxide or the oxides of nitrogen is randomly generated. The propagated error of the NO_x measurement is for this test case: $\Delta EI_{NO_x} = 0.685$ % and $\Delta NO_{x,dry}@15\%O_2 = 0.666$ %, whereas the influence on AFR, EI_{H_2} and η_b is up to five orders smaller and thus can be neglected. Additionally, the propagated error of the NO measurement is at least three orders smaller than the corresponding NO_x measurement uncertainty. Hence, the NO measurement uncertainty can also be neglected. The same holds true also for the CO_2 concentration of the inlet air. Therefore, setting a constant value for the CO_2 concentration is justified. Furthermore, the influence of the hydrogen measurement is again negligible in all cases.

CONCLUSION

As the number of emission species is reduced for hydrogen fuel, the evaluation of gaseous emissions of aircraft engines has also to be adapted. Thus, new relationships for emission indices, the combustion efficiency as well as the dry air–fuel–ratio have been derived in this paper. Therefore, a new mathematical model for the analysis of gaseous emissions as well as the main features of a sensitivity study are presented. Both were employed within a generic test case based on a chemical equilibrium computation. With the help of the sensitivity study, the propagated errors of several measurement uncertainties were examined.

It was able to be shown that the measurement uncertainty of the oxygen concentrations has the highest propagated error and is therefore the most crucial point during a measurement campaign. By contrast, the propagated error of the semidry dew point temperature measurement is very low. In addition to the statistical analysis, the influence of maximum and minimum deviations of semidry water vapour mole fractions on the emission parameters was also presented. Both analyses have shown a very small error of the semidry water vapour mole fraction on the emission parameters. Therefore, it is recommended that at least the semidry dew point temperature might be neglected. However, the semidry absolute pressure should be measured, as this can be accomplished with a standard pressure transmitter. This one is maybe already included in the emission measurement system. Additionally, the influence of the unburned hydrogen measurement itself was investigated. Due to the fact, that at least for lean conditions the unburned hydrogen concentration is very low, the influence of unburned hydrogen due to interference effects on the emission parameters is almost negligible. The relative propagated error due to measurement uncertainties on emission parameters based on the unburned hydrogen concentration, are either in the same order or even smaller compared to other emission parameters. Thus, if it is acceptable to always assume a combustion efficiency of 100 %, the measurement of unburned hydrogen might also be omitted.

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