Modelling of a Three-Shaft High-Bypass-Ratio Engine Performance and Emission Prediction Using Hydrogen Fuels

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Abstract—The price of oil has seen an unprecedented increase and the resulting demand for oil, especially from the transportation industries. The pollution emits from the vehicle has affected human health and environmental problems especially aviation industries because the emission covers much broader spectrums. Drop-in alternative fuels such as liquefied hydrogen fuel are believed to offer better engine performance and reduce the emission. An in-house computer tool, PYTHIA was used to model the performance of RB211 engine at a wide range of flight operations. Liquid hydrogen fuel will increase the thrust and the specific fuel consumption up to 63.9% reduction at higher speed. Liquid hydrogen fuel resulted in higher burning temperature which encourage the formation of NOx. At the sea level, it was found that EINOx was increased to about 5.5% when 20% blended ratio was used.

Keywords: Emission, Engine performances, Hydrogen biofuel, Jatropha biofuel

1. INTRODUCTION

In recent years, we are getting more conscious of the oil prices and oil consumption. The price of oil has seen unprecedented swings and the resulting demand for oil especially from the transport sector in the past decades [1]. This is because the fuel or natural gas is precious as energy resources and in transportation industries which grew over the year. Since the first oil crisis of 1973, this dependence is considered to be problematic; this is the “energy problem” of transport [2]. Land, air, and sea vehicles use crude oils as their energy resources and will soon diminish. Renewable energy resources potentially offer a solution to both energy and environmental crises.

Statistically, the fuel consumption has shown that annually the worldwide demand for energy is over 12 Billion Tons of Oil Equivalent (BTOE) results in the emission of 39.5 Gigatons of carbon dioxide (Gt-CO\(_2\)), and the annual CO\(_2\) emission would increase up to 75 Gt-CO\(_2\) when future energy demand will rise to 24 to 25 BTOE [3].

The emission produced by vehicles also contributes to health problems. Exposure to the particulate emission from the transportation can affect the adverse health outcomes including cardiopulmonary, ischemic heart disease and infant which lead to mortality [4].

The aircraft deposited gases like carbon dioxide (CO\(_2\)), water vapour (H\(_2\)O), nitrogen oxides (NO\(_x\) = NO+NO\(_2\)), various sulphur dioxide (SO\(_2\)), carbon monoxide (CO), various non-methane hydrocarbon (NMHC), and particles that may contribute to anthropogenic climate changes [5]. A modern turbofan engine consists of 72%CO\(_2\), 27.5% H\(_2\)O, 0.02% SO\(_2\), and 0.4% trace species where the trace species in turn contains 84% NO\(_x\), 11.8% CO, 4% UHC, and 0.2% soot for typical cruise condition [6]. CO\(_2\) deposition is the main contributors to the climate change because the emission are released in the upper troposphere [6]. Formation of the ozone leads to human health issues and local air quality due to the emission of NO\(_x\) in lower altitudes [7].

The regulations and legislation for aircraft manufacturers are expected to be more stringent in order to minimise the environmental impacts. Regulations imposed by the International Civil Aviation Organization (ICAO) is crucial to ensure safe and orderly growth of air transport. This organisation also committed to reduces and focused on the NO\(_x\) emission in the aircraft industries. NO\(_x\) had a linear relation with overall pressure ratio (OPR) as the regulation set by the ICAO in 1993 and has been revised three times in ICAO1993, ICAO1999 and ICAO2005 due to its high influence on climate change [6]. The Committee on Aviation Environmental Protection (CAEP) is a technical committee formed by ICAO to assist the council in making new policy and standards for aircraft emission and noise level are becoming more stringent on emission standard [6]. From the Figure 1, the NO\(_x\) emission standard has become more stringent since the first time being introduced. As the number of CAEP get higher means the rules and regulation is become stricter and should emits less NO\(_x\). To improve the Strategic Research Agenda dealing with accomplishing the targets of vision 2020 the Advisory Council for Aeronautical Research in Europe (ACARE) was established. It has announced its 2020 targets as in [8].

Alternative energy resources such as hydrogen, biofuels, electric powered, and fuel cells will potentially be being utilized in the next coming years. However, the feasibility and practicability of these alternative fuels being used in the existing engine are the primary concern and actively studied. Bio-fuel is extracted from agriculture and animal feed based

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biological materials with carbohydrate [9]. For instances, Jatropha, Camelina, Algae, halophytes, municipal and sewage wastes, forest residues were used in aviation fuel production process [9]. Numerous flight tests utilizing biofuels were conducted. Moreover, American Society for Testing and Materials (ASTM) standards were achieved in 2011 in order to allow aircraft and engine manufacturers to use biofuels in air vehicles after 2008 [9]. Biofuels have been tested and show a better result than the conventional fuels used regarding the emission. Furthermore, these biofuels can be blended with fossil fuel and can be used directly in internal combustion without any engine modification [9]. However, Jet-A1 fuel is only approved to blend with 50% of the others alternatives fuel according to the ASTM D7566 standard [9]. These kinds of mixing can reduce quite a significant amount of emission as compared to the pure kerosene. Regarding performance by using Jatropha biofuel, the gross thrust produce has been increased, and the reduction in specific fuel consumption also shows the advantages by using the biofuels [10]. The biofuel microalgae can obtain 76% reduction of lifecycle greenhouse gas emission based on the current research [9]. The biofuel still can be considered and reliable as the best alternatives fuel to reduce the emission as compared to conventional fuel.

1.1. Hydrogen Fuel

Beside biofuels, liquid hydrogen also has been studied actively. Hydrogen fuel has become attention since it does not emit any particulate CO and CO₂ [11]. From the molecular formula itself, it does not contain any carbon molecule unlike kerosene fuel. It has higher calorific value compared to the other alternative fuel and potentially give better performance and result in less emission. Hydrogen has been considered as an aviation fuel from early as 1918 [12]. There are many test engines which run completely using cryogenic liquid hydrogen, LH₂. However, conventional aircraft engine has to be modified and redesigned such as fuel supply substructure due to its chemical and physical properties [8]. Figure 2 has shown that hydrogen fuel can reduce fuel consumption as compared to the kerosene fuel. Less fuel consumption potentially reduces the emission. Comparison between conventional jet fuel and liquid hydrogen fuel have shown that gas emission from LH₂ can reduce toxic emission [8].

Abundant hydrogen gas available in nature and there are myriad ways to produce it. Currently, nearly 50% of the global hydrogen demand is generated via steam reforming of natural gas, 30% by oil/naphtha reforming, 18% by coal gasification, 3.9% by water electrolysis and 0.1% from other sources [13]. Methods such as gasification and electrolysis can be used to produce the hydrogen since it cannot be found freely [8]. However, producing H₂ by natural gas, reforming is the most commonly method used [8]. Hydrogen fuel has better thermochemical properties as depicted in Figure 3 Hydrogen fuel has double amount of heat of combustion than other hydrocarbon fuels. It gives an enormous amount of energy during combustion. Concise ignition time and wider flammability are significant characteristics of the LH₂ in reducing the emission since the emission of the NOₓ also depend on residence time. Using LH₂ as a fuel in the aircraft has many benefits with respect to kerosene usage such as [8]:

- Higher energy content per weight three times
- Less take-off gross weight obtained for both medium and long-range transportation
- Almost 22% more efficient flight for long-range transportation
- The life cycle of engines improved thus maintenance cost decreased
- If LH₂ burst into flame, it is handled more easily

Zero CO₂ emission and less NOₓ emission
1.2. Emission Formation

Hydrogen fuel offers clean combustion where no formation of carbon dioxide ($CO_2$), carbon monoxide (CO), and unburned hydrocarbon except for water [14]. Even though the $LH_2$ are more attracted however it also has disadvantages. Burning liquid hydrogen encourage $NO_x$ formation due to endothermic mechanism especially burning above 1800K [13]. Hydrogen fuel has a high flame temperature which strongly contributes to the formation of $NO_x$. Water vapour produces about 2.6 times more than conventional fuel, and water vapour is classified as one of the strongest greenhouse gases [8]. $NO_x$ has contributed to the acid rain and destruction of stratospheric ozone while $NO_2$ is the major factor that affects lakes and susceptible soils [11].

New aircraft engine has higher thermal efficiency and improved fuel consumption which then emits less $CO_2$. However, the $NO_x$ emission formation needs more attention because it involves non-linear effects of certain parameters, such as engine type, engine cycle, pressure ratio, combustor inlet temperature, flame temperature, air-fuel ratio, thrust, altitude and speed which may vary considerably during flight [15]. The only pollutant emission formed is $NO_x$ due to the oxidation of $N_2$ in the air at high combustion temperature when liquid hydrogen is used [14]. The difference between kerosene and hydrogen is the way of the $NO_x$ form from the combustion process. Liquid hydrogen produces $NO_x$ due to thermal mechanism when combustion occurs while both thermal and prompt mechanism are involved in hydrocarbon fuel [14].

$NO_x$ formation can occur in many ways depending on the temperature. As the turbine engine combust the air, NO and $NO_2$ are produced to form $NO_x$. At the first stage, the NO formation is taking place first before transform to the $NO_2$ since this conversion need the temperature reduction after some time in the atmosphere [16]. The nitric oxide (NO) formation is significant when the temperature above the 1800K. There are many types of formation on NO mechanism such as the Zeldovich mechanism or thermal mechanism, the prompt mechanism, the $N_2O$ intermediate mechanism, and through fuel-bound nitrogen [16], Konnov, Colson and De Ruyck [17] stated that the hydrogen-air system is dominated by thermal $NO_x$ since the flame temperature is above 2100K.

The thermal mechanism is the main factor that contributes to the $NO_x$ formation in high-temperature combustion over a wide range of equivalence ratio. The temperature of the flame has its peak at the stoichiometric condition. The flame temperature is the key towards the $NO_x$ formation. As close to stoichiometric conditions the $NO_x$ emissions are maximum (about 40 mg/MJ) and decrease as the equivalence ratio decrease [18]. The flame temperature seems strongly related towards the equivalence ratio which can reduce the $NO_x$ emissions as the equivalence ratio in the lean conditions [18]. The fuel mechanism also plays an important role in the production of $NO_x$ at very lean mixture, low-temperature combustion processes [11].

There are other factors encourage $NO_x$ formation such as the ambient temperature and relative humidity. However, $NO_x$ emission of the aircraft engine is more positive towards the ambient temperature instead of the relative humidity [15]. The ambient conditions in which the engine operates affect the environment inside a combustion chamber and the characteristics of the combustion process of the gas turbine engine. This problem seems to be true when the flight is operated at difference altitude since the altitude affects the density and ambient temperature. The fuel-air ratios also vary due to changes in ambient temperature which leads to produce emission. Based on the research provided, the higher the cruising altitude, the better the fuel efficiency, due to a decreasing drag force caused by lower density at higher altitude levels [15]. For example of the takeoff condition, increase in temperature will increase the $NO_x$ levels exponentially at the higher values of the combustor inlet temperature [16]. The $NO_x$ production increase at every equivalence ratio when the initial temperature increase [11].

Another factor that impacts the level of pollutants emitted from a combustor is the pressure at which combustion takes place. The flame temperature increase is also affected by the increase in pressure which leads to lower dissociation losses [16]. The effect of increasing pressure on flame temperature is shown in Figure 4. The $NO_x$ at combustor exit increase as the pressure increase in both stoichiometric and rich mixture of fuel [11].

The flame temperature of combustion also depends on the equivalence ratio of the primary zone of a combustor, which refers to the ratio of fuel and air [16]. The stoichiometric fuel-air ratio is the ratio of the fuel to the air which provides complete combustion. At the stoichiometric ratio, the temperature of reactions increases significantly [16]. Reducing the equivalence ratio will reduce flame temperature and resulting lower $NO_x$ formation. Modifying the fuel-air ratio toward leaner combustion regime at all engine load conditions is possible due to the wider flammability range of hydrogen in order to reduce $NO_x$ emission [13].

The residence time on the combustor also can affect the $NO_x$ production instead of temperature, pressure and equivalence ratio. Complete combustion needs a sufficient residence time to ensure that CO and UHC are reduced, on the other hand, prolong the residence time will provide excess $NO_x$ production [7]. Reducing the length of combustor, the alternative way uses to reduce the residence time. This longer reaction time and prematurely quench NO formation can be avoided by the short realistic combustor as an alternative [16]. The hydrogen fuel has the capability to endure the short combustor since it has high reactivity and velocity [14]. The previous work also has indicated that shorter combustor can be used when operated on hydrogen compared to kerosene due to the fast reaction rate of hydrogen [17].

Objectively, this paper studies feasibility and practicability of drop-in liquid hydrogen by modelling a variant of three-shaft high-bypass aircraft engine similar to RB211 using an in-house computer tool, PYTHIA at a wide range of flight operations. Given data extracted from PYTHIA, NOx correlations and NASA Chemical
Equilibrium Application (CEA) open software were used to compare and validate.

**Figure 5. PYTHIA data process flowchart [10]**

**Figure 6. PYTHIA engine model schematic diagram [10]**

**II. METHODS**

2.1. Performance Analysis

An aircraft engine model similar to of RB211 was used in PYTHIA to predict the engine performance parameters such as thrust, specific fuel consumption with different altitude are affected by the blended mixing ratio for both design and off-design conditions. Two fuels, kerosene and LH₂, are used at different blended mixing ratios. Kerosene fuel was set as a baseline fuel. A similar approach has been conducted in [10] was used. The PYTHIA process is illustrated in a flowchart as in Figure 5. PYTHIA provides library data and default setting configuration in order the engine type can be specified by the user. Since the engine model was selected, 13 block data were arranged as Figure 6. The data given by the PYTHIA will be extracted into Excel Spreadsheet to plot the graph for further analysis. The graph such are gross thrust and specific fuel consumption (SFC) against Mach number at different altitude are plotted. This type of graph shows how the different blended ratio percentage affect the performance of the turbine engine at different altitude.

2.2. Emission Analysis And Prediction

There are many NOₓ prediction model methods used by researchers. These models were used to see the relationship between the temperature and pressure at the combustor inlet P3 and T4 respectively. However, the model used for these correlations is specifically for the Jet-A fuel or kerosene based fuel. For the purpose of prediction of EINOₓ, AECMA, NASA and LEFEBVRE model was chosen for comparison with NASA CEA output.

NASA CEA open source software was used to obtain the product of molar fraction during the combustion process. This molar fraction data will be used to analyse and predict the emission produced from the engine specified. The results yield from the PYTHIA such as the temperature and pressure will be used in the NASA CEA. Chemical balance equation in (1) and (2) show the stoichiometric condition for kerosene and LH₂ respectively. Output parameters such as pressure, temperature, enthalpy, internal energy, entropy, percentage fuel, oxide to fuel ratio (O/F) and equivalence ratio (E.R) were selected as the properties that are interested in predicting the NOₓ emission.

In order to calculate the EINOₓ, the model like AECMA, NASA and Lefebvre model was used as shown in equation (3) - (5).

\[ C_{12}H_{26} + O_2 + 3.76N_2 = 12CO_2 + 13H_2O + 3.76N_2 \]  
\[ 2H_2 + O_2 + 3.76N_2 = 2CO_2 + 2H_2O + 3.76N_2 \]  
\[ EINO_x = 2 + 28.5 \left( \frac{P_3}{3100} \right)^{0.4} \left( \frac{T_3}{349.9} \right) \]  
\[ EINO_x = 33.2 \left( \frac{P_3}{432.7} \right)^{0.4} \left( \frac{T_3}{53.2} \right) \]  
\[ EINO_x = 4.59 \times 10^{-9} \times P_3^{0.25} \times F \times t_{res} \left( \frac{0.01(T_f - 273)}{349.9} \right) \]

Where \( P_3 \) is pressure before entering combustor, \( T_3 \) is temperature before entering combustor, \( F \) is air fraction in the primary zone which set to constant with value 0.1, \( t_{res} \) is the residence time which set to constant with value 0.5 second and \( T_f \) is the flame temperature for the hydrogen. On the other side the NOₓ emission standard is calculated through the equation (6).

\[ D_p/F_{oo} = \sum E_{i} \times T_{i} \times M_{i} \times W_{i}/R_{0} \]  

\( D_p \) is the mass of NOₓ emitted during landing take-off (LTO) cycle, \( F_{oo} \) is the rated output (RO) of the engine, \( E_{i} \) is the emission index of \( NO_x \) (EINOₓ), \( T_{i} \) is time in mode, \( W_{i} \) mass of fuel flow and RO is the gross thrust produce from the engine. The time in mode is set with value 240, 132 and 42 seconds for the cruise, take-off (TO) and climb respectively.

**Figure 7. The gross thrust produced against speed at sea level**
MODELLING OF A THREE-SHAFT HIGH-BYPASS-RATIO ENGINE PERFORMANCE AND EMISSION PREDICTION USING HYDROGEN FUELS

III. RESULTS AND DISCUSSION

3.1. Performance

Hydrogen fuel has shown better performance regarding thrust and specific fuel consumption. Liquid hydrogen fuel has higher calorific value compared to the kerosene fuel. Calorific value is the measure of heat energy content in the fuel. Liquid hydrogen fuel contains a higher percentage of water vapor, which leads to an increase in specific heat. Increasing in specific heat has resulting smaller pressure drop in the turbine, which leaves more energy to be converted into thrust in the exhaust nozzle [12]. More energy can be converted into thrust when the smaller pressure drop is considered based on energy conservation. Thus higher calorific value is desired in producing more power and thrust to the engine. Figure 7 shows thrust produced with the variation of the blended ratio percentage. It shows that, as the blended ratio goes up to 100% or pure, the thrust produced increase and perform better. The increment up to 7.4% of thrust produced using hydrogen fuel as compared with kerosene fuel.

However, at higher altitude, the thrust shows a slight reduction. Increase in altitude varies the inlet condition of the turbine engine. At higher altitude, ambient temperature and pressure are reduced. As the temperature lapse rate (rate of temperature decrease) is lower than the pressure lapse rate as altitude is increased, resulting in the density to decrease. Pressure lapse rate affects the density than the temperature lapse rate [19]. Thus, increasing altitude will produce low thrust generated. From Figure 8, the thrust produced for the different blended mixing ratio deteriorates as the altitude increases at the same speed. The percentage differences concerning kerosene fuel calculated show 7.2% 6.6%, 5.3% and 5.1% increment as the altitude increase from 0 to 500, 1500 and 2000 respectively.

Specific fuel consumption (SFC) of a blended mixing ratio of liquid hydrogen has improved significantly. The result shows that 100% blended ratio mixing gives better performance in terms of fuel consumptions. The lower SFC shows how efficient the fuel was consumed because the force generated is much higher compared to fuel flow rates. The comparison made from Figure 8 shows that SFC increase as the blended ratio of fuel increase. The percentage difference of the SFC in pure LH₂ has shown up to 62.9%, 63.3%, 63.6% and 63.9% reduction as the Mach number increases. From Figure 10, SFC has shown a slight decrease as altitude increases. Similarly, up to 63.3%, 63.2%, 63.0%, and 62.9% SFC reduction can be achieved at different altitudes. Conclusively, the SFC and percentage reduction in SFC with respect to kerosene are really decrease as the altitude increase. From the percentage difference, pure mixing blended gives more efficient in terms of the fuel consumption compared to the kerosene fuel. Thus, the fuel consumption can be reduced by fuel in the liquid hydrogen.
3.2. Emission

Liquid hydrogen has a higher flame temperature. At the primary zone of the combustor, the inlet burning temperature is higher at higher blended ratio percentage as depicted in Figure. 11. The hot temperature has increased to about 2.38% higher than kerosene. However, at higher altitude, the temperature reduces for every blended ratio as influenced by the ambient air temperature.

Liquid hydrogen fuel encourages \( NO_x \) formation. Higher temperature shows much higher \( NO_x \) formation. Thermal \( NO_x \) are formed in liquid hydrogen fuel at the flame temperature above 2400K. \( NO_x \) formation in kerosene fuel comes two ways which are the thermal and prompt mechanisms. NASA CEA software have shown that by increasing the inlet temperature of a combustor has increase the product of \( N_2 \) molar fraction. \( N_2 \) gas is the source of the \( NO_x \) formation due to oxidation of \( N_2 \) in high temperature condition.

Figure 12 shows the relation of the temperature and \( N_2 \) formation in the hydrogen combustion process. The dotted graph has shown the \( N_2 \) formation is linearly proportional to the temperature. Meanwhile, Figure 13 has shown different NOx correlation models against the temperature. These models have shown the similar trends even though there are many possibilities that the \( NO_x \) can form. The factors such as the residence time and length of combustor are also influencing the \( NO_x \) formation. However, those factors are not discussed in this paper since we are using drop-in liquid hydrogen fuel with no modification on the engine itself. Figure 14 shows the EINOx formation over a wide range of altitudes at different blended ratio percentages. At the sea level, the increase of EINOx is about 5.5% when 20% blended ratio was used. These percentage decrease as the altitude increases with up to 5.2% and 4.6% respectively when 20% blended ratio are compared. EINOx shows the highest value when pure liquid hydrogen fuel is used to about 13.1% increment with respect to kerosene at sea level. EINOx is reduced at higher altitude. EINOx measures the mass of the \( NO_x \) formed per kilogram of fuel burnt. This indicates that 1kg of liquid hydrogen fuel will produce 43.71g of \( NO_x \), which is higher compared to the kerosene fuel which only produces 38.63g of \( NO_x \). The EINOx will increase as the temperature increase undoubtedly. However, the thrust produce also plays an important role in reducing the \( NO_x \) emission standard. The overall \( NO_x \) emission standard for a flight envelope is determined by the equation (6).

\[
\frac{D_p}{F_{oo}} \text{ is used to determine the specific pollutant gas produces per thrust generated.}
\]

![Figure 13. EINOx formation at different temperature using different correlations](image)

Figure 13 shows the total amount of \( NO_x \) emission produced through the summation of \( NO_x \) at every flight condition; cruising, take-off and climbing mode. This value indicates that \( NO_x \) formation that can be reduced as the percentage blended ratio increases due to the better performance of the engine as discussed previously. Graph represented shows that the \( NO_x \) emission standard also reduced as the altitude increases. From the reduction given in the \( NO_x \) emission standard, it clearly understood that the amount of thrust generated by using the liquid hydrogen is higher compared to the EINOx produced. The reduction in \( NO_x \) emission standard has been calculated in percentage difference for the blended ratio to get the relations. As the blended ratio increase from 20, 40, 60, 80, 100 the percentage reduction decreases as 21.55%, 35.48%, 45.21%, 52.4% and 57.94% respectively.

IV. CONCLUSION

To conclude, the analysis that has been done and the data collected have shown that the liquid hydrogen is performed better than the kerosene fuel. Even though there are many alternatives fuel, however, the liquid hydrogen takes the priority as the best alternatives fuel for future aircraft. The hydrogen performs better in term of performance and also in reducing overall \( NO_x \) emission standards, not EINOx formation due to high temperature.

The performance, however, can be understood by the calorific value contained in the hydrogen fuel which tends to produce higher thrust and better SFC. At higher blended
ratio (pure liquid hydrogen fuel) will increase the thrust and the SFC up to 63.9% reduction obtained in hydrogen fuel at higher speed.

Increasing the blended ratio percentages will increase the burning temperature. At the sea level, it was found that EINO\textsubscript{x} was increased to about 5.5% when 20% blended ratio was used. EINO\textsubscript{x} formation continues to increase as the blended ratio is increasing. The temperature effects the EINO\textsubscript{x} formation. Higher temperature will produce higher EINO\textsubscript{x}. However, the NO\textsubscript{x} emission shows opposite trends. At higher blended ratio will reduce NO\textsubscript{x} emission due to better performance of the engine. Therefore, it is strongly believed that NO\textsubscript{x} emission can be reduced. However, other proprietary parameters such as equivalence ratio, residence time, combustor’s geometries, turbulent flows and other crucial parameters are not being considered here.

There are many ways to reduce the temperature inlet as the literature review state. The equivalence ratio could be reduced further by using the LH\textsubscript{2} fuel since it has high stability compared to kerosene. As the equivalence ratio decreases, the burning temperature decreases. The residence time should be reduced because LH\textsubscript{2} fuel has the higher rate of reaction. High rate of reaction gives the shorter period of time to combus. In such a high flammability, thus the combustor length could be reduced in order to reduce the EINO\textsubscript{x}. Thus, the reduction of emission can be optimum by using the LH\textsubscript{2} fuel instead of fuel in the LH\textsubscript{2} in an aircraft engine. However, many research and study should be conducted in order to optimum the NO\textsubscript{x} reduction while having higher gross thrust and efficiency.

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