Prediction of NOx Emissions for an RQL Aero-engine Combustor using a Stirred Reactor Modelling Approach

Atma Prakash1

School of Science and Engineering, Teesside University UK, TS1 3BA

The world has witnessed a drastic techno-economic development in the last century due to which transport, trade and logistics have improved the lifestyle of the public. The Aviation industry has transformed the way of travelling across globe. Now it is more economic, comfortable and accessible to travel. Unfortunately, this revolution in aviation has brought various environmental issues; gaseous emissions and noise nuisance. These gaseous emissions disrupt the eco-system normal operating process. These gases have serious implications on the global environment and pose a great risk for human health. The NOx (NO and NO2) is a major concern; especially around the airports locality, where it can create ozone gas which is harmful to the wellbeing. In spite of much advancement in fuel-efficient and less polluting turbofan and turboprop engines, the rapid growth of air travel in recent years has contributed to an increase in total emissions. According to the ICAO, the contribution of civil aircraft to global greenhouse emissions has been estimated at around 2%. The Committee on Aviation Environmental Protection (CAEP), which assists ICAO in the formulation of new policies on aircraft noise and emissions, has presented a number of policies in the last decade in order to curb down the aviation emissions. Due to these emission regulations, the aviation industry is looking into the ways to cut down its global emission imprints. The primary objective of this paper is to assess the suitability of the stirred reactor modelling approach to predict NOx emissions of a Rich-Burn Quick-Quench Lean-Burn (RQL) combustor concept. This paper further illustrates the axial variation in the main parameters such as equivalence ratio, NOx mass fractions and temperature for a NASA test rig experiment combustor geometry from the RQL combustor model based on the stirred reactor method. The paper also comments on the NOx emission regulations development by ICAO for different operating conditions.

Nomenclature

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CO2 = Carbon Dioxide

NO = Nitrogen Oxide

 NO_2 = Nitrogen Dioxide

NOx = Oxides of Nitrogen

UHC = Unburned Hydrocarbons

I. Introduction

THE world has witnessed a drastic techno-economic development in the last century due to which transport, trade and logistics have improved the lifestyle of the public. The Aviation industry has transformed the way of travelling across globe. Now it is more economic, comfortable and accessible to travel. Unfortunately, this revolution in aviation has brought various environmental issues; gaseous emissions and noise nuisance. These gaseous emissions disrupt the eco-system normal operating process. In addition to the CO_2 released by in-flight jet engines, aviation industry also contributes to greenhouse gas emissions from ground airport vehicles and transport used by passengers and staffs to access the airport. While the principal greenhouse gas emission from powered aircraft in flight is CO_2 , other emissions include nitric oxide, nitrogen dioxide, water vapor and particulates (soot and sulphate particles), Sulphur oxides, carbon monoxide, and unburned hydrocarbons (UHC).

These gases have serious implications on the global environment and pose a great risk for human health. The NO_X (NO and NO_2) is a major concern; especially around the airports locality, where it can create ozone gas which is harmful to the wellbeing. Moreover, aviation is the only reason for high altitude cruise NOx which plays a major role in the ozone layer depletion in the stratosphere¹. Depletion of ozone layer allows the solar Ultra-Violet (UV) rays to penetrate the Earth leading to skin related diseases.

Contribution of civil aviation to global greenhouse emissions has been estimated at around 2% by the International Civil Aviation Organization (ICAO). According to the 2010 ICAO Environmental report, air travel is

¹ Lecturer, Aerospace Engineering, School of Science and Engineering, Teesside University, UK and AIAA Member

growing at an average rate of 4.8% per year and it is expected to increase further². The Advisory Council for Aeronautical Research in Europe (ACARE) which is a European advisory body in a public-private partnership between the European Commission, aviation industry leaders and academia has established ambitious goals in flightpath 2050 to reduce CO_2 emissions by 75% per passenger kilometer, NO_X emissions by 90% per passenger kilometer and to reduce perceived noise by 65% by 2050^{3; 4}. The ICAO has been taking continuous efforts to regulate the aircraft emissions by formulating stringent policies on emission reduction. Therefore, aviation industry is looking ways to reduce the emissions not only due to its global climatic impact and health hazard, but to meet stringent emission standards set up by ICAO, CAEP & ACARE.

In case of stationary gas turbines, emission regulations tends to vary from one country to another due to different legislations which is supplemented by local or site-specific regulations and ordinances governing the size and usage of the plant under consideration and the type of fuel used⁵. The NOx emission for stationary gas turbines engines in the USA is regulated by EPA (United States Environmental Protection Agency), more details may be found in⁶. The formation of pollutants during combustion depends on various parameters such inlet pressure, temperature, combustor as geometry, airflow, and fuel distribution inside the combustor⁵. The formation rate of NO_X increases with flame temperature, peaking at airfuel ratios close to stoichiometric⁷.

In particular, requirement for the larger aircraft to carry more passengers with lower fuel cost has led the aviation industries in moving to the higher bypass ratio engine designs. As, the bypass ratio of large turbofans increases, the

resulting power requirements of the larger fan mandate increases requiring more energy to be extracted from the low-pressure turbine. This typically leads to higher pressures, combustion temperatures, and therefore higher NO_x production. In fact, the increase in total aviation NO_X emissions has grown rapidly than total fuel consumption over the last few decades because of the higher pressure ratios (and therefore combustion temperatures) demanded by the more fuel-efficient high-bypass-ratio engines8. Carbon dioxide and water vapor are not considered as the pollutants because they are usual by products of complete combustion of a hydrocarbon fuel. However, both contribute to global warming and only



Figure 1. Effect of Temperature on NOx and CO formation ⁵



way to reduce their production is by burning less fuel. Thus, improvement in engine thermal efficiency not only reduces operating costs but carbon dioxide and water vapor pollutants as well.

Therefore, in order to minimize the NO_X emission in the combustor, the time spent in the high flame temperature region must be minimized. Novel combustor design concepts limits the temperature, varies the mass flow distribution in different zones, and resident time in order to reduce the overall NO_X emission below the current ICAO legislation levels. As, novel low emission combustors show a promising way to curb down the aircraft emissions and compliance with the stringent regulations, this research focuses on the novel combustor designs

concept and the suitability of a NO_X emission prediction method for an aircraft engine. Figure 2 shows the gas turbine engine emissions characteristics for different engine power settings.

Generally, most of the nitric oxide (NO) formed during combustion process inside gas turbine engine subsequently oxidizes into NO₂. Therefore, usually NO and NO₂ are lump together to express the results in terms of oxides of Nitrogen (NO_X). NO_X is pollutant from aero engine exhausts which plays a major role in disturbing the atmospheric ozone concentration. NO_X is responsible for low level ozone formation near airport area which is toxic. If inhaled may lead to many respiratory illness, impaired vision, headaches and, allergies. Similarly, NO_X emission emitted by aircraft at high altitudes can deplete the ozone layer.

The factors which play a pivotal role in NO_x formation during combustion are; degree of uniformity/nonuniformity of the fuel distribution within the combustor, flame temperature, pressure, residence time and fuel atomization. Non-uniform fuel distribution creates small pockets of fuel which burns in a diffusion mode at near stoichiometric fuel/air ratios, giving rise to many local high temperature regions in which NO_x forms in considerable quantities. Reduction in mean droplet size of fuel hampers the formation of envelope flames, so that a larger proportion of total combustion occurs in premixed mode thereby producing less NO_x. Major part of the NO_x is generated in the higher temperature region known as thermal NO_x. Figure 1 shows, NO_x formation is exponentially dependent on temperature; an obvious way of reducing NO_x emissions is by lowering the temperature in the combustion primary zone. One way to reduce the thermal NOX is by introducing additional air but if used in excess, it can raise the primary-zone velocity, which has an adverse effect on ignition and stability performance. An alternative way to reduce NOX emission is to inject water or steam in the primary zone of the combustor. But, this technique is not feasible for aircraft engines as carrying large amount of water amounts to increase in weight therefore not fuel efficient. On the other hand, stationery gas turbine engines have been using water or steam injection in order to control NOX emission to the level required by the regulations ⁹.

II. NOx Emission Regulations

The Committee on Aviation Environmental Protection (CAEP) is a technical committee of 2.4 International Civil Aviation Organization (ICAO) council established in 1983, superseding the Committee on Aircraft Noise (CAN) and the committee on Aircraft Engine Emissions (CAEE). CAEP assists the Council in formulating new policies and adopting new Standards and Recommended Practices (SARPs) related to aircraft noise and emissions, and more generally to aviation environmental impact. CAEP undertakes studies as and when requested by the ICAO. Its scope of activities encompasses noise, air quality and basket of measures today considered for reducing international aviation CO2 emissions, including aircraft technology, operations improvement, market-based measure and alternative fuels.

The ICAO reviews and adopts CAEP recommendations, including amendments to SARPs and in turn reports to ICAO Assembly where the policies main on environmental protection are ultimately defined ¹⁰.

CAEP meets every three years to report on the civil aviation and to recommend changes in the emission policies to be accepted by the states. In its 8th meeting held 2010, it in has recommended more



Figure 3. Illustration of ICAO Emissions Certification Procedure in the LTO Cycle ¹²

stringent NOx emission standards of up to 15 % on large engines and 5 to 15 % on small engines certified after 31st December 2013. Main concern about the Local Air Quality (LAQ) is in the vicinity of an airport which is the hub

for all the aircraft flying and out of any city. Therefore, ICAO emission standards focuses on the aircraft engine emissions released below 3,000 feet and emissions from airport sources, such as airport traffic, ground service equipment, and de-icing operations. The current ICAO standards for emissions certification of aircraft engines state that to achieve certification, it must be demonstrated that the characteristic emissions of the engine type for HC, CO, NO_X and smoke are below the limits defined by ICAO. The certification process is based on the Landing Take-off (LTO) cycle, as shown in Figure 3.

The engine certification process is performed on a test bed where the engine runs at each thrust setting to generate the data for each of the modes of operation. The result of the engine emissions certification test includes: fuel flow (kg/s), emissions index for each gaseous pollutant (g/kg), and the measured smoke number. All of these data are stored in the publically available ICAO emissions databank ¹¹. The Standard for NO_X was first adopted in 1981, and then made more stringent based on the recommendations of four CAEP meetings in 1993 (CAEP/2), 1999 (CAEP/4), 2005 (CAEP/6) and 2011 (CAEP/8) ¹⁰. In addition, in 2011 a NO_X production cut-off requirement was adopted stating that individual engines produced on or after 1st January2013 have to comply with the previous 2005 (CAEP/6) NO_X Standard. Together, these two measures will help to ensure that the most efficient NO_X reduction technologies are being employed in the

production of aircraft engines ¹⁰.

Technological innovations in aviation continue to lead the way towards effective and efficient measures in support of ICAO's environmental goals of limiting or reducing the impact of aircraft emissions on LAQ. To standard-setting complement the process, CAEP developed, with the assistance of a panel of independent experts, medium and long-term NOx technology goals (10 and 20 years, respectively). Figure 4 depicts the graphical representation of the CAEP LTO NO_X cycle limits from 1981 up until in 2010, which was last time CAEP conducted a NO_X technology review including the mid-term and long term



Figure 4. CAEP LTO Cycle Limits

goals to be achieved. Figure 4 shows emission standard set by CAEP for small to large size jet engines. The graph is between NO_X characteristics verses overall pressure ratio of an aircraft jet engine. DP/F_{00} represents the total NO_X emissions for the engine during the landing/take-off (LTO) cycle divided by the engine take-off thrust at sea level static, and is a parameter used for emissions regulation.

These ICAO certification limits apply only to newly certificated types and with industry standard production lives of 15+ years for most aircraft types coupled with the even longer in-service lives of 30+ years for passenger aircraft and about 45 years for freight types, total fleet NOx is slow to respond to a change in the stringency of the NO_x standard. The incorporation within these ICAO standards of a slope against OPR was in response to the characteristic for the mass of NOx emitted to increase along with increasing OPR and temperature.

These higher pressures and temperatures have been used in a drive to improve fuel and thermal efficiency of the engine. As most of the aero-engines at that time were designed with OPR of greater than thirty in order to curb down the fuel consumption and carbon dioxide emissions, it was decided at CAEP meeting to give a leeway to aircraft manufactures on that occasion by relaxing for the NO_X emissions. Hence in the Figure 4, there is a kink in CAEP/6 & CAEP/8 NO_X characteristics after the overall pressure ratio (OPR) of thirty. Nevertheless, CAEP/8 meeting proposed medium and long term goals with stringent NOx characteristics guidelines without giving any leeway to the engine manufactures even for overall pressure ratios greater than thirty to emit less NO_X emissions by 2030¹² and hence no kink in the later future goals.

III. DEVELOPMENT OF RQL NOX EMISSION PREDICTION MODEL

A. RQL Combustor

The research on Rich-Burn Quick-Quench Lean-Burn (RQL) combustor concept has been in progress since the late 1970s but it was first introduced in 1980 as a strategy to reduce NOx emission from gas turbine engines ¹³.

The concept was then furtherdeveloped by the NationalAeronautics and Space

Administration (NASA) later in the 1990's, for the reduction of NOx in next generation High Speed Civil Transport (HSCT) aero-propulsion engines ¹⁴ described in the next section. Pratt & Whitney is currently working on the RQL combustor technology in aero engines commercially under the name TALON (Technology for Advanced Low NOx) ¹⁵.

In the RQL design as shown in Figure 5, combustion is initiated in the fuel-rich primary zone operating in the equivalence ratio of 1.2-1.8 and due to the combined effects of low temperature and oxygen depletion, the rate of NOx formation is lower in the flame front zone. Whereas in Conventional combustor design, a continuous admittance of air in the primary zone raises both the temperature and oxygen content, thereby greatly accelerating the rate of NOx formation as shown in Figure 6, the high NOx route. If, however, the additional air required to complete the combustion process is mixed uniformly and instantaneously with the flame front gases without the substantial temperature rise, the combustion process follows the low NOx route as shown in Figure 6. This demonstrates that in order for the rapid and effective quick-quench mixing section, its design is of critical importance to the success of the RQL concept 16.

As shown from the combustor stability loop Figure 7, the RQL combustor being a rich initiated combustion have a wider flame stability limit when compared to the lean burn combustor designs. Therefore, the RQL combustor is preferred over lean premixed options in aero engine applications



Figure 5. RQL combustor with equivalence ratio shown in zone ²³



Figure 6. Principle of RQL Combustion ⁵



Figure 7. Combustor Chamber Stability Loop ²²

due to the safety considerations and overall stability throughout the duty cycle. RQL combustor design reduces not only thermal NOx but due to its initial fuel-rich combustion process, it reduces Fuel Bound Nitrogen (FBN) NOx emission by converting large amount of FBN into N2¹⁷.

Once the fuel-rich combustion effluent gases from rich-burn enters into quick-quench zone, they encounter jets of air that rapidly reduces the temperature below 1800K reducing the NOx formation substantially. As mentioned above, this transition from rich to lean zone has to take place quickly to prevent the formation of near-stoichiometric NOx. The temperature of the lean zone has to be high enough to consume any remaining CO, UHC, and soot left from quick-mix section. Thus, the equivalence ratio for the lean-burn zone has to be carefully selected to satisfy all emissions requirements. Generally, lean-burn combustion occurs at equivalence ratios between 0.5 and 0.7¹⁸.

B. Development of the stirred reactor model for NOx prediction

ROL combustor is divided mainly into three sections as shown in Figure 9. The first part is the richzone, where fuel and air mix and burn in fuel rich conditions with the equivalence ratio normally in between 1.5 and 1.8. The second section is the quick-mix zone, where almost all the remaining compressor exit air mixes with the fuel-air effluent gases from the rich zone very quickly. The equivalence ratio is in the range of 0.6-0.8 for quick quenching. Third section is the lean zone, where all the mixture blends with the remaining air and the mixture itself is lean because of highest percentage of air. The equivalence ratio is in the range of 0.3-0.4.

As in all the zones the temperature doesn't exceeds critically required for NO_X formation, the emission is considerably less compared to the



Figure 9. Reactor layout of RQL combustor in the model ²⁰



Figure 8. RQL Combustor Zones ²¹

conventional combustor. But, it demands careful designing to control the air flow and requires highly efficient instantaneous quick-quench mixing section.

The reactor layout of RQL is shown in the Figure 8. The rich-burn zone has one flame front reactor selected as partially stirred reactor. This assumption has been taken into account as the flame front area is fuel rich, thus the fuel/air mixture is heterogeneous with equivalence ratio of 1.8.

The second is quick-quench region and is modelled with two series of perfectly stirred reactors, one at the near wall and the other at the core. These assumptions take into account the quick mixing and abundance of air present in this zone. Eventually, both the near wall and core flow of the quick-quench zone mix together and enters the leanburn zone. By the time the mixture reaches the lean-burn zone the mixture is assumed to be fully homogenous and hence it is assumed to be a series of perfectly stirred reactors.

From Figure 8, F1 is the fraction of air entering the flame front rich-burn zone, F2 is the fraction of the burning gases entering the near-wall reactor at quick-mix zone from rich-burn reactor and F3 is the fraction of air initially assigned for quick-mix zone entering the near wall quick mix reactor. The rest of F3 air left from near-wall quick-quench enters the quick-quench core section of the combustor denoted by F4. The reactor arrangement and the air flow inside the combustor are based on a NASA test rig combustor ¹⁹. The RQL Combustor geometry details have been taken from that NASA test rig experiment ¹⁹ and is shown in Table 1.

	Rich-Burn (RB)	Quick-Quench (QQ)	Lean-Burn (LB)
Length (m)	0.203	0.127	0.610
Diameter (m)	0.152	0.102	0.178
Area (m ²)	0.031	0.013	0.108

Table 1. Combustor Geometry from NASA Test Rig Experiment²⁰

Based on the geometry given by the NASA test rig experiment ¹⁹, the area and corresponding length of the Rich-Burn (RB), Quick-Quench (QQ) and Lean-Burn (LB) region of the different reactors within the RQL combustor is

modelled as shown in Table 2. The input parameter for the model is combustor inlet temperature (T_3) , pressure (P_3) , combustor inlet airflow (W_A) , fuel flow (W_F) , ambient relative humidity and the air distribution within the different regions.

Inlet area RB (m ²)	Outlet Area RB (m ²)	Length RB (m)	Inlet Area QQ (m ²)	Outlet Area QQ (m ²)	Length QQ (m)	Inlet Area LB (m ²)	Outlet Area LB (m ²)	Length LB (m)
0.031	0.013	0.203	0.013	0.108	0.127	0.108	0.108	0.610

Table 2. RQL Reactor Geometry in Hephaestus²⁰

C. Assumptions and constraints in modelling the RQL combustor

All the assumptions and constraints in modelling the RQL combustor in the stirred reactor model "Hephaestus" is kept same as in the NASA test rig experiment ²⁰ in order to verify the result with their experimental data. As the RQL combustor is an air staged low NOx and not fuel staged, all the fuel is fed into the flame-front rich burn zone after airblast atomization. So, 100% fuel enters the Rich burn section of the combustor. The air is fed into rich-burn and the quick-quench section of the RQL combustor was not the priority for the NASA test rig experiment. The emphasis of the NASA RQL combustor test rig experiment was on NO_X emission prediction. Hence, similar assumption of not ingesting air in the lean-burn section has been taken in Hephaestus for RQL NO_X emission prediction modelling using stirred reactor approach. The distribution of air in the rich-burn and quick-quench section of the combustor. Therefore, for different measurement points from the rig test experiment, the input air varies in the rich burn section of the right accordingly for the stirred reactor model.

The rich-burn section in the NASA test rig experiment is fuel rich with heterogeneous mixture of fuel and air. The air and fuel is fed from the front section of the combustor and there are no further air intakes in the chamber which means the rich-burn section acts a single cylindrical tube with two openings; one for the intake of fuel and air and the other for the effluent gases emanating from it to go to quick-quench section. Therefore, a single partially stirred reactor is chosen to capture the chemical kinetics within the rich-burn region. It is assumed that the effluent gases emanating from the section mixes quickly in the second quick-quench region and attains the state of chemical equilibrium instantaneously in the series of discrete sections. Hence, the quick-quench region is modelled with series of perfectly stirred reactors. The aim of developing a preliminary NOx emission prediction model for RQL combustor using stirred reactor approach is to be able to predict NO_X emission results comparative with the NASA test rig experiment and to be able to capture the chemical kinetics within the RQL combustor for predicting NO_X emissions for an aero engine.

IV. Results and Discussion

A. Comparison between the model and NASA test rig NOx emissions

Table 3 shows the outcome of the Hephaestus for the RQL combustor and comparison of $EINO_X$ with the NASA test rig experiment. Here, the input into the RQL combustor model such as combustor inlet temperature (T3), Pressure (P3), Air mass-flow and fuel flow has been taken from the NASA test rig experiment as shown in Table 3.

T3 (K)	P3 (atm)	Air mass flow (kg/s)	Fuel Flow (Kg/s)	EINO _X (g/Kg) (NASA rig)	EINO _X (g/Kg) Hephaestus
795	7.8	2.808	0.0894	5.4	5.38
585	5.4	2.717	0.1057	1.7	1.41
797	8.0	3.048	0.0889	4.9	4.54
583	10.5	2.567	0.0984	4.5	4.70
583	10.0	2.784	0.0989	3.9	2.27

848	10.0	3.361	0.1048	8.6	7.02

Table 3. Comparison of EINOx from Hephaestus and NASA test rig

As it can be seen from the Table 3, the RQL Hephaestus model has been able to predict the EINO_X comparatively close to the experimental results from the NASA test rig experiment. The reason for variation of EINO_X for few points is due to the assumption and constraints in model; one being not taking the jet-to-crossflow momentum flux ratio into account during the RQL combustor modelling using stirred reactor approach.

B. Axial Position Results for NASA test rig combustor

This section describes the axial variation in the main parameters such as equivalence ratios, NO_X mass fractions and temperature for the NASA test rig experiment combustor geometry from the developed stirred reactor RQL combustor model. The Figure 10 shows the variation of equivalence ratios in the core and near wall region of the RQL combustor axially along the length.

It is inferred from Figure 10 that the equivalence ratio is 1.8 for the first two points in core and near wall. These points are from the flame front rich-burn region where a single partial stirred reactor for core was used to model the region and the equivalence ratio was fixed to 1.8 according to the NASA test rig experiment. Hence, the inlet and outlet equivalence ratio of the rich-burn region is unchanged. However, the steep decline in both the near-wall and core section of the second quick-mix region is due to the addition of large amount of quenching air in the midsection.

As per the NASA test rig experiment requirement, there is no air added further in the lean-burn section. Therefore, the effluent gases emanating from the quick-quench section reaches to equivalence ratio of 0.5; it remains same for the whole lean-burn section. For real engine case, air would further be added for a uniform temperature traverse at the end of the dilution zone and hence the equivalence ratio would vary in the dilution zone.

The Figure 11 shows the temperature variation in the near wall and core region along the length of the RQL combustor. It is inferred from Figure 11 that there is a steep drop in the near-wall region temperature; this is due to the addition of abundance compressor exit air which is comparatively cooler than the combustor in the quick-quench region. When, the air first enters in the quick-mix section, it first quenches the near-wall region reducing its temperature before entering into the core section of quick-mix section.

There is a rise in temperature in the core



Figure 10. Equivalence ratio vs RQL combustor axial positions









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section of the quick-quench region before a sharp decline because the combustion in the core region moves towards stoichiometric ratio from 1.8 as shown in Figure 10 and, as further air is added, the combustion moves towards leaner equivalence ratio of 0.5 as shown in Figure 11 which reduces the core temperature. Eventually, the fuel-air mixture become homogeneous and reaches to a point of almost constant temperature which shows in the lean-burn section of the RQL combustor.

The Figure 12 shows the mass fraction of Oxides of Nitrogen along the length of the RQL combustor. The mass fraction is defined as the ratio of the mass of the substance to the total mass of the mixture.

The NO_X formation in a combustor is mostly thermal NO_x and forms at higher temperature of more than 1800K. The Figure 12 of NO_X formation follows the same trend as in the Figure 11 of temperature variation in the near wall and core of the RQL combustor. As, most of the air is added in the quick-quench zone the mass fraction of NO_X decreases. The slight continues increase of mass fraction in the lean burn zone is due to the temperature in the range of more than 1800 K in Figure 11, no further addition of air and longer residence time.

V. Conclusion

The preliminary RQL stirred reactor model is able to predict the NOx emissions reasonably comparative to the public domain NASA test rig experiment data. This has demonstrated that the model is capable of fairly capturing the chemical kinetics process inside the RQL combustor and can provide a representative estimation of NO_X for an RQL combustor. The model was able to predict NOx by varying the amount of air in various zones, but in order to carry out the test rig equivalent scenario, major design changes needs to be taken for the RQL combustor. The varying geometry RQL combustor would be able to vary the amount of air in different zones.

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