

Genetic Algorithm optimised Chemical Reactors Network

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Genetic Algorithm optimised Chemical reactors network: A novel technique for alternative fuels emission prediction

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Abstract

Sustainability of the conventional jet fuels and climate change has attracted the aviation sector to diversity to alternative fuels. However, fuel diversification requires an assessment of the long term impact to engine performance and engine emissions through the combustion process, as alternative fuels are not as well understood as conventional jet fuel. A detailed experimental study on alternative fuels emissions across the entire aircraft fleet is impractical. Therefore a plausible method of computer modelling combined Genetic algorithm and Chemical reactors network was developed to predict alternative fuels gaseous emissions, namely, Carbon Monoxide, Nitrogen Oxides and Unburned Hydrocarbons in aircraft engines. To evaluate the feasibility and accuracy of the technique, exhaust emission measurements were performed on a re-commissioned Artouste Mk113 Auxiliary Power Unit, located at the University of Sheffield's Low Carbon Combustion Centre. The simulation produced results with good agreements with the experimental data. The optimised model was used to extrapolate emissions data from different blends of alternative fuels that did not operate during the campaign. The proposed technique showed that it can develop a data base of alternative fuels emissions and also act as a guideline for alternative fuels development.

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†passed away in 2013

Glossary and Nomenclature

Glossary	•
CO	Carbon Monoxide
NO _x	Nitrogen Oxides
UHC	Unburnt Hydrocarbon
CRN	Chemical Reactors Network
PSR	Perfectly Stirred Reactor
GA	Genetic Algorithms
CFD	Computational Fluid Dynamics
APU	Auxiliary Power Unit
ICAO	International Civil Aviation Organisation
Nomenclature	•
apu_{nk}	APU experimental emissions data
cal_{nk}	Calculated emissions data
h_k	Specific enthalpies (kJ/kg)
\dot{m}_i	Mass flow rates (kg/s)
v_i	Volumes (m ³)
Q_i	Heat losses (J)
W_k	Molar masses (kg)
Y_k	Mass fractions
$\dot{\omega}_k$	Molar rates of production
Subscripts	•
i	PSR numbers
n	Engine conditions
k	Emission numbers
GAS	Combustion gases
I	Maximum number of PSR
N	Maximum number of engine conditions
K	Maximum number of emissions

Introduction

Conventionally refined jet fuel from crude oil is unlikely to meet future demand for the aviation sector alone. It is likely that the aviation industry will need to diversify into the use of alternative fuels derived from other fossil fuel feedstocks such as Gas to Liquid (GTL) and Coal to Liquid (CTL) fuels [1] or fuels with a Life Cycle Analysis carbon emission lower than conventionally refined fuel. Fuel diversification requires an assessments of the long term impact to engine performance and engine emissions through the combustion

process, as fuels derived from these resources are not as well understood as conventional jet fuel, particularly as advanced, low emission, combustor designs can be more sensitive to changes in fuel composition [2]. The large variety of aircraft engine configurations in use around the world make undertaking a detailed experimental study on alternative fuels emissions across the entire aircraft fleet impractical. Computer modelling could provide a faster assessment than an experimental study since comparable results can be obtained in a relatively short time frame. However, detailed simulation of the emissions of specific combustors by methods such as computation fluid dynamics (CFD) needs detailed knowledge of the engine combustor which is often the proprietary design of engine manufacturers. Therefore, an alternative method to simulate the aviation fleet is required by using publicly available data on specific combustors and engine performance such as the International Civil Aviation Organisation (ICAO) engine emissions data bank [3] or experimental data for specific engines.

A simulation method called Genetic Algorithm optimised Chemical Reactors Network (GACRN) [4, 5] was developed to tackle the problem in predicting alternative fuels gaseous emissions of Carbon Monoxide (CO), Nitrogen Oxides (NO_x) and Unburned Hydrocarbons (UHC) in aircraft engines. The amounts of these gaseous emissions are regulated by the ICAO during the landing-take off cycles. Both CO and UHC emissions are at their highest level while the engine is running on idle and NO_x is at its highest level during full power condition. The focus of this paper is to review this novel emissions predicting technique aimed at reverse engineering the air splits ratios of a gas turbine combustor to predict the gaseous emissions from the combustion of alternative fuels.

Methodology of the Chemical Reactors Network

CRN is a technique that connects discrete reactors together to discretise a non-homogeneous chemical species concentration in a fixed volume. Gas turbine combustors are designed with air entrainment at various locations through the combustor which generates intense turbulence and mixing the reacting gases and fuel. These combustion reaction taking place in these regions of high mixing in the combustor are limited by the rate of chemical reactions, rather than the rate of mixing and can be approximated by a network of perfectly stirred reactors (PSR). Therefore, the concentrations of specific chemical species in the PSR are only governed by the chemical kinet-

ics applied to the model. The chemical balances in each PSR are determined by initial chemical concentrations and thermodynamics properties of the PSR volume such as pressure, temperature and residence time. The Swithenbank model [6] was one of the first CRN to be used in simulating combustion processes in gas turbine engines with a seven reactors model consisting of PSR and plug flow reactors. The flow rate distributions were evaluated by the area of the holes and its corresponding discharge coefficient. In the vicinity of the air entrainments, the kinetic energy in the impinging jet is dissipated in turbulent eddies which result in a high degree of mixing, and can be modelled using zero dimensional perfectly stirred reactors. The CRN model can also be defined by using CFD calculations [7, 8, 9, 10, 11]. Integrated CRN and CFD approach has been applied extensively in evaluating emissions in gas turbine combustors, but both of the Swithenbank model and the CFD-CRN models require knowledge of the detailed geometry of engine combustors in advance of any assessment. Without this information, the CRN cannot be developed unless an engine is in a design stage. K.Choo et al.[12] recognised that CFD was too computational costly for predicting soot emissions of aircraft engines in conceptual designs, so they developed a combined CRN and empirical equations model by using polynomial regression methods to apply the data to the actual operating conditions at the primary combustion zone. In the case of working with established gas turbine combustors without the access of the design, a search method that can estimate the flow rates and sizes of reactors by comparing the results of the network against a set of output criteria is needed, e.g. calculated and measured emissions data in this respect. A Genetic Algorithm approach [4, 5] was selected as the most suitable method for this purpose because it is easy to implement without the need to rearrange the governing equations. This is a self-contained solution for problems of a black box process rather than a competition with methods using CFD.

What do Genetic Algorithms do?

The concept of GA was originally introduced by John Holland et al. [13] to simulate the adaptive process of nature in artificial systems which retains the important mechanisms of nature such as selection, breeding and mutation. It was then widely adapted into engineering by Goldberg and Michalewicz [14, 15]. It also found its use in optimising chemical kinetics [16, 17, 18] and design of gas turbine engines [19] where both applications involved large number of variables to optimise. The GA has an adaptive and self-guiding yet random behaviour. Practically, the fitness of the calculated results is

weighted towards relatively more important goals because computer models are usually simplified and research projects are limited by time. Therefore the fitness function determines the fitness of the results from a weighted solution map rather than the real solution space. For example, provided that there are known number of variables and the favourable goals are big and strong for human being, then the GA will tune the variables until it finds the right values to build the biggest and the strongest human. The goals to be met are problems dependent but since the GA only needs access to the variables, it is easy to implement by giving it the variable to alter. However, the GA has no access to the auxiliary information of the system which it only sees the solution map governed by the variables. A solution domain can be imagined as a landscape with a lot of peaks and valleys of different altitudes. If one wants to search for the highest peak in the entire landscape (global optimum) and searched with one team, then the chance of finding the highest peak in a limited time is very small and in most cases it is only realistic to assume that a local peak (local optimum) will be identified. However, if one sends multiple teams to search the whole landscape at the same time, allowing them to communicate (breeding or crossover of information) with each other and randomly exploring areas for the whole process, the chance of finding the highest peak will increase dramatically. In short, the GA searches for optima in parallel over various locations on the solution map and it gets the direction by combination of information and random exploration of the whole solution space.

In this paper, the GACRN method was implemented to search for the entrained air flow splits ratios and the volumes of the reactors forming the discretised combustor volume. Data from experimental emissions dataset was used to compare with the calculated emissions data from the GA searched air flow splits ratios and volumes of the reactors.

The Auxiliary Power Unit (APU) alternative fuels emissions campaign

To evaluate the feasibility and accuracy of the GACRN, exhaust emission measurements were performed on a re-commissioned Artouste Mk113 APU, located at the University of Sheffield's Low Carbon Combustion Centre. This engine found application in the RAF Victor Bomber (retired 1993), supplying both pressurised air for main engine starting and electricity to the aircraft systems. Despite the apparent age of the hardware, the simplicity and the small size of the APU provided an ideal laboratory platform. The Artouste is

a single spool gas turbine engine, in which a centrifugal compressor is driven by a two stage turbine through a single rotating shaft as shown in Figure 1. The APU combustor has a reverse flow annular combustor such that a proportion of the total air from the compressor enters the primary combustion zone [2] directly at the outer holes, while some goes through the hollow nozzle guide vanes before entering the primary combustion zone. The amount of air entering in different location of the combustor is controlled by the air flow split ratios which is defined by the size of the holes. The fuel injector design is a slinger system which injects the fuel into the primary combustion zone through a row or two rows of holes from the shaft by taking advantage of centrifugal forces acting on the fuel spray by rotating the shaft to assist fuel atomisation. The CO, NO_x and UHC emissions of Jet fuel (JetA-1), synthetic gas to liquid jet fuel (GTL), JetA-1 and GTL 50/50 by volume blend and rapeseed bio-diesel were collected during the campaign [1, 4, 20]. The APU was started on Jet A-1 and once stabilised, it was switched over to an alternative fuel. The APU was set to run for approximately 6 minutes at idle then 6 minutes on full power, before returning to idle. Continuous logging allowed for the identification of stable emission data. Table 1 shows the engine conditions for various fuels. The APU was controlled to a constant shaft speed, which drives, via a gear box, the fuel pump. The higher viscosity and lower energy content of the bio-diesel fuel prevented the engine from running at the same engine conditions as Jet A-1.

Flow of the GACRN

The procedures of the GACRN are shown in Figure 1 together with the Artouste APU and an illustrative CRN. Initially a template CRN with two rows of PSRs was constructed to represent the outer and inner side of the annular combustor. At the end of the dilution zone, one PSR was used to combine the two streams of hot air together before the combustor exit. In total, there were sixteen PSR in the CRN and the total volume of the network was kept constant but the discretisation of this volume by the network was a variable in the optimisation method. The shape of the reactor network show in figure is illustrative, and prior knowledge of the combustor geometry is not assumed by the optimisation method. It is a process that purely focused on matching emissions output by tuning the air splits/volume ratios. No exact geometry of this combustion zones were known and will know from the optimisation. This gave the speed to this method while sacrificing an accurate representation of the fluid dynamics of the combusting flow.

The GACRN started with a randomly generated parent population of air splits/volume ratios. Both of the air splits and volume ratios were treated as float point decimal numbers. This first population was evaluated in the CRN. Fitness values were given by comparing the calculated emissions to experimental data. Based on the fitness values, the GA selected relatively fitter solutions for breeding with a tournament selection process [17]. Then the selected parents were bred to form three children by using the linear crossover method [21]. After the crossover process, the children had small chances to mutate several of the air splits/volume ratios by the non-uniform mutation method [15]. The children population was evaluated and then consolidated into the intermediate population with a 3 to 2 process from each family. The new population favoured the make up by children unless there are some air splits/volume ratios in the children population that could not generate any results, such as the air splits/volume ratios caused flame out in the network. In that case, individuals from the parent population are chosen in descending order of fitness to fill the new population. This cycle repeated until the arbitrarily chosen maximum number of generations is reached. Once the model is converged, the engine CRN model was ready to predict alternative fuels emissions performance.

Table 1: Engine conditions

Power Settings	Fuel Flow(g/s)	Fuel Temperatures(K)	Air pressure(MPa)	Air Temperatures(K)	Air flow rate(g/s)
Full power(all other fuels)	30.19	306	0.312	477.8	2308
Idling(all other fuels)	15.9	301	0.1404	373	1298
Full power(Bio-diesel)	31.79	306	0.34	474	2525
Idling(Bio-diesel)	15.4	301	0.122	357	1130

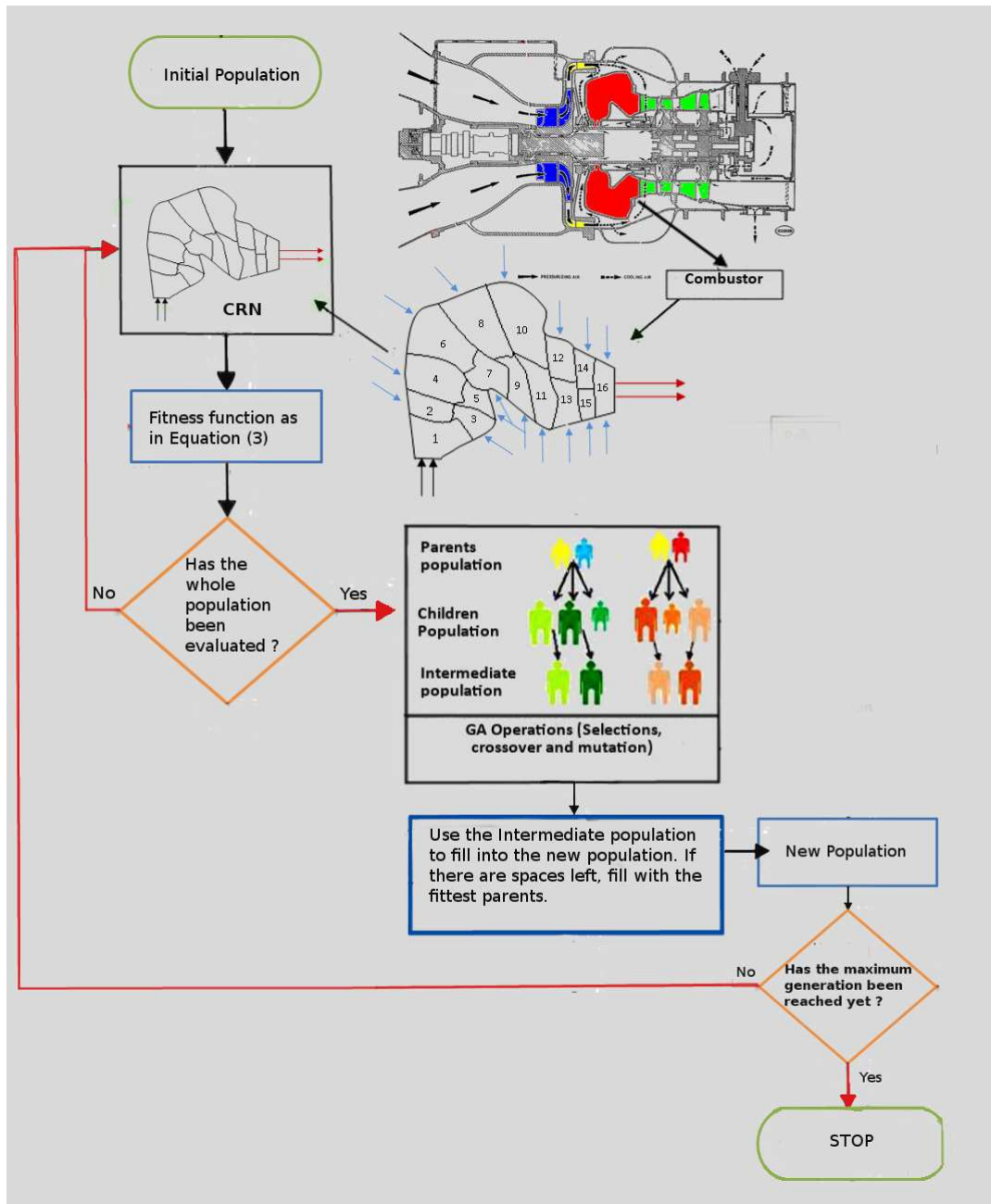


Figure 1: Schematic diagram of the APU, CRN and the procedures of the GA

Implementation of the GACRN

Since the aim of developing the GACRN is to create CRN models of different engines to predict future alternative fuels emissions output, so the optimisa-

tion process is based on using current Jet A-1 emissions data. Jet A-1 consists of thousand kinds of hydrocarbons [22], so it is impossible to simulate without reducing the number of components. Therefore the Jet A-1 was mimicked by a surrogate fuel of 89% n-decane ($C_{10}H_{22}$) and 11% toluene (C_7H_8)[23]. The PSR [24] was operated in conjunction with the CHEMKIN II [25] library. A semi-detailed chemical kinetics scheme namely, AFRMv1.0 [23] consisted of 84 chemical species and 440 reversible reactions. This scheme is small compare to the proposed detailed schemes of approximately 220 variables and 1500 equations [26]. The scheme was small enough to allow every CRN calculation to complete within few minutes. For a fair comparison, all alternative fuels were simulated with a combined AFRMv2.0 [27] and Heptane [28] chemical kinetics scheme in the optimised CRN. By following the guidelines in previous works [27, 29], all repeated chemical routes in the Heptane scheme were removed and no reaction rate parameters were changed in the combining process. The structure of bio-diesel is very similar to fatty acid methyl esters while GTL synthetic fuel is essentially a mixture of linear alkanes of different C-chain lengths [29]. Therefore it is possible to simulate them with simpler surrogates. With the same surrogate methodology, the GTL and the bio-diesel were mimicked by Heptane C_7H_{16} and Methyl-Butonate (MB) $C_5H_{10}O_2$ respectively. Note that the MB has less energy content than the rapeseed bio-diesel, which are 26.7MJ/kg and 40MJ/kg respectively [30, 31], so the fuel flows in the model had been increased to compensate this difference. The assessment of the technical suitability of alternative fuels however is broader than just focusing attention on combustion performance. The specification and approvals process for alternative aviation fuels is rigorous and robust. It is also known that MB have poor low temperature properties and thermal stability performance [32] but these concerns are beyond the scope of the simulation process focused on the emissions.

The governing equations of the PSR output are presented in the following simplified equations:

$$EnergyConservation : (\dot{m}_i + \dot{m}_{GASi}) \sum_{k=1}^K (Y_k h_k - Y_k^* h_k^*) + Q_i = 0 \quad (1)$$

$$MassConservation : (\dot{m}_i + \dot{m}_{GASi})(Y_k - Y_k^*) - \dot{\omega}_k W_k v_i = 0 \quad (2)$$

Where for the k th species, Y_k is the mass fraction, W_k is the molar mass, h_k is the specific enthalpy, $\dot{\omega}_k$ is the molar rate of production. \dot{m}_{GASi} \dot{m}_i ,

v_i and Q_i are the combustion gases mass flow rate, the air mass flow rate, reactor volume and heat loss of the i th PSR respectively. The upper case * stands initial condition. Note that the volume of the reactors are defined as a three dimensional Cartesian space contained by the virtual reactors. For details of the chemistries, readers are recommended to follow CHEMKIN II [25] and chemical kinetics mechanisms [23, 27, 28, 29] for further information.

A real number encoded GA was implemented which is a closer resemble of the real space and as shown by Elliott et al. [17] that it has a better chance to find the global optimum in smaller number of generations with local fine tuning by the non-uniform mutation than binary representation. The air mass flow rates and reactor volumes were presented in the following format for each individual in a population:

$$(\dot{m}_1 v_1 \dot{m}_2 v_2 \dot{m}_3 v_3 \dots \dot{m}_I v_I) \quad (3)$$

Where I is the maximum number of PSR. The GA's job was to alter the \dot{m}_i and v_i . The combustion gases mass flow rates are depended on the upstream PSR's mass flow rates. The code would repair the air splits/volume ratios to keep the total mass flow rates and total volume constant. The optimisation of the air splits/volume ratios were analysed by the following maximisation fitness function [17]:

$$fitness(\dot{m}_1 v_1 \dot{m}_2 v_2 \dots \dot{m}_I v_I) = [10^{-8} + \sum_{n=1}^N \sum_{k=1}^K w_k (\frac{cal_{nk} - apu_{nk}}{apu_{nk}})]^{-1} \quad (4)$$

Where n is the index for engine conditions and N is the maximum number of engine conditions, k is the index for number of emissions and K is the maximum number of emissions, cal_{nk} , apu_{nk} are the calculated emissions data and APU experimental data respectively. The constant 10^{-8} is designed to stop numerical overflow, however it must be small enough to not intervene the GA optimisation. The optimisations were weighted on the larger emissions in each engine condition. Due to the size of the APU, it does not produce significant amount of NO_x even at the full power condition. Both the CO and UHC emissions formed in larger proportions of the emissions than NO_x , thus they were weighted more heavily than the NO_x in the fitness function. The control settings of GA are presented in the Table 2. These values were adopted and fine tuned by previous works [17, 4, 33]

Table 2: GA control settings

Control Settings	Values
Parents Population	50
Children Population	60
Maximum number of generations	1000
Selection Probabilities	0.8
Crossover Probabilities	0.65
Mutation Probabilities	0.05
Elitism	2

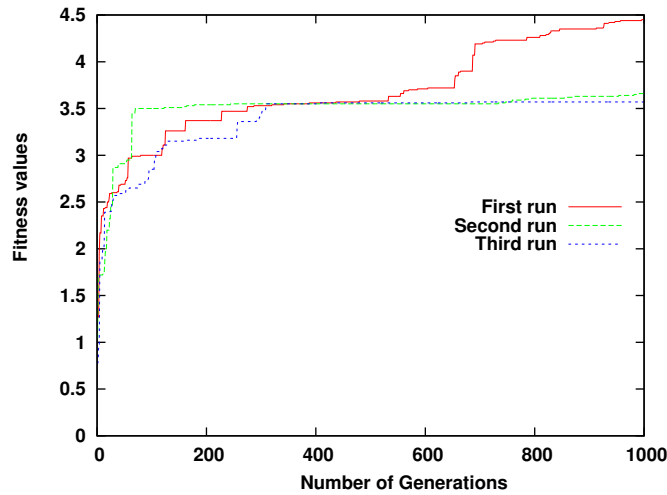


Figure 2: Convergence of the GA searches

Optimisation Results

Due to the embarrassingly parallel nature of the GA, each potential solution were organised to be calculated in recurring job arrays in the ICEBERG [34] cluster and the fitness results at the end of each generation were collected for the GA to breed the next generations. This method was shown to have less waiting time for the resources than implicitly parallelising the GA. Three separate runs were performed for 1000 generations. The modelling results were obtained with seventy five 2.4GHz AMD Opteron nodes over 65 hours of computation on each run. The numerical calculations in the PSRs consumed over 99% of the computational time and less than 1% of the time was assigned for the GA optimisation. Figure 2 shows the convergence graph of

the three GA runs which the large improvements of the fitness values were mostly occurred in the early stages and the later changes are restricted to some fine tuning of the air splits volume ratios. The best air splits volume ratios from the three runs were averaged before operated with the combined scheme to access the emissions performance of the alternative fuels and compared to the APU experimental data without any further optimisation.

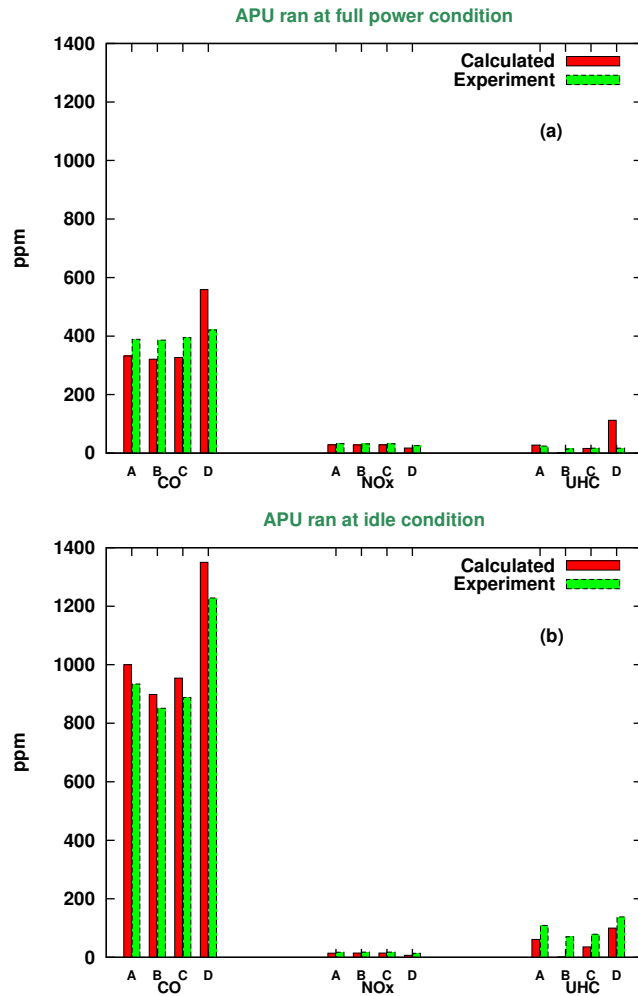


Figure 3: a) Full power b) Idle, A stands for Jet A-1 emissions ,B stands for GTL emissions ,C stands for Jet A-1 and GTL 50/50 blend, D stands for Bio-diesel emissions

The results are compared to the measured emissions data in Figure 3 obtained from the APU while running with Jet A-1, rapeseed bio-diesel, GTL

and JetA-1/GTL 50-50 blend (JetA-1/GTL blend). It is important to notice that the engine outputs varied from different fuels due to the APU struggled to maintain similar engine conditions during the campaign. At both engine conditions, the CO and NO_x emissions are very well replicated with minimal errors. Lower amount of CO and equal amount of NO_x emissions compared to JetA-1 can be observed in GTL and JetA-1/GTL blend. Due to the lower flame temperatures of bio-diesel combustion, a reduction of NO_x and an increased in CO emissions were observed in the model. The most challenging calculation is the UHC emissions. The modelled UHC emissions disappeared completely for the GTL case which suggests that the surrogate fuel is more efficient than the actual fuel in the combustion. A large spike in the modelled bio-diesel UHC emissions for the full power condition was observed in comparison to the experimental data. Although the chemical kinetics scheme was validated against designed conditions with accurate prediction of the main combustion products such as CO₂, CO and H₂O, the trends in the smaller chemical species are less accurate. Due to the low concentrations of hydrocarbons, the discrepancies in these hydrocarbons do not affect the accuracy of the chemical kinetics scheme. However, the UHC emissions have also cumulated the discrepancies in each hydrocarbon which affected the prediction in the CRN. The same apply to the CO and NO_x but both are less sensitive to the cumulative errors than UHC because the numbers of chemical species involved are relatively less. The change to the combined scheme for alternative fuels had added another layer of uncertainty. This is why the GA optimisations were weighted to maximise the accuracy. It was found that most of the UHC in the modelling were coming from the break down of toluene in the CRN model. Without the toluene present in the GTL surrogate, not enough UHC were formed. In the MB combustion, the fuel flows were increased to match the CO₂ emissions in the bio-diesel combustion, as a result, the air/fuel ratio has been changed which in term increased the CO and UHC emissions.

Extrapolation with the optimised CRN

Next, two component fuel blends of different percentages were tested in the optimised CRN model. This test assumed that all the fuels were working at the same engine conditions as the Jet A-1 and the output temperatures were brought to 1037K and 918K in the full power and idle conditions respectively to ensure equal energy output. The results are shown from Figure 4. The first chart suggests that NO_x reduction is favourable with the increase of MB

and reached its minimum with 100% MB. NO_x production is highly temperature dependent, so the lower combustion temperatures of MB would result in less NO_x emissions. Jet A-1/GTL blends produced similar amount of NO_x because of their minimal difference in flame temperatures. In these cases, the NO_x emissions were depended on the proportion of MB component in the fuel and therefore the Jet A-1/MB blends and GTL/MB blends almost mirrored each other in the NO_x emissions.

Figure 4b suggests that CO emissions of the blended fuels. When the blends were closed to 100% GTL, the CO emissions dropped slightly. This result suggests that GTL component has reduction effect in the CO emissions. On the other hand, when the blended fuels increased with the MB component, the CO emissions were also increased. GTL contains only a linear alkane which burns more efficiently than the other two fuel components. In general, the GTL/MB blends performed better than Jet A-1/MB blends in combustion efficiencies with lower CO emissions.

Figure 4c shows a dramatic increase in UHC emissions with any MB blends which suggested that the MB component is less combustion efficient than the other two components. Since there was only linear alkane in the GTL component, only low UHC emissions were able to form with the GTL blended fuels. The lack of UHC emissions in the GTL component and spiking increase of UHC emissions by the MB component produced two different sizes of semi oval shapes connected together in the graph. As suggested by the results, a 50% GTL and 50% MB blended fuel is desirable for the most optimum solution where all three emissions are reduced, i.e. improved combustion efficiencies and lower flame temperatures. Also, this fuel blend is potentially more sustainable than Jet A-1. In other words, a fuel that formed by linear C chain alkanes such as Heptane and biologically derived methyl-esters such as MB can be a better alternative than conventional Jet A-1. Clearly, however other considerations such as energy density, temperature properties and thermal stability performance are required for the approval of alternative aviation fuels.

Further discussions

The GACRN was developed to save time and be accurate enough to access the emissions performance of the entire fleet of aircraft engines. This paper presented a fast method to emissions prediction by sacrificing detailed

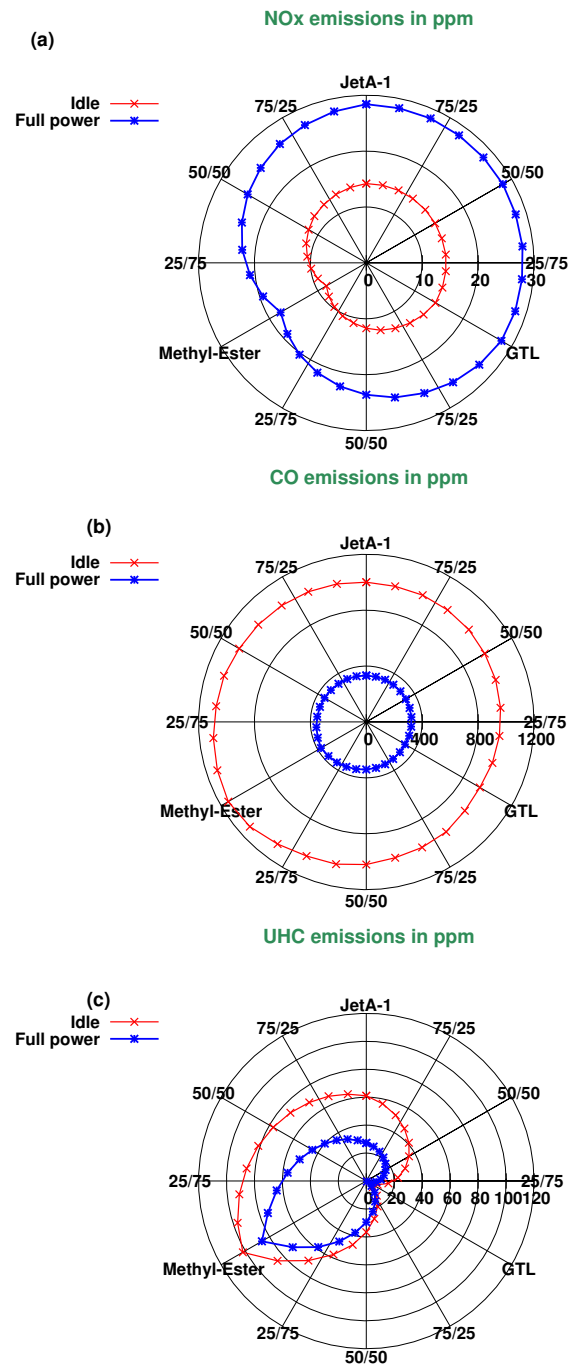


Figure 4: Emissions of JetA-1/GTL blends, JetA-1/MB blends and GTL/MB blends a)NO_x, b) CO, c) UHC

information of combustion gas fluid dynamics in the combustor. This simplification showed that the results on predicting the emissions from an APU operating on different fuels were producing similar trends to the experiment data. It also demonstrated that the optimised model can be used as a tool to identify a fuel blend that is potentially beneficial to both emissions reduction and sustainability of supply. However, there were more errors found in UHC emissions than CO and NO_x emissions.

The real fuels have been simplified by the semi-detailed chemical kinetics schemes and multi-component fuels. Then the previously validated chemical kinetics schemes have been applied to an engine model built with a CRN which the geometry of the combustor was neglected. Finally, this solution space was weighted and then searched by the GA which also assumed that an optimum or optima exist in the space. The errors existed in each layer affected the UHC emissions substantially while the other two emissions are almost resilient to these errors. It could be that the volatility in UHC prediction are caused by the larger number of chemical species involved in the formation process in comparison to CO and NO_x emissions. Indeed, this type of modelling restriction is true regardless whether it is a GACRN or a CFD-CRN approach because both will rely on the completeness of the chemical kinetic scheme. After all, even there is a perfect chemical kinetics scheme, the trade off between the potential upside and the increase in computation time is too large. Therefore development of simple approaches that can tackle certain problems directly is more important than developing a perfect tool. In areas such as redesigning air flow splits ratio for alternative aviation fuels to fit within a pre-set emissions criteria, the GACRN approach would contribute to reduce the time in setting up experiments for multiple designs.

Conclusion

A model of an APU combustor based on the GACRN approach has been created and it demonstrated that it can closely replicate the emissions data of alternative fuels combustions in the experiment. It demonstrated that a model could be built within a week without knowledge of the detailed geometries and flow splits ratios. The CRN model is not restricted to use with any particular fuel, therefore any further alternative fuel tests could be implemented without any further modifications to the model. Thus, the generation of an alternative fuels emissions data base of an entire fleet of aircraft engines would be feasible with the GACRN approach. The resulting model was used to extrapolate emissions results in combustion of different blends of Jet A-1, GTL and MB in the same APU CRN without further optimisations

needed. Analysis based solely on the results of this model suggests that a fuel blend of 50% linear alkane and 50% bio-methyl ester would reduce overall emissions. Due to the use of bio-methyl ester in the fuel, it would increase the sustainability of the jet fuel. Clearly, however other considerations are required for the approval of alternative aviation fuels. Finally, the GACRN approach would also find its use in area such as assisting air flow splits ratio modifications for specific alternative fuel according to pre-set emissions criteria.

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References

- [1] S. Blakey, L. Rye, and C. W. Wilson, *Aviation Gas Turbine Alternative Fuels: A Review*. Proceedings of the Combustion Institute, 2011, 33, p. 2863 - 2885
- [2] A. H. Lefebvre and D. R. Ballal, *Gas Turbine Combustion - Alternative Fuels and Emissions*, 2010, Chapter 1 and 10
- [3] *ICAO Data Bank*, <http://www.caa.co.uk/default.aspx?catid=702>.
- [4] C. C. Leong, S. Blakey, L. Rye, and C. W. Wilson, *Reverse Engineering Gas Turbine Emission Performance: Applied to An Aircraft Auxiliary Power Unit*. ASME Turbo Expo, 2010, June 14-18 2010, Glasgow, UK.
- [5] M. Akram, C. Leong, and S. Blakey, *Chemical Kinetic analyses of Combustion for Carbon Capture from Gas Turbines using Exhaust Gas Recycle*. Journal of Energy Challenges & Mechanics, 2014
- [6] J. Swithenbank, I. Poll, D. D. Wright, M. W. Vincent, *Combustor Design Fundamentals*. Symposium (International) on Combustion, 1973(1): p. 627 - 638.

- [7] M. Falcitelli, S. Pasini, N. Rossi, L. Tognotti, *CFD+Reactor Network Analysis: An Integrated Methodology for the Modeling and Optimisation of Industrial Systems for Energy Saving and Pollution Reduction*. Applied Thermal Engineering, 2002. 22: p. 971–979.
- [8] I.V. Novosselov, P.C. Malte, S. Yuan, R. Srinivasan, J.C.Y. Lee, *Chemical Reactor Network Application to Emissions Prediction for Industrial DLE Gas Turbine*. ASME Turbo Expo 2006: Power for Land, Sea and Air, Barcelona, Spain.
- [9] I. V. Novosselov, *Eight-Step Global Kinetic Mechanism on Methane Oxidation with Nitric Oxide Formation for Lean-Premixed Combustion Turbines*, Master of Science in Mechanical Engineering , University of Washington, . (2001)
- [10] M. Kanniche, *Modelling Natural Gas Combustion in Gas Turbine: Coupling 3D Combustion Simulations with Chemical Reactor Network for Advanced NOx Prediction*. EDF, Research and Development Division, 6 quai Watier 78401 Chatou cedex, France
- [11] R. F. D. Monaghan, R. Tahir, G. Bourque, R. L. Gordon, A. Cuoci, T. Faravelli, A. Frassoldati, and H. J. Curran, *Detailed Emissions Prediction for a Turbulent Swirling Nonpremixed Flame*. Energy and Fuels, 2014, 28 (2), pp 1470–1488
- [12] K. H. Choo, S. Lee, R. K. Denney and D. N. Mavris, *A Semi-Empirical Model to Predict Aircraft Soot Emission in Rich Zone of RQL Combustor*. ASME Turbo Expo 2015: Turbine Technical Conference and Exposition Volume 4B: Combustion, Fuels and Emissions Montreal, Quebec, Canada, June 15–19, 2015. GT2015-43659
- [13] J. H. Holland, *Adaptation in Natural and Artificial Systems*. (1975).
- [14] D. E. Goldberg, *Genetic Algorithms in Search, Optimization, and Machine Learning* (1989).
- [15] Z. Michalewicz, *Genetic Algorithms + Data Structures = Evolution Programs*. (1999).
- [16] L Elliott, D.B. Ingham, A. G. Kyne, N. S. Mera, M. Pourkashanian, C.W. Wilson, *Genetic Algorithms for Optimisation of Chemical Kinetics Reaction Mechanisms*. Progress in Energy and Combustion Science, 2004. 30: p. 297 - 328.

- [17] L. Elliott, D. B. Ingham, A. G. Kyne, N. S. Mera, M. Pourkashanian, C.W. Wilson, *A Novel Approach to the Optimisation of Reaction Rate Parameters for Methane Combustion Using Multi-Objective Genetic Algorithms*. Journal of Engineering for Gas Turbines and Power, 2004. 126: p. 455 - 464.
- [18] W. Polifke, W. Geng, K. Döbbeling, *Optimization of Rate Coefficients for Simplified Reaction Mechanisms with Genetic Algorithms*. Combustion and Flame, 1998. 113: p. 119 - 135.
- [19] A. Despierre, P.J. Stuttaford, and P.A. Rubini, *Gas Turbine Combustor Design Using Genetic Algorithms*, Int. Gas Turbine and Aeroengine Congress & Exhibition, : Orlando, Florida, June 2 - 5, 1997.
- [20] S. Blakey, L. Rye, and C. W. Wilson, *Emissions from an APU Operating on a Range of Alternative Fuels*, SWAFEA members meeting, Paris, France (2010).
- [21] A. H. Wright, *Genetic Algorithms for Real Parameters*. 1991.
- [22] M. Colket, T. Edwards and S. Williams, N. P. Cernansky, D. L. Miller, F. Egolfopoulos, P. Lindstedt, K. Seshadri, F. L. Dryer, C. K. Law, D. Friend, D. B. Lenhart, H. Pitsch, A. Sarofim, M. Smooke, W. Tsang, *Development of an Experimental Database and Kinetic Models for Surrogate Jet Fuels*. AIAA, 2007.
- [23] P. M. Patterson, A. G. Kyne, M. Pourkashanian, A. Williams, C. W. Wilson, *Combustion of Kerosene in Counterflow Diffusion Flames*. Journal of Propulsion and Power, 2000. 16(2): p. 453 - 460.
- [24] P. Glarborg, R.J. Kee, J.F. Grcar, J.A. Miller, *PSR: A FORTRAN Program for Modelling Well-Stirred Reactors*. Sandia National Laboratories SAND86-8209, 1988. SAND86-8209.
- [25] R. J. Kee, F. M. Rupley, E. Meeks, J. A. Miller, *CHEMKIN-II: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics* Sandia National Laboratories Report SAND89-8009 (1989)
- [26] P. Dagaut and M. Cathonnet, *The Ignition, Oxidation and Combustion of Kerosene: A Review of Experimental and Kinetic Modeling*. Progress in Energy and Combustion Science, 2006. 32: p. 48 - 92.
- [27] M. Pourkashanian, K. Hughes, I. Shafagh, E. Catalanotti, I. Uryga-Bugajska, C.W. Wilson, *Combustion of Alternative Aviation Fuel:*

Multi-scale, First-Principles-Based Development of Predictive Kinetic Mechanism and its Application to CFD Modelling and System Simulation. Omega Report 2009

- [28] R. Seiser, H. Pitsch, K. Seshadri, W.J. Pitz, H. J. Curran, *Extinction and Autoignition of n-Heptane in Counterflow Configuration.* Proceedings of the Combustion Institute, 2000. 28: p. 2029 - 2037.
- [29] E. Catalanotti, K. J. Hughes, M. Pourkashanian, C. W. Wilson, *Development of a Chemical Reaction Mechanism for Alternative Aviation Fuels.* Energy & Fuels, 2011(25): p. 1465 - 1473
- [30] I. Uryga-Bugajska, M. Pourkashanian, D. Borman, E. Catalanotti, C.W. Wilson, *Theoretical Investigation of The Performance of Alternative Aviation Fuels in an Aero-Engine Combustion Chamber,* CEAS 2009, 26 - 29 October, Manchester, UK
- [31] A.K. Jasuja and J.B. Moss, *Sustainable Fuels for Aviation: Final report: Combustion Characteristics of Kerosene - Biofuel Blends.* Omega report, 2008.
- [32] A.M. Mohibbe, A. Waris, and N.M. Nahar, *Prospects and potential of fatty acid methyl esters of some non- traditional seed oils for use as biodiesel in India.* Biomass and Bioenergy, 2005. 29: p. 293-302.
- [33] C. C. Leong, *A Novel Technique for Predicting Alternative Fuels Emissions in Aircraft Engines: GACRN,* Chapter 2 and 3, PHD thesis in Mechanical Engineering, University of Sheffield, (May 2012)
- [34] *Iceberg cluster,* <https://www.shef.ac.uk/wrgrid/iceberg/specs>.