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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.

1. 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. The information is often the proprietary design of engine manufacturers. Therefore, an alternative method to simulate the aviation fleet is required by using engine performance data and emissions data from the public domain. These include engine performance and experimental emissions data from literatures and from the International Civil Aviation Organisation (ICAO) engine emissions data bank [3].

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 further explore this novel emissions predicting technique aimed at reverse engineering the air splits ratios of a gas turbine combustor

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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

to predict the gaseous emissions from the combustion of alternative fuels.

2. 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 kinetics 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 [7–11]. 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.

3. 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 [16–18] 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