CRANFIELD UNIVERSITY

KADAMBARI LOKESH

TECHNO-ECONOMIC ENVIRONMENTAL RISK ANALYSIS OF ADVANCED BIOFUELS FOR CIVIL AVIATION

SCHOOL OF AEROSPACE, TRANSPORT AND MANUFACTURING

PhD
Academic Year: 2012 - 2015

Supervisor: Dr Vishal Sethi

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This thesis is submitted in partial fulfilment of the requirements for the degree of PhD
(NB. This section can be removed if the award of the degree is based solely on examination of the thesis)

ABSTRACT

Commercial aviation has demonstrated its ability to be a key driver of global socio-economic growth to this date. This growth, resulting from an ever increasing need for air-travel, has been observed to be environmentally unsustainable. Any technological enhancements to the upcoming fleet of aircraft or operational improvements have been overshadowed by this very demand for air-travel. Any further investigation into innovative concepts and optimisation approaches bring in trade-off difficulties due to limitations in current technology. This creates a constraint on design space exploration. The need to mitigate civil aviation's environmental impact has necessitated this sector to expand its frontier and seek radical technologies. Among a range of other technologies, advanced biofuels for civil jet engines have been claimed to be one of the most promising solutions.

"Techno-economic Environmental Risk Analysis (TERA) of Advanced Biofuels for Civil Aviation" is a study that contributes to knowledge through conception plus application of quantitative/ qualitative approaches to assess the technical viability, financial feasibility and environmental competence of 2nd and 3rd generation biojet fuels, through their application into the existing scenario of civil aviation, against that of the fossil-derived conventional jet fuel (Conv.Jet fuel). TERA of advanced biofuels aims to accomplish the aforementioned through a holistic, multi-disciplinary study entailing life cycle studies, carbon-foot printing, sustainability analysis, fuel chemistry, virtual studies comprising combustion thermodynamic, engine/aircraft performance and emission prediction, economic studies entailing biofuel price prediction and business case analysis as opposed to earlier studies.

TERA of Advanced biofuels study entails development of elaborate life cycle models, ALCEmB (**A**ssessment of **L**ife **C**ycle **Em**issions of **B**iofuels) and ALCCoB (**A**ssessment of **L**ife **C**ycle **Co**st of **B**iofuels) to predict life cycle emissions and costs, respectively, of the advanced biofuels from the point of raw material generation to the point of finished product consumption (a "cradle-grave" approach). A virtual experiment, to assess the impact of the "performance" properties of the advanced biofuels on a representative twin-shaft turbofan/airframe combination, relative to that of Conv.Jet fuel, was also undertaken through numerical modelling and simulation.

Evaluation through ALCEmB revealed that Camelina-SPK, Microalgae-SPK and Jatropha-SPK delivered 70%, 58% and 64% savings in life cycle emission, relative to Conv.Jet fuel. The Net Energy Ratio (NER) analysis indicates that current technology for the biofuel processing is energy efficient and technically feasible. An elaborate post-combustion gas property evaluation infers that the Bio-SPKs exhibit improved thermodynamic behaviour. This thermodynamic effect has a positive impact on mission-level fuel consumption which reflected as fuel savings in the range of 3 - 3.8% and, therefore, emission savings of 5.8-6.3% in CO_2 and 7.1-8.3% in LTO NOx, relative to that of Jet-A1. An economic feasibility analysis which entails prediction of hypothetical biofuel price prediction and its impact on direct operating cost (DOC) of an aircraft which infers that Bio-SPKs, over a user-defined medium-range mission profile, costs an additional 95-100% in terms of aircraft DOC, relative to that operated with conventional Jet-fuel, within short (2020) and medium (2020). However, the advanced biofuels are able to exhibit financial competence from 2020 onwards, relative to that of Conv.Jet fuel. However, the Bio-SPKs exhibit this economic feasibility only against a backdrop of persistent Conv.Jet fuel price volatility and severe environmental taxation between the analysis periods (2020-2075)

Keywords:

Bio-Synthetic Paraffinic Kerosene, Life Cycle Assessment, Thermodynamics, Engine/Aircraft analysis, DOC.

Dedicated to Lokesh and Anurag………

ACKNOWLEDGEMENTS

I kindly wish to convey my deepest gratitude to my supervisor Dr Vishal Sethi and Dr Eric Goodger for their dedicated support and guidance through the course of this research. I would like to extend my thanks especially to Prof Pericles Pilidis for having provided me the opportunity to pursue this PhD at Cranfield University.

I am obliged to my beloved husband Dr Lokesh Aresh, my son Anurag, my mother Preethi, my father Gopal Raja, my brother Vignesh and all my family in general for all their limitless support and understanding.

I am thankful to all the postgraduate and PhD students who guided me through the complicated scenarios that I encountered during my study as a visiting research student in Gas turbine technology. I hope to cherish their valuable advices and friendship for life.

My heartfelt thanks to Dr Theoklis Nikolaidis, Dr Devaiah Nalianda, Dr Hugo Pervier and Alex Nind, whose guidance and contribution enabled the completion of this research. This study is dedicated to all those who motivated my efforts and were supportive/ tolerant towards the completion of this research, by direct and indirect means. My heartiest thanks to all those mentioned above for sharing their most cherished lives and knowledge with me.

I also would like to thank the Department of Power and Propulsion for funding and supporting this PhD research.

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LIST OF ABBREVIATIONS

ACARE	*Advisory Council for Aviation Research and Innovation in Europe*
ALCCoB-BP	*Assessment of Life Cycle Cost of Biofuels – Biofuel pricing*
ALCCoB-DOC	*Assessment of Life Cycle Cost of Biofuels – Direct operating cost*
ALCEmB	*Assessment of Life Cycle Emissions of Biofuels*
ALCEmB	*Assessment of Life Cycle Emissions of Biojet fuels*
ASTM	*American Society for Testing and Materials*
ATM	*Ait Traffic Management*
atm	*atmosphere (unit)*
AW	*Airframe Weight (kg)*
BC_{cost}	*Biomass Cultivation Cost*
B_CC	*Biomass Cultivation Cost (£/kg Bio-SPK)*
BcY	*Bio-crude yield (kg)*
BH_{cost}	*Biomass Harvest Cost*
BhC	*Biomass harvest Cost (£/kg Bio-SPK)*
Bio-SPK	*Bio-derived Synthetic Paraffinic Kerosene*
Bio-SPK Conv.eff	*Bio-crude to Bio-SPK conversion efficiency (%)*
BT_{cost}	*Biomass Transportation cost*
BY	*Biomass Yield (kg)*
BY	*Biomass Yield (kg)*
CAEP	*Committee on Aviation Environmental Protection*
CEA	*Chemical Equilibrium with Application*
Cp	*Isobaric Specific Heat*
CU- Jet-C	*CU-Jet operated with 100% Camelina SPK*
CU- Jet-J	*CU-Jet operated with 100% Jatropha SPK*
CU- Jet-M	*CU-Jet operated with 100% Microalgae SPK*
CU-Jet	*Cranfield University Jet*
CU-Jet-K	*CU-Jet operated with Jet-A1*
CW	*Crew Weight (kg)*
DC	*Diesel Cost (£/l)*
DEF-STAN	*UK Defence Standard*
DP	*Design Point*
Ds	*Diesel Supply (l)*
DZ	*Dilution Zone*
e	*Potential energy*
EC	*Energy Cost (£/MJ)*
ElC	*Electricity Cost (£/kWh)*
ESFC	*Energy Specific Fuel Consumption (MJ/kN.s)*
EW	*Engine Weight (kg)*
FAR	*Fuel-Air Ratio*

FC	*Feedstock cost (£/kg Bio-SPK)*
FDE	*Fossil-derived Energy*
FFZ	*Flame front zone*
F_n	*Net Thrust, kilonewton*
F_{oo}	*Take-off net thrust, kilonewton*
FPR	*Fan Pressure ratio*
FT_{cost}	*Fuel Transportation cost*
FTP	*Fluid Thermodynamic Properties*
FW	*Fuel Weight (kg)*
gCO_2e/MJ *fuel*	*Grams of* CO_2 *equivalent per megajoule of fuel*
GHGs	*Greenhouse Gases*
gui	*Graphic user interface*
gui	*Graphic User Interface*
GWP	*Global Warming Potential*
H	*Specific Enthalpy, kilojoule per Kelvin*
H/C	*Hydrogen-Carbon atomic ratio*
ha	*hectare*
HC	*Hydrogen Cost (£/kg)*
HeC	*Harvest energy Cost (£)*
HPC	*High Pressure Compressor*
HT_{cost}	*Hydrotreatment Cost*
ICAO	*International Civil Aviation Organisation*
iLUC	*Indirect Land Use Change*
IPCC	*Intergovernmental Panel on Climate Change*
IZ	*Intermediate zone*
kg	*kilograms*
kWh	*Kilo-watt hour*
LC	*Labour Cost (£/hr)*
LCA	*Life Cycle Assessment*
LCE	*Life Cycle Emissions, grams of* CO_2 *equivalent per MJ of fuel*
LHV	*Lower Heating Value, megajoule per kilogram*
LokAir-C	*Model Aircraft operated with 100% Camelina SPK*
LokAir-J	*Model Aircraft operated with 100% Jatropha SPK*
LokAir-K	*Model Aircraft operated with Jet-A1*
LokAir-M	*Model Aircraft operated with 100% Microalgae SPK*
LS diesel	*Low Sulphur Diesel*
LTO NOx	*Landing Take-off NOx emissions*
Mm_C	*Molar Mass of carbon,g per mol*
Mm_{CO2}	*Molar mass of* CO_2*, g per mol*
MPW	*Maximum Payload Weight (kg)*
m_s	*Stoichiometric moles*

MT $ha^{-1}.yr^{-1}$	*metric tonnes per hectare year*
MTOW	*Maximum Take-Off Weight (kg)*
MZFW	*Maximum Zero Fuel Weight (kg)*
NER	*Net Energy ratio*
NgC	*Natural gas Cost (£/MJ)*
ODP	*Off-design point*
OE_{cost}	*Oil Extraction cost*
OeC	*Oil Extraction Cost (£/kg Bio-SPK)*
OEW	*Operating Empty Weight (kg)*
p	*pressure*
$PC_{Bio\text{-}SPK}$	*Production Capacity of Bio-SPKs*
$PC_{Jet\text{-}K}$	*Production Capacity of Jet-Kerosene*
PR	*Pressure ratio*
PW	*Payload Weight (kg)*
PZ	*Primary zone*
R	*Gas constant, Joule per kilogram Kelvin*
RPK	*Revenue-Passenger Kilometre*
S	*Entropy, kilojoule per kilogram Kelvin*
SC	*Solvent Cost (£/kg)*
SFC	*Specific Fuel Consumption, grams per kilonewton sec*
SPK_{Yield}	*Bio-SPK Yield (kg)*
T	*temperature*
T_{amb} & P_{amb}	*Ambient Temperature & pressure, K & kPa*
UHC	*Unburned Hydrocarbon*
v	*volume*
W	*Air mass flow, kg/s*
W_{ff}	*Fuel flow, kg/s*
WsC	*Water supply Cost (£/l)*
x	*Carbon number*
y	*Hydrogen number*
γ	*gamma*
η_{comb}	*Combustor efficiency*
$\eta_{is\ booster}$	*Isentropic booster efficiency*
$\eta_{is\ fan}$	*Isentropic Fan efficiency*

RESEARCH PUBLICATIONS

Journal Publication

Lokesh, K., Sethi, V., Nikolaidis, T., Goodger, E. and Nalianda, D. (2015), "Life cycle greenhouse gas analysis of biojet fuels with a technical investigation into their impact on jet engine performance", *Biomass and Bioenergy,* vol. 77, no. 0, pp. 26-44.

Conference Publication

Lokesh,K. Sethi,V. Nikolaidis,T. Nalianda,D. (2014), "System-level performance and emissions evaluation of renewable fuels for jet engines", Proceedings of the ASME 2014 Gas turbines India Conference, Vol. Combustion, Fuels and Emissions, Dec 15-17, New Delhi, India, American Society for Mechanical Engineers, pp. 1-13.

Lokesh,K., Prakash, A., Sethi, V., Goodger, E., Pilidis, P., (2013), "Assessment of Life cycle emissions of Bio-SPKs for Jet engines (GT2013-94238)", Proceedings of ASME TurboExpo ASME Turbo Expo 2013: Turbine Technical Conference and Exposition. Volume 2: Aircraft Engine; Coal, Biomass and Alternative Fuels; Cycle Innovations. San Antonio, Texas, USA, June 3–7, 2013, pp 1-24

1 GENERAL INTRODUCTION

1.1 Context of Research

Civil Aviation is a highly complex, yet a well-organised sector among the transportation industry. This sector has been instrumental in connecting 220 countries with scheduled services bringing different parts of the world within the reach of the travellers [62]. Besides travel for leisure, civil aviation facilitates establishment of international business infrastructures which boosts the nation's GDP (Gross Domestic Product). With business infrastructure comes skilled workforce, competition, capital investments, cultural diversity and tourism all of which contribute to cultural and socio-economic development through job creation.

The growth of civil aviation has been observed to be phenomenal in the last 5 decades. This industry currently faces 80 times more passenger volume compared to just over 30 million passenger departures recorded in the 1950s [5]. Environmental organisations such as the International Panel for Climate Change (IPCC) have acknowledged civil aviation to be "one of the fastest growing means of transport" in 2007. The ultimate driver of this growth is air travel which is generally measured from the metric for the airline's passenger volume called as Revenue Passenger-Kilometre (RPK). International Air Transport Association (IATA) reported that the RPK, attributable to global international travel, fell to -1.1% in 2009 (due to global economic recession) from 8.9% in 2007 and surreally recovered to 8% in 2010. This demonstrates the perpetual demand for air-travel [65] & [66]. Besides the globe trotters, competition among the airline operators and subsequent marketing strategies (loyalty schemes, frequent flyer points and seasonal offers) contribute to such an increase in air-traffic. Besides the unequivocal benefits of globalisation, unsustainable growth of civil aviation also leads to two major consequences as.

- Environmental: through uncontrolled emission of aviation based pollutants into the atmosphere leading to greenhouse effect and eventually global warming. This effect is alarming due to direct injection of pollutants into the upper atmosphere leading to prolonged pollutant life and thus enhanced greenhouse impact.

- Economic: through constant creation of instability in jet-fuel supply-demand, a major cause for its price volatility.

The “Four-pillar” strategy, conceived by the International Air Transport Association (IATA), to mitigate aviation carbon di-oxide (aviation CO_2) emissions from the ever-increasing air-traffic demand clearly indicates the need for the environmental impact through the following four measures

- **Technology**- engine, airframe development and alternative fuels
- **Operations**- efficient engine/ aircraft operations and weight reduction
- **Infrastructure**- harmonisation of air routes, air-traffic management (ATM) and improvement of airport operations
- **Market Measures** – emission Trading, taxations and incentives.

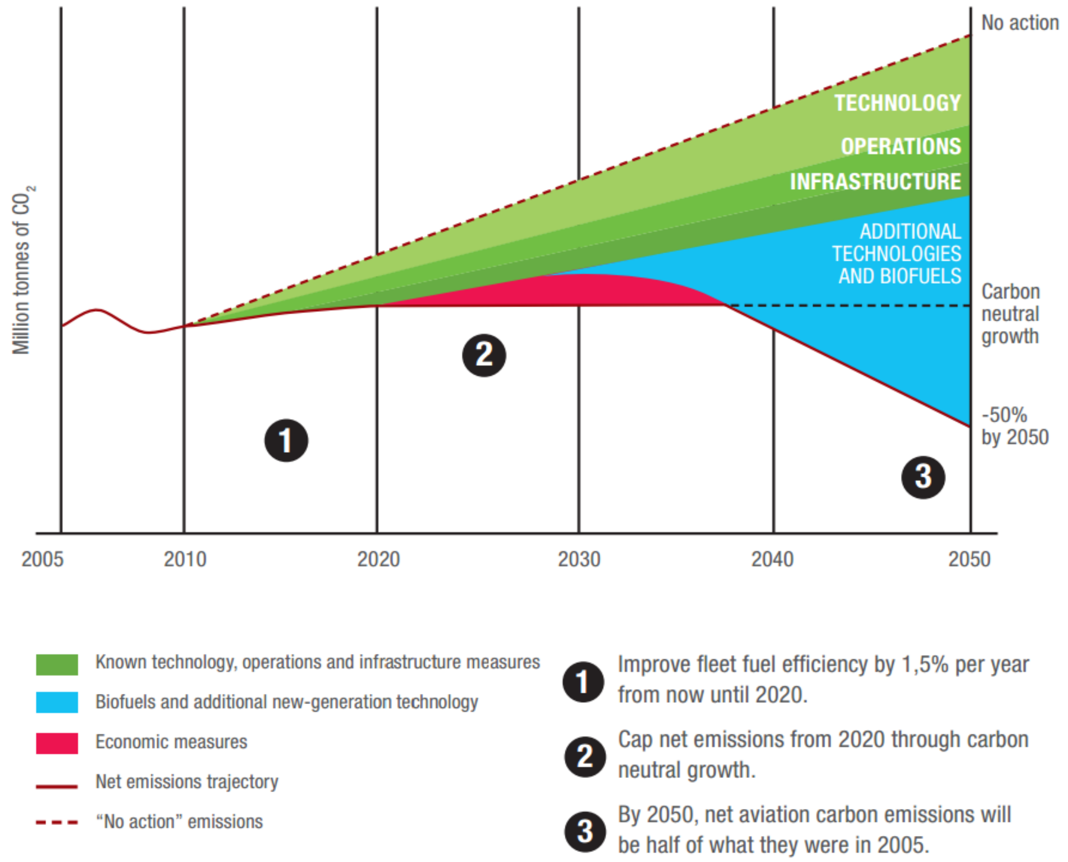


Figure 1-1: A Schematic of “Four Pillar approach” [70]

A schematic of the "Four-pillar" approach [presented in Figure 1-1] indicates the "business-as-usual" (No Action) scenario which without any environmental actions could lead to roughly 150% increase in aviation CO_2 emissions (by 2050) from international air travel. However, infusion of existing state-of the art technology, fleet renewal, modernisation of air-traffic management and infrastructure bring about a gradual reduction of roughly 50%. The inevitable need for advanced biofuels to bridge the gap and to attain carbon neutral growth by 2050 is clearly evident. This perspective on the need for the advanced biofuels is also the fundamental driver of this PhD research.

A flight test was conducted by Airbus to demonstrate the feasibility of the "four pillar" strategy leading to carbon neutral growth. This test was conducted in collaboration with Air France in 2011 and Air Canada in 2012, with A321 and A319 respectively. Overall aviation CO_2 savings of 42% and 50% respectively, was achieved through incorporations of the following [6].

- **Biofuel** – use of 50% blend of used cooking oil
- **Aircraft efficiency** – Use of light weight carpets/ alloys for seats and trolleys and pre-flight fuselage wash
- **Engine Efficiency**- Compressor cleaning and relatively reduced take-off thrust
- **Operational efficiency** – Optimised routing (flight speed and altitude), modified descent approaches (reduced use of flap and reverse thrust), reduction of traffic congestion in the landing space, reduced use of Auxiliary Power Unit (APU) through single engine taxiing on ground.

The financial implications of conventional Jet fuel (Conv.Jet fuel) price volatility to airline operators is also a motivation to research into renewable jet fuel. The price of Conv.jet fuel is clearly influenced by the supply-demand ratio (or supply/demand equilibrium[1] in economic terms) where the supply of its feedstock (crude oil) is determined accounting the crude oil reserve to production ratio (R/P ratio). This dependence on estimated reserve make fuel-price forecast "a challenge" in profitability prediction to airline operators. Ironically, fuel cost is a variable operating cost which currently amounts to 35% of the total operating cost [66]. Airline

[1] Supply Demand equilibrium is achieved when the quantity of the commodity supplied is equal to the quantity demanded. When this equilibrium is achieved, stability in product price is also established.

operators expect to achieve some level of profitability from fuel efficiency through technological improvements to engine/ airframe combinations, without compromise on passenger safety considerations.

Continuous technological development contributed by original equipment manufacturers (OEMs) and operators have led to present fleet of civil aircraft being 70% more fuel efficient than those introduced 40 years ago [5]. This efficiency has been achieved through some of the major developments in technological and operational research and industrial implementation which are as follows.

Engine based developments

- Exploitation of engine's propulsive efficiency (advanced high bypass turbofan engines)
- Thermal efficiency improvement through incorporation of intercoolers
- Design based improvements e.g. component weight reduction through use of advanced durable and light weight composites for blades

Aircraft based Developments

- Use of wingtip devices to reduce wingtip vortices and reduce drag (avg. 6% reduction in CO_2)
- Use of high strength to weight airframe material e.g. Carbon fibre enforced polymer in Boeing 787 Dreamliner.
- Use of light weight alloys for seats and other interiors

Besides those mentioned above, further technological /operational improvements have been overshadowed by the very demand for air-travel which is also responsible for the growth of civil aviation. Any additional investigation into concepts and optimisation approaches bring in trade-off difficulties due to limitations in current technology. This creates a constraint on design space exploration. Therefore, the aviation industry is in pursuit of radical solutions to mitigate its environmental impact. The assertion of the benefit of advanced biofuels from IATA's "four pillar" strategy sets this PhD research in motion. To establish a clear insight into how biofuels contribute to mitigate aviation's environmental impact, an assessment from "cradle-grave" perspective has been undertaken. "Cradle-Grave" is a common term in Life Cycle Assessment

(LCA) which entails holistic evaluation of a given product from the point of raw material generation (cradle) to the point of its consumption (grave). This method of evaluation establishes the environmental impact and the sustainability of the examined product. To evaluate the prospects of biofuels in an existing aviation infrastructure, such a life cycle study is required.

“Techno-economic Environmental Risk Analysis of Advanced Biofuels in Civil Aviation” is an inter-disciplinary study which contributes to knowledge through conception plus application of quantitative/ qualitative approaches to assess the technical viability, financial feasibility and environmental competence of advanced biofuels from their application into the existing civil aviation infrastructure, relative to conventional jet fuel. Advanced biofuels, unlike first generation candidates, do not compete with food crops for land. The advanced biofuels, which have been chosen for this study are called Bio-Synthetic Paraffinic Kerosene (Bio-SPK) which is renewable synthetic jet fuel processed from plant lipids, developed for application in civil aero-engines. The plant lipids are thermochemically tailored to a composition similar to that of conventional jet fuel, through a dedicated technology called Hydroprocessing. This resulting composition enables Bio-SPK compatibility with the existing civil turbofan engine configurations, thus avoiding the need for major modifications that could prove to be economically unsound. The Bio-SPKs are also claimed to be “Drop-in” for this particular reason. Advanced biofuels chosen for this TERA analysis are Camelina SPK, Jatropha SPK and Microalgae SPK. The above mentioned Bio-SPKs were chosen for this assessment since they offer broader coverage of processing techniques dictated by their feedstock’s morphological characteristics and specific geographical locations. Such variations enable this study capture the carbon intensity and thus the environmental impact of these factors into the overall life cycle emissions analysis. Carbon Intensity is defined as the grams of emissions released per unit mega joule of the fuel.

There are inter-continental authorities that have establish standards and specifications for commercial aviation fuel upon extensive visual, laboratory and site based- performance evaluation e.g. ASTM (American Standard for Testing and Materials) and DEF-STAN (UK Defence Standards). In accordance to ASTM (American Standards for testing and materials) D7566, the physico-chemical specifications and hardware compatibility issues of these biojet fuels have restricted their use to 50% blends in existing aero-engines. Further study into this analysis may uncover the fact the Bio-SPKs possess better fuel “performance” properties including lower heating value and lower density, which theoretically hints a potential towards better jet engine performance. However, the technical abilities and limitation of Bio-SPKs can be ascertained only through an elaborate engine/aircraft performance analyses. Successful test flights on business jets and twin engine propellers operated with 100% biofuels have marked an affinity for purely alternative-fuelled air-operations [138] & [146]. Such a dedication towards commercial intrusion of advanced biofuel has been supported and recommended by the aviation authorities and environmental organisations including IATA (International Air Transport Association), ICAO (International Civil Aviation Organisation) and ACARE (Advisory Council for Aviation Research and innovation in Europe) as evident from consultation of available literature [3], [14], [68] and [127]. In fact, IATA expects biofuels to contribute a share of 6% of overall jet fuel supply to commercial deployment by 2020 [67].

An array of low/ no carbon alternative fuels (e.g. natural gas and Hydrogen) exist. However, a number of challenging factors including existing technological limitations, systemic technical viability and supply management have forced these candidates to become futuristic options. In the existing phase of technological progress, advanced biojet fuels appear technically and environmental feasible options and hence, have been adopted for this analysis.

The financial implications of introducing biofuel into commercial aviation have also been assessed as a part of this TERA study. As mentioned earlier, inability to establish supply-demand equilibrium is the contributor to fuel price volatility. Unlike, Conv. Jet fuel, the productivity of Bio-SPKs is certainly foreseeable, controllable and can be optimised to the needs of consumers with relative ease. Full-fledged establishment of Bio-SPKs to singularly manage this jet fuel supply-demand ratio, against Conv.Jet fuel [which had a 50 years kick start], will be quite a challenge. However, it is essential for a radically-changing aviation industry to wean away from the fossil-based energy source. Beside the industrial and environmental significance, the global/ societal acceptance, ethical benefits and issues associated with the advanced biofuels are also required to be evaluated. In spite of creation of jobs and the overall socio-economic development of rural community, the need for manual labour may, in turn, demand the need for establishment of ethical obligations by the biofuel producers to the local community.

1.2 Research Aim and Questions

The aim of the study is to evaluate the Bio-SPKs in terms of technical viability, economic feasibility, environmental competence, sustainability and societal impact, in view to consider for commercial deployment in the existing civil aviation infrastructure. “Techno-economic Environmental Risk Analysis of Advanced Biofuels for Jet engine” is a study that is expected to answer the following queries

- How to quantify the life cycle GHG savings delivered by the selected Bio-SPKs and judge their environmental impact?
- Are Bio-SPKs sustainably produced (in terms of land use, feedstock availability and costs, water footprint and energy demand)?
- Are the Bio-SPKs compatible with the existing engine configurations and for application on a representative mission with a suitable engine/ airframe combinations? If not, what are the technical implications?
- Will Bio-SPKs be an economically viable option relative to Conv. Jet fuel in civil aviation today? How will Bio-SPKs cope with varying emission taxation and fuel price scenarios in the future?
- What is the societal impacts related to large scale deployment of aviation biofuels?
- Are there other alternatives to Conv. Jet fuel other than the advanced biofuel assessed in this study?

1.3 Methodology

Techno-economic Environmental Risk Analysis (TERA) of Advanced Biofuels for civil engines is a multi-disciplinary study that motivates the development, use of a models and tools of a variety of specialism indicated below

- Life cycle studies
- Fuel chemistry
- Thermodynamic analysis
- Engine/ mission level performance modelling and simulation
- Environmental and
- Economic assessments

This study utilises elements of the Cranfield university-conceived "TERA" framework to achieve its objectives. TERA a versatile concept composed of computational programs to evaluate/optimise the technical viability, environmental intensity and economic feasibility of an existing/ new technology and operation within user-defined boundaries. TERA of advanced biofuels has customised the essential elements of TERA to achieve the objectives of this research [as presented in section 1.2]. However, a brief highlight of the method of analysis to achieve the objectives of this TERA study have been summarised below.

- Development of a comprehensive "Cradle-Gate" emission prediction tool titled ALCEmB (Assessment of Life Cycle Emissions of Biofuels) to report the life cycle carbon footprint, water consumption and the energy intensity of existing and prospective aviation biofuels.
- Development and integration of a robust thermodynamic model into the gas turbine performance simulation code, TURBOMATCH towards the following
    - Prediction of engine performance when operated with biofuel candidates against reference fuel, Jet-A1
    - Prediction of aircraft performance when operated with biofuel candidate over a user-defined medium-range flight trajectory
- Development of a two-part life cycle economic model titled ALCCoB (Assessment of Life Cycle Costs of Bio-SPKs) comprising the following modules
    - ALCCoB-BP (Biofuel pricing) to predict the hypothetical cost of the Bio-SPKs

- ALCCoB-DOC (Direct operating cost) to predict aircraft operating cost over a user defined mission towards, medium (2020), long (2050) and very long-term (2075) periods in varying environmental taxation and fuel price scenarios

The methods of analyses have been provided in a greater detail in the respective chapters of this thesis, in addition to a brief elaboration provided in this section. A general schematic of TERA customised to this study has been presented in Figure 1-2.

This study has chosen three Bio-SPKs, Camelina SPK, Microalgae SPK and Jatropha SPK. The reason for the choice of the two second generation (Camelina and Jatropha) and one third generation (Microalgae) biofuel feedstock is to facilitate broader coverage of varying process technology, process demands (material/energy specs) and the corresponding impact of all these factors on the life cycle cost and emissions of the candidate fuels. In addition to the above mentioned reasons, these Bio-SPKs were also determined by the consumer industry to be more readily available for gradual implementation into commercial usage.

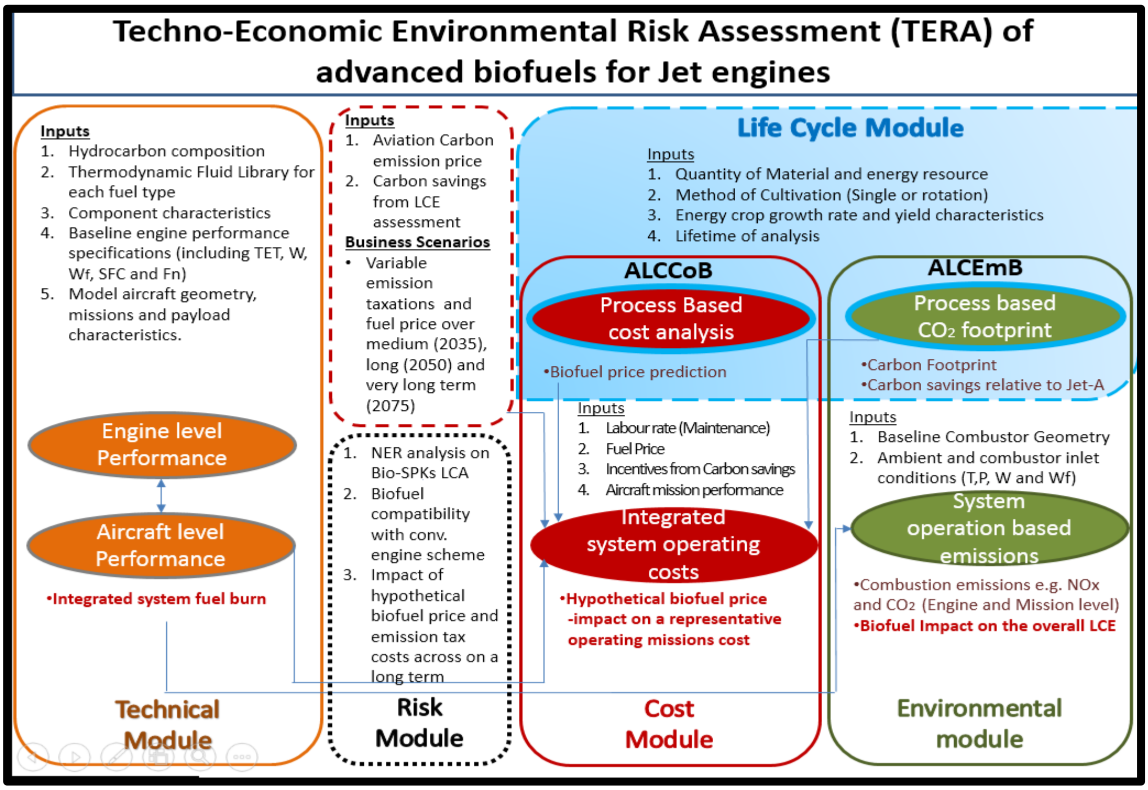


Figure 1-2: Method and Flow of data within TERA of advanced biofuels for Jet engines

1.3.1 Technical Module

Bio-SPKs are plant lipids that have been thermochemically altered to Conv. Jet fuel like compositions. Similarity in composition with the conventional fuel renders the Bio-SPKs compatible with the existing engine configurations, without the need for major technical modifications that could only prove to be economically unsound. Bio-SPKs are also claimed "drop-in" for this reason. However, certain discrepancies in their thermal, physical and chemical properties (dictated by the method of their synthesis) theoretically hints possibilities for variation in systemic fluid behaviour and subsequent impact on the integrated system performance. The technical investigation is, therefore, initiated with the development of a gas model for Camelina SPK, Microalgae SPK and Jatropha SPK as a function of temperature (T), pressure (P) and Fuel Air Ratio (FAR). This was achieved through use of industrially accepted chemical equilibrium software called NASA CEA (NASA Chemical Equilibrium with Application). Integrated system level performance delivered when operating the engine with the advanced biofuels was also undertaken. Fuel-specific gas models were implemented into the virtually constructed civil turbofan engine (*CU-Jet: Cranfield university Jet*) and fully-rigorous simulation of engine/ aircraft performance analysis was conducted. A FORTRAN-based gas-turbine modelling and performance simulation software called TURBOMATCH, conceived by the Cranfield University, was used to achieve this objective. The engine performance (when operated with the different fuel candidates) was measured in terms of SFC (Specific Fuel Consumption - g/ kN. sec). This evaluation is zoomed out into mission analysis where the performance of a virtually modelled aircraft, "LokAir", operating with the alternative fuel candidate was simulated and assessed. This task was accomplished using another Cranfield university- conceived FORTRAN based aircraft performance simulation code called HERMES for dynamic mission performance analysis. A virtual aircraft is modelled with user-defined weight and range specifications from an existing baseline aircraft. The validated aircraft (LokAir), equipped with the modelled turbofan engines (CU-Jet), is subjected to a virtual flight simulation under user-defined mission specifications. The typical mission is over a range of 4650m, typical flying distance between London Heathrow (LHR) and Bahrain International (BAH). The effect of fuel properties on flight level performance is measured as mission fuel burn. Quantification of combustion emissions of alternative fuels forms an important aspect of this technical module. These emissions have been predicted over the range of following mission phases

1. Engine Level estimation through use of ICAO-Landing-Take off Cycle specifications for the baseline engine.
2. Aircraft level emissions from fuel burn data established earlier over user-defined trajectory (comprising Taxi, Take-off, Climb, Cruise, Descent, Landing and Taxi).

Aviation CO_2 emission is predicted as a function of fuel burn assuming the fuel undergoes complete combustion. Aviation NOx (Engine Emission Index NOx), attributable to each of the fuel candidates was predicted (through stirred reactor approach) using a modelled conventional combustor. The degree of NOx emission formation is assumed to be influenced by factors including combustor inlet conditions, combustor characteristics and fuel compositions. Therefore combustion of the three biofuel candidate were numerically modelled and simulated using the above mentioned input specifications on a FORTRAN based -emission prediction software called HEPHAESTUS. Such an elaborate assessment has two- fold benefits: explore the “Drop-in” capabilities of the biofuels in question and carefully quantify the figures for combustion emission (Aviation CO_2) predicted towards the environmental module.

1.3.2 Environmental Module

Life Cycle emission assessment is a comprehensive discipline that examines the environmental impact of a product or process using their process inventory (material/ energy specifications). The depth of such an analysis is study-specific and can be conducted at different levels, e.g.

- Cradle-Cradle: Raw Material generation to recycle product
- Cradle-Grave: Raw material Generation – Product end life
- Cradle-Gate: Raw Material Generation – Factory gate

The Life Cycle Emissions (LCE) of the advanced biojet fuels quantifies and reports their carbon intensity from "cradle-grave" perspective i.e. the point of feedstock cultivation to the point of wake emissions upon fuel consumption. It is achieved through development of an elaborate life cycle emission model (ALCEmB- Assessment of Life Cycle Emissions of Biofuels) which calculates carbon intensity attributable to the life processes of each of the Bio-SPKs restricted to user-defined specification (material/ energy inputs). A key feature, attributable to the Bio-SPK, which causes it to offset its overall life cycle emissions, is termed "Biomass Credit". Biomass credit (measured in gCO_2e/MJ of the fuel product) is the ability of bio-derived fuel products /co-products to offset their overall life cycle emissions through a natural carbon sequestration process called photosynthesis. Biomass credit is exclusive to the biofuel feedstock and is a function of the feedstock's carbon fixation rate. This study also sheds light on the sustainability of Bio-SPK synthesis by defining the life-cycle based energy, resource and water intensity. GHG emissions attributable to water (a feedstock which is significant as land use) have been captured by ALCEmB, unlike earlier studies. Life cycle studies generally encounter a number of uncertainties due to the proprietary and uncommercial nature of the adopted technology. However, these shortcomings have been resolved with carefully considered assumptions suggested by earlier studies and industry experts. The environmental impact of a product (in accordance to ISO 14040/ ISO 14044 of Life Cycle Assessment) reports emissions to air, water and soil attributable to a given product or a process. As required by the above mentioned standards, these emissions are adequately allocated among the co-products through mass, energy and displacement allocations. The final life cycle emissions of the product or a process may vary depending upon the type of allocation chosen by the assessor. Further details on this environmental module have been provided in Chapter 3.

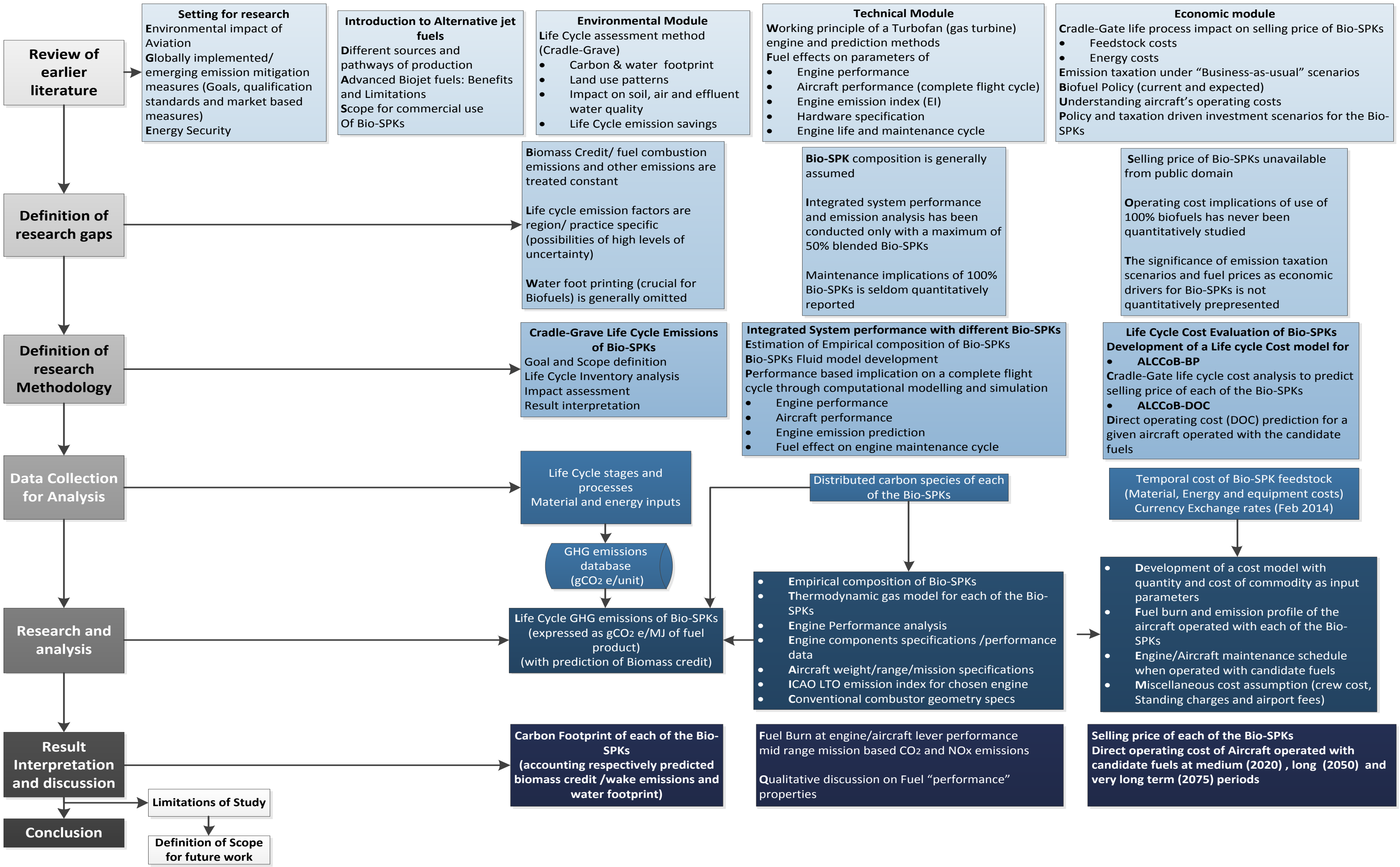


Figure 1-3: Research Methodology

1.3.3 Economic Module

The Economic module entails the development and use of a an elaborate cost model called ALCCoB (Assessment of Life Cycle Cost of Biofuels) which reports the economic feasibility of the chosen advanced biofuels through a "two-part" assessment approach

- **ALCCoB-BP** for life cycle costs analysis to predict the hypothetical *biofuel price*
- **ALCCoB-DOC** for *Direct Operating Cost* of an aircraft operated on biofuels

"Cradle to grave" material/ energy specifications of the candidate biofuels were sourced from ALCEmB. These specifications were incorporated with an integrated inventory cost database to calculate the manufacturing costs. The gate-cost of the final product estimated from the fixed operating cost and plant production capacity were designated as the retail prices for Camelina SPK, Microalgae SPK and Jatropha SPK. In order to overcome uncertainties associated with commodity (material) prices, regional average prices have been adopted for stage based cost calculations. Regional energy prices specific for Feb 2014 were adopted towards this study.

The Direct operating cost module is expected to establish the cost of using Bio-SPKs as the fuel of choice for a specific mission as a function of fuel price, carbon emission taxation and implications of variation in maintenance schedule. This study incorporates mission costs (fuel and emission costs), maintenance costs (spare costs, time between overhaul), standing charges, and airport and crew costs as well. Any studies of similar nature may have been conducted but extensive consultation of earlier literature resulted in very limited recovery of data. Therefore, the method of this economic analysis had to be conceived from scratch. The uncertain parameters and their impact on the resulting mission cost were further scrutinised with appropriate sensitivity studies. Further information on this economic module has been provided in Chapter 7.

1.4 Contribution to Knowledge

"Techno-economic Environmental Risk Analysis of Advanced Biofuels in Civil Aviation" is an inter-disciplinary study which contributes to knowledge through conception plus application of quantitative/ qualitative approaches to assess the technical viability, financial feasibility and environmental competence of advanced biofuels from their application into the existing civil aviation infrastructure, relative to conventional jet fuel. This PhD research motivated the development/ use of models and tools of a variety of specialisms indicated below

Quantitative analysis

1. Fuel chemistry
2. Life cycle assessments
   i. Environmental impact assessment (carbon intensity)
   ii. Economic Impact- fuel price and operating cost analysis at varying time scales and emission taxation scenarios
3. Thermodynamic fluid property analysis
4. Engine/ mission level performance modelling and simulation

Qualitative discussion

5. Handling and Combustion properties of candidate fuels- impact on existing engine scheme
6. Societal impact and ethical concerns

Any earlier literature on advanced biofuels, upon literature review, have been found to be specialism specific, as opposed to a holistic view that is required to judge their need and potential. This section briefly provides a view of the literature consulted, limitations of the studies and how the TERA aims to address these limitations thus setting a contribution to knowledge.

Fuel chemistry

Any fuel-centred study is initiated with the knowledge of the chemical composition of the biofuel candidate. A major limitation that is often encountered in most virtual experimental studies that involve advanced biofuels is as follows

Limitation:

- The novel nature and the consequential lack of information of the Bio-SPKs, in earlier studies, have forced the use of assumed empirical compositions [10], [15], [61] and [142].

Actions Taken:

The fundamental chemical composition of each of the Bio-SPKs has been predicted from the published data on paraffinic carbon species predicted through GCXGC [in accordance to D6379 of the ASTM fuel testing standards analysis] [107]. This can be noted a novel addition to earlier studies of such nature and contributes to all the upcoming investigations including prediction of biomass credit, fuel combustion emissions, gas model development for engine/aircraft performance and aviation NOx emission. Further details on method of analysis and outcome have been presented in section 3.3.1 and 3.4.1 respectively.

Life cycle assessments - Environmental impact assessment (carbon intensity)

Life Cycle Assessment (LCA) is a means of evaluating the emissions and costs of a given product (fuel in this study). A “cradle-grave” fuel-centred LCA requires the prediction of two key elements: biomass credit (GHG offset by biofuel plantation) and fuel combustion emissions which are predicted from fundamental fuel composition. Life cycle assessments on the Camelina SPK [18], [21], [60] and [119] Microalgae SPK [21], [29], [55], [58], [60], [77], [120] and [121] and Jatropha SPK [1], [15], [21], [29], [49] and [111] have been conducted earlier. Major limitations encountered in such studies have been indicated below

Limitations

- Failure to calculate and incorporate fuel-specific empirical information which is significant to the calculation of biomass credit and combustion ([15], [29], [58], [60], [119])
- Failure to account for emissions from water usage which is also key criterion for competition with food crops [15], [18], [29], [77], [119] and [123]
- Assumptions of biomass and fuel transportation emissions to be similar to that of Conv.Jet fuel [15], [18], [29], [60], [77] and [119].
- Lack of an elaborate quantification of systemic combustion emissions through representative engine/ aircraft performance evaluation [15], [71], [97] [114], [119], [123] and [143].

Action Taken

Careful quantification of feedstock-specific biomass credit is crucial to ranking the biofuels based on their carbon footprint. Unlike earlier studies where assumptions were adopted, ALCEmB precisely predicts the biomass credit attributable to each of the biofuel plantation through incorporation of hydrocarbon chemistry and tracking of carbon cycle within the life processes.

GHG emissions attributable to water supply are assumed to be energy-demand dependent, especially with the type of fossil fuel used to lift ground water to surface. In addition to the above mentioned, ALCEmB predicts carbon footprint attributable to the water consumptions unlike earlier studies. Further details have been elaborated in the sub section 3.3.2.1.

When the functional unit of the study is gCO_2e/MJ of fuel, adoption of standardised emission figures neglects the fuel's energy factor. ALCEmB uses fuel-specific composition and properties to predict LCE through underpinning life-process and engine/aircraft system based investigations.

Life cycle assessments- Economic Impact

The assessment of financial impact of advanced biofuels when deployed into existing civil aviation is undertaken in two parts. It is initiated with prediction of hypothetical biofuel prices, under an assumed set of constraints, followed by prediction of aircraft operating cost analysis. Life cycle cost analysis of alternative fuels has been conducted earlier in studies of reference [20], [30], [59], [71], [72], [121], [131]. Due to the uncommercial nature of the biofuels in question, the "Life Cycle Cost" analysis have primarily been used as a tool to deduce the feasibility of establishment and maintenance of the biofuel production plant , in the earlier studies. As a result of such a commonality in these earlier studies, the following limitations were identified

Limitations

- The price of the advanced biofuels deduced were generalised over the feedstock chosen, location of the biofuel production plant and plant capacity [72] and [121].
- Failure to account for the effect of changing fossil-fuel prices (energy feedstock) on the biofuel prices is major limitation [20], [30], [59], [71], [72], [121], [131].
- Lack of representative business case studies to deduce consumer-level financial feasibility [involving mission cost evaluation when using the advanced biofuels]

Actions Taken

ALCCoB-BP (Assessment of Life Cycle Cost of Biofuel- Biofuel Pricing) is the first half of the 2-part economic model developed as a part of TERA analysis. This model has adopted contemporary elements of LCC analysis such as process inventory based cost calculation. However, the cash flow analysis has been replaced with prediction of biofuel prices bound by carefully considered assumptions. This analysis has adopted the life cycle inventory for Camelina SPK, Microalgae SPK and Jatropha SPK from ALCEmB to standardise the economic and environmental analysis.

A sensitivity analysis to account for the effect of changing fossil-fuel prices (FFP) on the hypothetical biofuel price has also been included, unlike any other earlier studies.

An elaborate mission cost analysis which entails the use of hypothetical fuel price (predicted from ALCCoB-BP) to represent fuel cost and aviation CO_2 emission tax has also been conducted. This section of the ALCCoB will be called ALCCoB-DOC (Assessment of Life Cycle Cost of Biofuels – Direct operating Cost). ALCCoB-DOC also incorporates a sensitivity study which predicted the mission cost of a representative medium-range mission over medium (2020), long term (2050) and very long term (2075) periods as a function of varying fuel prices and emissions taxations scenario. This is once more a novel attempt in this analysis and an evaluation of such a nature has been seldom encountered by the author in any published literature.

Thermodynamic fluid property analysis

The significance of an accurate gas model for engine level performance evaluation of alternative fuels is well acknowledged by this study. Studies of reference [10], [60], [134] & [142] carried out a technical evaluation of FT-SPK blends that operated a turbofan engine. However, the technical module of this TERA study entails the use of fuel model attributable to for rigorous engine % pure Bio-SPKs performance simulation of this nature. The uncommercial nature of the biofuels in question resulted in a rare recovery of studies from the open domain, most of which had adopted hypothetical fuel compositions besides other studies which undertook elaborate laboratory based rig and flight test programs.

Limitations

- Quantitative thermodynamic property analysis on pure (100%) Bio-SPK has seldom been reported in the open literature. Available literature closely related to this study is of reference [29] and [142] which, however, do not cover the content in greater detail.

- The virtual experiments failed to account for fuel's "performance" properties, such as H/C ratio, LHV and most commonly overlooked aromatic content, on an operational gas turbine engine [10], [21], [29] and [44].

Actions taken

Thermodynamic fluid properties of significance to engine performance [Enthalpy (h), Entropy (s), Gamma (γ), Gas constant (R) and Isobaric specific heat (Cp)] were predicted and analysed for each of the candidate fuels. These gas properties were predicted as a function of temperature (T), pressure (P) and fuel-air ratio (FAR) to contribute to rigorous approach of engine performance simulation.

Some studies [78] & [137] have appreciated the precision achieved with fully rigorous engine cycle estimation and also indicate that its inaccuracies are influenced by the quality of the chosen thermodynamic models. The current version of TURBOMATCH employs thermodynamic definitions from Walsh and Fletcher (2004), [139], for rigorous engine-cycle calculation. The authors of these definitions have also indicated that these polynomials are only suitable for non-dissociated combustion-gas modelling up to a temperatures of only 2000K [139]. A segment of this technical module was devoted to identification and implementation of a valid thermodynamic model which accounts for variations in temperature/ pressure and dissociated combustion products with the best achievable accuracy.

<u>Engine/ mission level performance modelling and simulation</u>

Evaluation from fuel-property viewpoint enables one to appreciate and dedicatedly decide the most technically viable alternative fuel for their choice of aircraft, trajectory and mission-range. However, uncommercial nature of Bio-SPK has led to very limited numbers of studies. For instance, the only available literature on virtual evaluation engine/aircraft performance is [29] and [73]. Other limitations are as follows.

Limitations

- Most studies on biofuels entails investigation of blended fuels alone with insufficient information on impact of fuel compositions and its caloric properties on engine performance. E.g. Studies of reference [29] and [73] carried out an extensive experimental investigation on varying blends of UOPs Bio-SPKs, FT-SPK, and GTL from Sasol, Syntroleum and Shell (25% and 50% with JP-8).

- Representative engine level performance is seldom extended to a representative mission level assessment to obtain an insight into any discrepancies in mission fuel burn.
- Earlier studies on emission index of engine operated with blended Bio-SPK (25% and 50%) [29] and [73]. Lack of information on Emission Index of engines operating with 100% Bio-SPKs is a limitation encountered.
- Failure to discuss the impact of blended biofuel's handling and combustion properties on an existing engine scheme can also be considered a gap in literature

Actions Taken

Representative engine/ mission level assessments have been conducted through virtual experimentation using numerically modelled and validated engine/ airframe combination. The integrated system is assumed to be operated with 100% Camelina SPK, Microalgae SPK and Jatropha SPK. This analysis employs the gas model developed from the fundamental biofuel composition unlike earlier studies.

The quantified engine fuel consumption is zoomed out to a representative mission level performance assessment with the three Bio-SPKs. The purpose of this assessment is to precisely quantify combustion based emissions from Camelina SPK, Microalgae SPK and Jatropha SPK relative to Conv. Jet fuel.

The outcome of this assessment feeds into the ALCEmB towards the "fuel combustion" phase. It is essential to predict these emissions with utmost precision as this phase is the highest life cycle emission contributor (≈70%). A qualitative attempt to discuss the impact of pure Bio-SPKs on engine and hardware specifications has been made in this module in chapter 6.

1.5 Thesis Structure

Chapter 1 sets the context of study by introducing the reader to the need for this research. In this study, the ever-expanding nature of commercial aviation and its allied environmental impact has been briefly described. Key factors attributable to environmental, industrial and societal significance with respect to the alternative fuels of choice are drawn. These factors are multi-disciplinary in nature thus aiming to cover all possible aspects of the novel concept, from the point of conception to associated ethical concerns. This is followed by an elaboration of contribution of this research to existing literature coupled with the methodology adopted for this analysis.

Chapter 2 provides the literature review for each of the industrial drivers listed below and they include

- Existing/ upcoming emission standards and tax initiative
- Economic implications of volatile fossil fuel process
- and the need for a sustainable alternative fuel

Existing/prospective, renewable liquid fuels developed for aero-engine applications have been presented in this section. The purpose of this section is also to inform the reader about developments, achievements and limitations in earlier studies of similar nature. Owing to the multi-disciplinary nature of this study, an elaborate account of specialist literature review on earlier literature, its ideology, limitations have been detailed in the dedicated chapters. Techniques opted by this study to address the gaps in literature could also be found in the same.

Chapter 3 analyses and presents Bio-SPKs from the environmental perspective reporting their carbon footprint from a “Cradle to Grave” perspective ALCEmB. This study follows a life cycle assessment approach which involves definition of goal and scope of the study, inventory analysis, environmental impact assessment and interpretation of results. This study specifically reports air emissions and energy intensity resulting from the life processes of Camelina SPK, Microalgae SPK and Jatropha SPK.

Chapter 4 is the initiatory segment of the technical module. This chapter is devoted to the evaluation of thermodynamic behaviour of the Bio-SPKs. A deeper understanding of post-combustion gases attributable to the Bio-SPK is essential to understanding their behaviour within an integrated engine/ airframe combination.

Chapter 5 presents Bio-SPKs from technical perspective where their innate thermodynamic effects on the performance of integrated engine/ aircraft systems is analysed. This effect is studied virtually through numerical modelling and rigorous simulation of gas turbine performance. This evaluation is extended to mission-level assessment through virtual modelling of integrated engine/airframe and performance simulation over pre-determined flight trajectory. Fuel combustion emissions predicted from operation of a given engine/airframe configuration with candidate fuels completes he technical module and also contributes to the validation of “grave” phase emissions predicted through the ALCEmB.

Chapter 6 is dedicated to an elaborate qualitative assessment of the Bio-SPKs entailing their expected handling and combustion behaviour as a function of their composition and physical properties, in relation to the baseline fuel, conventional jet kerosene.

Chapter 7 is devoted to the economic evaluation of Bio-SPKs. This chapter reports the method of assessing the economic feasibility of each of the Bio-SPKs accounting their “Cradle-gate” specific material and energy input to predict reasonable market costs of these non-commercial biojet fuels under varying fossil fuel prices. Aircraft operating cost evaluation includes sensitivity analysis reporting the DOCs of a given aircraft at varying emission taxation and fuel price scenarios.

Chapter 8 briefly and qualitatively discusses about the industrial and societal challenges faced by these sustainable alternative fuels in terms of immediately available alternative fuel.

Chapter 9 summarises the conclusions drawn from this TERA research in terms of ranking the Bio-SPKs from environmental economic and technical perspectives.

Chapter 10 is devoted to identifying the deficiencies of this research and thus indicating the actions to be undertaken in the future to contribute to development of this study.

2 LITERATURE REVIEW

"*Although it is less than 100 years since the first powered flight, the aviation industry has undergone rapid growth and has become an integral and vital part of modern society. In the absence of policy intervention, the growth is likely to continue*."

was stated by the International Panel for Climate Change in their special report on aviation and global atmosphere [19]. The environmental impact of civil aviation has been comprehended for the past 3 decades. However, the tools to quantify and ascertain the actual effect have been available only since the 90s.

2.1 Environmental impact of Aviation

The Kyoto Protocol (1997) was the only international agreement devoted to regulation of greenhouse gas emissions and was addressed to the United Nations framework for control of climate change. Kyoto Protocol, has indicated under Section 2 of Article 2, that,

"The Parties included in Annex I shall pursue limitation or reduction of emissions of greenhouse gases not controlled by the Montreal Protocol from aviation and marine bunker fuels, working through the International Civil Aviation Organization and the International Maritime Organization, respectively".

The Kyoto Protocol was then followed by the regional directives for emission mitigation which include Carbon Tax in US and European Union Emission Trading Scheme in EU. International Civil Aviation Organisation (ICAO), a UN-agency, aimed to mitigate the environmental impact by setting strict standards for new aircraft and introducing market-based measures (emission taxation policies). Committee on Aviation Environmental Protection (CAEP), a sub-committee of ICAO is responsible for exploring advanced technologies and setting strict standards towards improvement of environmental performance of upcoming fleet of aircraft.

Typical emissions released from the combustion of aviation hydrocarbons and their corresponding sources have been listed in Table 2-1. High concentrations of these pollutants at ground level affect local air quality. Ground level and atmospheric concentrations of these components pose varying category of effects beside their impact on climate change [Table 2-2].

Pollutants	Designations	Source
Carbon dioxide	CO_2	Carbon content of the fuel
Water Vapour	H_2O	Hydrogen content of the fuel
Nitrogen dioxide	NO_2	Combustion with air (78% Nitrogen)
Nitric oxide	NO	Fuel bound nitrogen
Sulphur dioxide	SO_2	Sulphur additive for Lubricity
Carbon monoxide	CO	Incomplete combustion of fuel
Unburned hydrocarbons	UHC	Partially degraded fractions of parent fuel
Soot	-	Incomplete hydrocarbon combustion

Table 2-1: Typical aero-engine pollutants from combustion of fossil derived fuels

<table>
<tr><th>Pollutant</th><th>Impact Category</th><th>Effects</th></tr>
<tr><td>CO_2</td><td>Environmental</td><td>• Positive radiative forcing</td></tr>
<tr><td rowspan="2">NOx</td><td>Environmental</td><td>• Depletion of stratospheric ozone concentration
• Formation of tropospheric ozone concentration</td></tr>
<tr><td>Health</td><td>• Exposure to Ozone leading to skin cancer
• Respiratory issues in vulnerable population</td></tr>
<tr><td rowspan="2">Contrails (H_2O)</td><td>Environmental</td><td>• Formation of Contrails
• Radiative forcing
• Disturbance in the Day- night temperature patterns, local wind and pressure conditions</td></tr>
<tr><td>Agricultural</td><td>• Variation in wind and temperature patterns affect agricultural practices</td></tr>
<tr><td>CO</td><td>Health</td><td>• Asphyxiation and fatality</td></tr>
<tr><td rowspan="2">SOx</td><td>Engine life</td><td>• Formation of corrosive acids
• Damage to post combustor components
• Condensation nuclei. Aids contrails</td></tr>
<tr><td>Environmental</td><td>• Acid rain</td></tr>
<tr><td rowspan="2">Soot</td><td>Environmental</td><td>• Radiative forcing through contrail intensification
• Visibility issues</td></tr>
<tr><td>Health</td><td>• Serious respiratory issues</td></tr>
<tr><td rowspan="2">UHC</td><td>Environmental</td><td>• Photochemical smog</td></tr>
<tr><td>Health</td><td>• Heart and lung conditions in vulnerable age-group of population</td></tr>
</table>

Table 2-2: Categorical impact of typical Aero-engine emissions

According to IPCC studies of reference [19] & [64], escalating demands for air transportation and subsequent growth of the aviation industry is currently contributing to 2% of global anthropogenic CO_2 emissions. The most understated and under-documented by-product of combustion that also causes of global warming is water vapour. Many studies in the past decades were able to report the most direct link between contrails and global climate change [51], [53] and [60]. Further information on specific pollutants of interest can be found in the upcoming sections.

2.1.1 Fuel Combustion and Emissions

Combustion is a chemical process by which a fuel is completely oxidised facilitating conversion of chemical energy to thermal energy, in addition to pollutants formed.

$$C_xH_y + Air \rightarrow CO_2 + H_2O + N_2 + NO_x + CO + UHC + SO_x + heat \qquad \textbf{Eq 1}$$

The mechanism and degree of formation of each of the pollutant, with respect to the combustion process, is influenced by a number of environmental and technical factors some of which have been mentioned below

1. Ambient temperature and pressure
2. Engine Power setting influencing Inlet and Outlet conditions (Temperature and Pressure) at each reactor zone
3. Fuel composition and specifications
   a. *Thermo-physical properties* - Stoichiometric flame temperature, caloric properties (Cp, γ, h, s, ɳ), fuel density, bulk modulus, viscosity, flash point, boiling point, thermal conductivity, vapour pressure, LHV
   b. *Chemical properties* – Thermal stability, aromatics, sulphur and nitrogen content
4. Thermodynamic properties of the combustion products
5. Liner wall cooling characteristics
6. Fuel injector characteristics and location
7. Fuel spray characteristics
8. Equivalence ratio and degree of homogeneity of the fuel-air mixture
9. Combustor residence time.

2.1.1.1 **Carbon Di-Oxide (CO_2)**

Carbon-di-oxide is direct and dominant product of hydrocarbon combustion. Aviation emission account for approximately 13% of global transportation based anthropogenic CO_2 [84] and approximately 3% relative to total anthropogenic CO_2. Since CO_2 emissions are a function of the fuel composition, the mitigation efforts must primarily focus on efforts to reduce fuel burn. ACARE have quoted fuel burn as the underpinning cause of CO_2 emissions. According to their projections, CO_2 emissions can be reduced by 15-20% improvement to engine efficiency, 25% increase to airframe efficiency and robust air-traffic management and route optimisations techniques [3] and [4].

2.1.1.2 **Nitrogen Oxides (NOx)**

NOx emission, the third most abundant and unavoidable emission of typical combustion process, is required to be intricately understood to determine the factors that drive their synthesis. NOx (NO, NO2 and N_2O) emissions released on ground and the upper troposphere create and deplete ozone (O_3) respectively, the health and environmental hazards of which have been presented in Table 2-3. With respect to the degree of cruise NOx emissions, Faber et al, (2009) have reported about NOx emissions related to long-distance air-transportation falls in the range of 1.7-2.5 Tg (Teragrams) NOx /yr [46].

2.1.1.2.1 Radiative Forcing

Radiative forcing is a measure of change of energy at the tropopause as a function of the GHG's ability to disrupt the energy balance and cause climate change. Simply defined, radiative forcing helps measure the rate of climate change influenced by anthropogenic and natural causes. Radiative forcing can be termed positive or negative based on the warming or cooling effect inflicted by the respective GHG. Radiative forcing is measured as watts per square meter of earth surface. The degree of radiative forcing is influenced mainly by the weather conditions which is a complex system to model and GHG concentrations, which in current scenario is uncontrollably emitted. It is also essential to note that the forcing is influenced by concurrent GHG emissions of the local tropospheric zone, the method of deducing radiative forcing related to each of the GHGs has been provided in literature by IPCC [19] and [64]. The radiative forcing can be measured by two approaches: Global Warming Potential and Global Temperature Potential; Global Warming Potential is defined as "the radiative forcing of one kilogram of emitted gas relative to one kilogram of reference gas (CO_2) [64]. Global Temperature Potential refers to change in average surface temperature influenced by one kilogram of the emitted gas relative to one kilogram of the reference gas (CO_2). Global Warming Potential is an unsuitable metric to measure aviation emissions owing to the shot-span of the gases released in the upper troposphere. Hence, it is difficult to measure the radiative forcing of other gases such as NOx and particulate emissions released at an altitude. Attempts to develop a model integrated with mechanisms to predict the GWP of aviation GHGs has been listed in open literature.

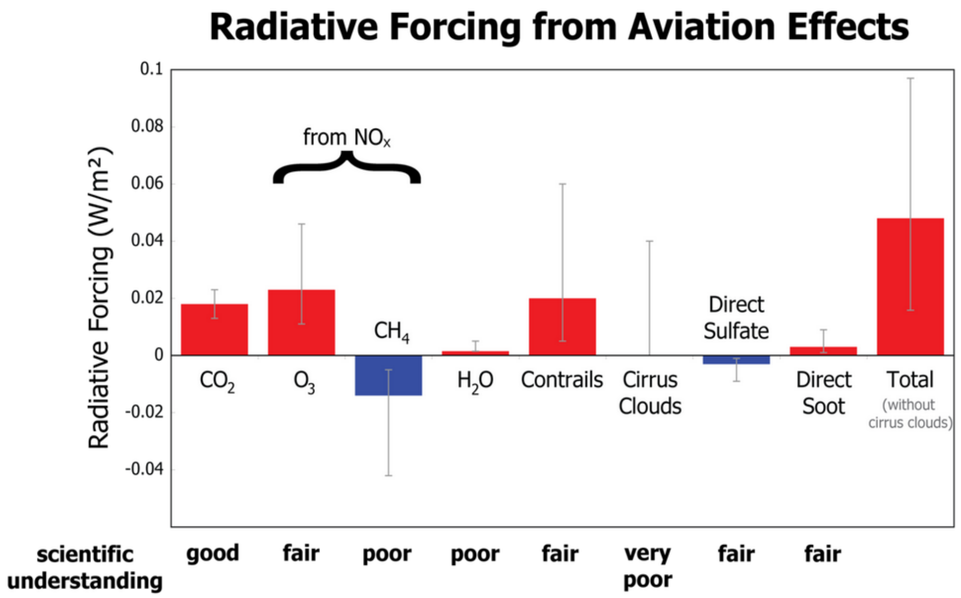


Figure 2-1: Radiative Forcing from Aviation Emissions [82]

According to these studies, the GWP of O_3 produced through induced ozone perturbation is variable with ambient temperature and pressure conditions, degree of ozone formed, local weather and wind patterns [51], [82], [96] and [145]. However, it is essential to note that these studies are assumptions based and the lack of scientific understanding [Figure 2-1] coupled with the extremely unpredictable weather patterns makes these models a less robust virtual instrument for scientific evaluation.

2.1.2 Global Environmental Measures

Environmental, health and engine life level impact of typical combustion emissions listed in Table 2-2 are compelling reasons for the aviation industry to regulate the same. In order to ensure its sustainable growth, international goals/ policies and regional market-based taxation mechanisms were introduced. An essential example of an environmental standard being ICAO based CAEP-NOx regulation which is required to be met by new fleet of aircraft to enter commercial operation. Unlike the land and marine based gas turbine applications jet engine tend to inject emissions in the upper atmosphere thus accelerating the atmospheric deterioration and cause global warming. In comprehension of this implication, aviation authorities, research establishments and collaborations have initiated global efforts to mitigate aviation emission mitigation. Some of the key contributors that research, develop, test and implement environmentally-efficient technologies and operational strategies has been schematically presented in Figure 2-2.

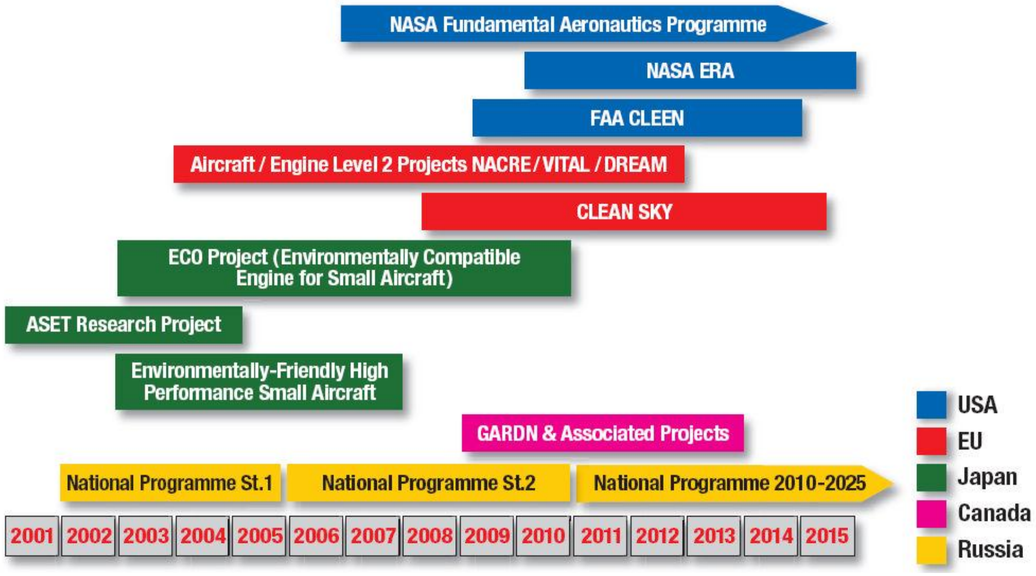


Figure 2-2: International environmental research initiatives to mitigate aviation emissions

2.1.2.1 Advisory Council for Aeronautical Research in Europe – ACARE

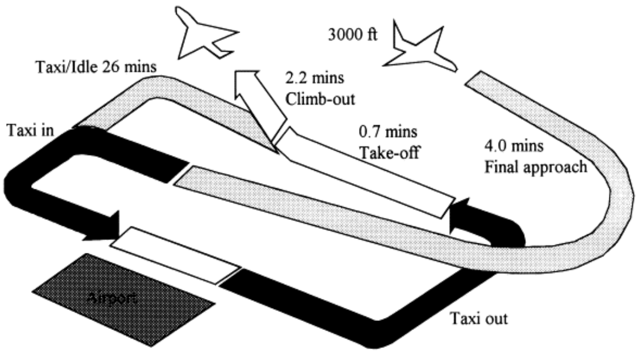
ACARE is a European seventh framework program, initiated to conceive, assess and optimise the aeronautical sector in Europe through regularly updated "Strategic Research Agenda (SRA)". In 2012, ACARE conceived goals for 2020 and 2050 providing ambitious but achievable targets for a cleaner and sustainable future. ACARE's research programmes have influenced R&D in the EU member state and initiatives of stakeholders including EUROCONTROL and EASM (European Aeronautics Science network). The ACARE recommends the following target for 2020 and 2050 by reducing overall emissions to levels relative to the average emissions in 2000 [Table 2-4]. ACARE suggests boosting aircraft fuel efficiency as a primary measure to achieve the 2020 target for CO_2 reduction. According to ACARE, this can be achieved through strategies including improvement of engine/airframe efficiency, sound air-traffic management and use of alternative fuels as presented in Figure 1-1.

Parameters	ACARE Vision 2020	Flightpath 2050
CO_2 emissions (kg per pass km)	-50%	-75%
NOx Emissions	-80%	-90%
LTO NOx (margin to CAEP 6)	-60%	-75%
Cruise NOx (kg/pass.km)	-80%	-90%
Engine Noise reductions	-50%	65%

Note:
All values relative to 2000 values
Values sourced from [3] and [4]

Table 2-4: ACARE targets for environmental impact reduction

2.1.2.2 **CAEP- NOx Certification Standard**



Flight Phase	Time in mode (min)	Power setting (%)
Take-off	0.7	100
Climb	2.2	85
Approach	4.0	30
Idle	26.0	7

Figure 2-3: Typical Definition of Landing- Take-off (LTO) Cycle

Committee on Aviation Environmental Protection CAEP initiated (1986) strict LTO-NOx standards for new aircrafts as a qualification criterion for certification towards commercial service. Establishment of such a standard entails rigorous technical investigation and feasibility analysis of low emission technologies and their economic feasibility for commercial implementation. These standards are renewed regularly and new “achievable” standards are introduced upon assessment of commercially viable low-NOx technologies. The historic, present (CAEP/8) and proposed standards for future LTO-NOx regulations have been presented in Figure 2-4.

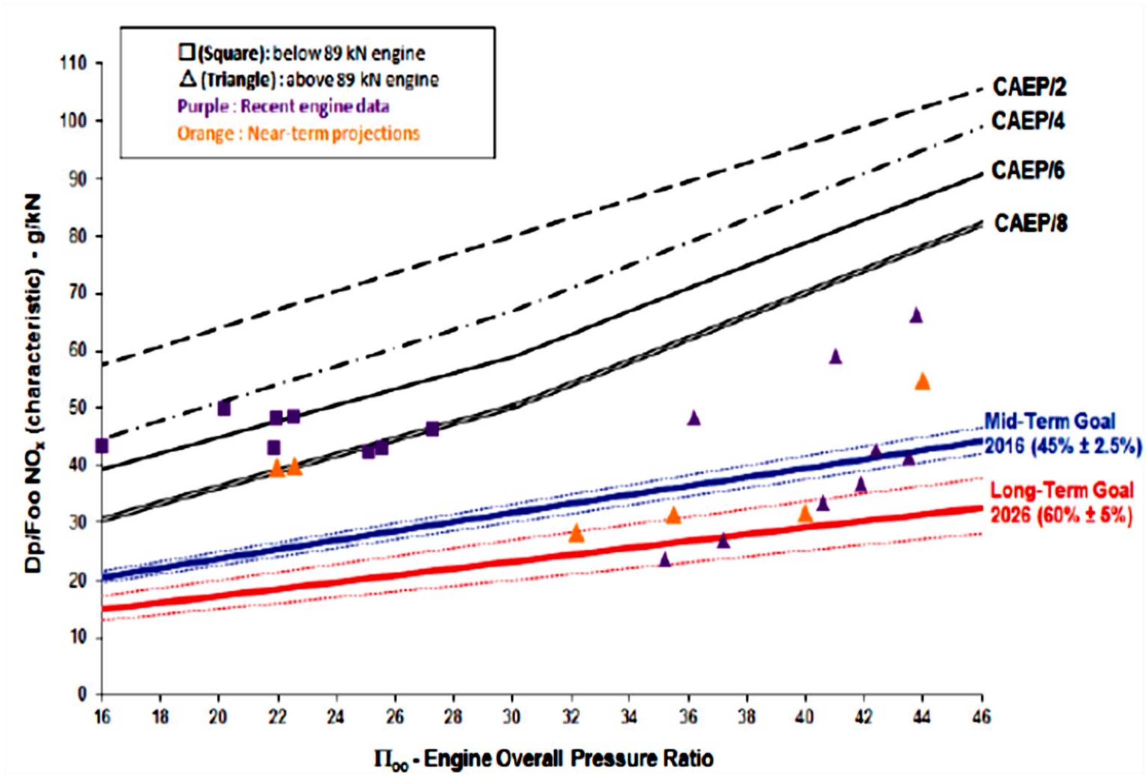


Figure 2-4: Definition of CAEP-NOx standards for civil engines [46] and [48]

Engines aiming to qualify for commercial operation certification are required to fall below the indicated CAEP-NOx limit. LTO NOx was chosen as the benchmark for certification due to its relatively higher concentration as wake emissions during the cycle and its immediate environmental and health impacts on local air quality. Earlier literature indicates of probable taxation and regulation scenarios for cruise NOx which are, however, currently non-existent [46].

2.1.2.3 **European Emission taxation Policies – EU-ETS**

In 2007, the European Union Emissions Trading Scheme (EU-ETS) proposed to consider aviation into its taxation policies. This proposal was the outcome of an alarming 87% increase in air pollution from commercial air traffic between 1990 and 2006. These efforts took effect from 2013 with a goal to reduce carbon emissions by 5% relative to average emissions between 2004 and 2006. EU-ETS has fully included commercial aviation into taxation from 2013, which if successfully executed, could have potentially cut back 73 million tons of CO_2 equivalent emissions between 2013 and 2020 [84]. The EU-ETS enforcement plans to allocate 85% of allowances to airline free of charge whereby the rest of the 15% of allowances will be auctioned. These allowances are annually allotted on the basis of fuel consumption and revenue passenger kilometre (fuel consumption and RPK- functions of air traffic) attributable to an airline as a share from that of the total aviation industry. Regrettably, the full-fledged global deployment of aviation emissions taxation faces protests from intercontinental aviation associations which has resulted in the EU having to "stop the clock" on carbon emission taxation. After the "Stop the clock" deadline that ended in 2012, the aviation CO_2 emissions are anticipated to be taxed at £4.28/tonne of aviation CO_2. This rate is likely to increase annually and be capped at £18/ tonne between 2016 and 2020 [12]. The existing carbon cap of 95% is expected to fall by 1.74% from 2013 and by 2.2% from 2020 to achieve overall CO_2 emissions reduction by 20%-30%. The European skies are under EU-ETS radar and therefore inter/intra-regional aviation authorities are under the pressure to reduce their emission footprint by every possible means. The consequential environmental impact of incessant air travel has led the aviation sector on a quest for ways of sustainable growth.

2.2 Economics of Aviation Fuel –an Overview

When accounting the existing/newly discovered mineral oil reserves and at the current rate of consumption (excluding shale reserves), global jet fuel supply has been roughly estimated to last only up to 50 years.

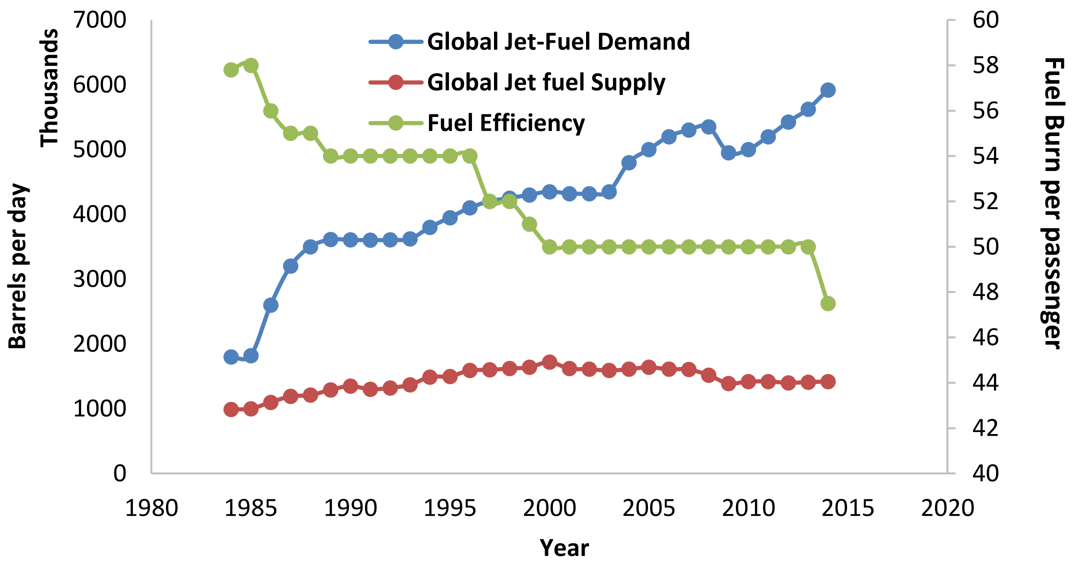


Figure 2-5: Jet fuel Supply-Demand balance over the last 2 decades [Sources: [105] & [129]]

This inability to establish a balance between the future fuel demand and supply causes fuel price volatility. Supply/demand equilibrium refers to a point where the price of a given product achieves stability when the quantity of product produced is equal to the quantity demanded. The cost of jet fuel has increased by 80% (from $0.55/gal in 1990 to $2.98/gal in 2014) [105]. Positively quoting, the volatility in fuel process influences the profitability of the end-users, the airline operators. In order to ensure a stable profit margin, some airline operators "hedge" or "fix their fuel prices" a year in advance, to avoid losses from price hike. However, the fuel price is volatile to an extent that fuel price "hedging" can either protect or penalise the operators in billions of dollars at a global level. Fuel cost from total operating expenses, in 2014, amounted to just 35% relative to 15% in 2006 [62].

Investment into technologies for the improvement of fuel efficiency and air-traffic management are some of the mandatory strategies followed by most airlines. In fact, voluntary fuel efficiency upgrades contributed by the OEMs have aided the airline operators manage this financial uncertainty (fuel cost) by reducing fuel use and thus fuel costs. The relation between global fuel supply/demand and fuel efficiency improvement is evident from the Figure 2-5. Technological improvements (fuel efficiency measures) levelled out and managed increasing fuel demand amidst relatively constant fuel supply scenarios. However, further technological developments bring in trade-off difficulties which pose restrictions to design space exploration in engine/airframe configurations. Any gains from technological improvement are rapidly over-shadowed by equivalently growing demand for air travel. Demand for air-travel which is crucial for profitability has also been identified and criticised as a factor for unsustainable growth of commercial aviation.

There is immense pressure to establish a balance between profitability and sustainable growth which has led the industry to explore ways of achieving equilibrium. Aviation industry has theoretically ascertained short, medium and long terms solutions to mitigate its environmental impact that have been mentioned below

- Technological improvements to boost the overall aircraft efficiency
    - Retrofit with regular updates such as tech insertion packages
    - Modifications to engine configurations for improved thermodynamic cycle

    - Conception, development and deployment of low emissions concepts like low emission combustor and airframe design (e.g. blended wing body), hybrid electric propulsion systems and advanced high bypass ratio engines
- Use of “cutting edge” light weight material composites for blade designs and paint/ polymers for wings and fuselage construction.
- Global efforts for fleet renewal
- Development and robust implementation of GHG conscious ground and air traffic management strategies. For instance, TIACA (The International Air Cargo Association) have determined that improvised ATMs that can potentially reduce flight time by 1 min, on a global scale, could benefit the airline industry environmentally by 4.7 million tons of CO_2 savings and economically (through fuel savings) by $1.5 million for the operators, according to a source of reference [126]. This can be achieved through the following strategies.
    - Direct routing between destinations through harmonisation of air-space, e.g. SESAR- Single European Sky ATM Research Programme
    - Avoiding unnecessary taxiing
    - Modernisation of air traffic management e.g. use of GPS instead of conventional radar and transponder system [as proposed by NextGen (Next Generation air transport systems) to replace radars by 2025]
    - Flexible routing to take advantage of wind patterns en-route
    - Organised ground traffic management e.g. continuous descent to prevent avoidable flight hold and diversions
- Conception of strict emission mitigation goals to encourage and guide the industry into environmentally sustainable growth.
- Enforcement of stringent emission standards and taxations. E.g. ICAO-CAEP limits for LTO-NOx
- Encouragement and speedier certification of environmentally efficient engine/ airframe concepts

2.3 Alternative Jet fuels- Environment, Economics and Ethics

Extensive research and development have expanded the frontiers of aviation. From Technical perspective (aerodynamics and engine /airframe design), existing and new fleet of aircraft are 70% more efficient than those in 1960s [5]. However, this benefit is shadowed by the escalating demand for air travel. Bio-derived jet fuels have recently captured the attention of aviation authorities and environmental organisations as a viable short-medium term solutions. A more elaborate insight into biofuels developed for civil aviation could aid comprehend their significance in environmental impact mitigation, energy security and be introduced on the range of alternative fuel choices available for now and the future.

Synthetic Paraffinic Kerosene is a classification of synthesized jet fuels produced through two pathways: Fischer-Tropsch (FT) process and Hydroprocessing. Natural gas, biomass, coal and other feedstock are initially gasified to produce syngas which follows the Fischer-Tropsch pathways to produce syncrude. The syncrude is converted to synthetic jet fuel (FT-SPKs) through Hydroprocessing technology. The Fischer-Tropsch pathway can be specifically termed as Gas-Liquid (GTL), Biomass-Liquid (BTL) or Coal-Liquid (CTL) depending upon the feedstock used. However the fuels produced through FT process are collectively termed as FT-SPK.

Bio-derived Synthetic Paraffinic Kerosene (Bio-SPKs) which are group of jet fuels of biological origin is synthesized solely through the hydrotreatment process which follows a complex set of thermochemical process: Deoxygenation, hydrocracking and isomerisation. In general, fuels synthesized through hydrotreatment are termed Hydrotreated Renewable Jet (HRJ). The fuel candidate chosen for this multi-disciplinary evaluation follows similar fashion of synthesis and is collectively called as Bio-SPKs by their manufacturers (UOP LLC). The lipids and fatty acid extracted from biomass, called bio-crude, is altered by a thermochemical process called Hydrotreatment and converted to hydrocarbons which are similar in thermal and chemical properties to that of Conv.Jet fuel. These biofuels are also claimed to be “Drop-in” for they are claimed to be compatible with existing aero-engines. The physico-chemical and thermal properties of the advanced biofuels sourced from manufacturer’s literature [73] and chosen for this study have been presented in Table 6-1.

Fuel type	Source	Method of Synthesis	Test /Commercial flights	Destinations
Fossil derived Jet fuels	Shale oil Shale Gas	In-situ conversion and Fractional Distillation Fracking	In test phase	- -
	Coal	Fischer-Tropsch (GTL, CTL) Direct & Indirect Liquefaction Pyrolysis	Oct 2009 Airbus A340	London to Doha
Bio-jet fuels	Camelina	Renewable Jet Process ™ (Bio-SPK/HRJ)	Jul 2011 Airbus A321	Frankfurt to Washington
	Algae	Renewable Jet Process ™ (Bio-SPK/HRJ)	Nov 2011 Boeing 737-800	Houston to Chicago, US
	Jatropha	Renewable Jet Process ™ (Bio-SPK/HRJ)	Aug 2011 Boeing 777-200	Mexico to Madrid
	Rapeseed[1]	Hydroprocessing (Bio-SPK /HRJ)	April 2013 Airbus A320	-
	Pennycress[1]	Hydroprocessing (Bio-SPK /HRJ)	-	-
	Soybean[1]	Hydroprocessing (Bio-SPK /HRJ)	April 2013 Airbus A320	-
	Coconut[1]	Hydroprocessing (Bio-SPK /HRJ)	Feb 2008 Boeing 747	London to Amsterdam
	Cellulosic crops Switchgrass, Miscanthus Wood	Pyrolysis Genetically engineered microbial fermentation Alcohol to Jet pathway (ATJ) (Dehydration-Deoxygenation and oligomerisation)	ATJ fuel in test phase	- -
Waste derived Jet fuel	Waste Vegetable Oil* Agricultural residues Forest residues Municipal waste	Gasification and Fischer-Tropsch (Syngas/ Syncrude)	May 2014 Airbus A330	Aruba to Netherlands
	Industrial exhaust	Carbon capture and (GTL) Pathway	Production phase	-
Sunlight derived Jet fuel	Sunlight, Air	Solar-jet & Fischer Tropsch Process	In R&D phase	-

Table 2-5: Alternative sources of Jet fuel- Past, Present and Future

Feedstock associated with the Bio-SPKs chosen for this analysis have been studied extensively from agricultural perspective and have been identified as sustainable feedstock to qualify for further evaluation through the following characteristics.

Camelina sativa

- Camelina seeds can germinate at very low temperatures and are extremely frost resistant.
- Camelina species have been determined to perform very well in drought stress [149].
- Biomass cultivation requires very minimal inputs of fertilizers [119].
- Sustainable cultivation by crop rotation with food plants (Winter wheat) and in marginal lands eliminates “Food vs. Fuel” concern and reclaims soil fertility as well.

Microalgae sp

- High levels of lipid/ oil accumulation
- Rapid biomass growth rate [55]
- Relatively low land usage.
- Relatively higher CO_2 absorption/ uptake rate [relatively higher biomass credit] [35].
- Comparatively higher sustainability of bio-crude production

Jatropha curcas

- Resistance to poor soil conditions and high temperatures [1]
- Wasteland/ soil reclamation & opportunity for afforestation [2]
- Sustainable yield of oil bearing seed from the second year of plantation and year round production upon irrigation.
- Jatropha oil is non-edible and performs well on average soil; this eliminates food vs. fuel conflict [15]
- Pharmaceutical by-products from bark and leaves
- Economic enhancement of the agricultural sector.

In accordance to ASTM D7566, the physico-chemical specifications and hardware compatibility issues of these biojet fuels have restricted their use to 50% blends in existing aero-engines. The aromatic content of any hydrocarbon ensures swelling of elastomer seals with greater efficiency compared to the pure paraffinic components of biojet fuels. Sulphur content of the fuel offers lubrication/ longer life to the moving parts of fuel pumps and injectors. Existing fuel system are used to innately aromatics-containing jet fuel thus posing restrictions to biojet fuels (contains <0.001 by vol.). Therefore, ASTM D7566 specifications in the US and DEF-STAN 91-91 has certified use of just 50% biofuels in blend with conv. jet fuel for commercial purposes. However, some test flights with 100% Camelina and Algae derived biofuels operated, on business jets and twin engine propeller engines respectively, have marking the interest into purely alternative-fuelled air-operations [138] and [146]. It is crucial to note that fuel experts [21], [36], [39] and [61] have indicated that the required aromatic content (which was conceived 50 years ago) must be reviewed and updated to pave way for deserving renewable fuels.

3 LIFE CYCLE GREENHOUSE GAS EMISSION ANALYSIS OF BIO-SPKS

(Environmental Module)

3.1 INTRODUCTION

The Environmental module of TERA of advanced biofuels aims to evaluate the environmental competence of Camelina SPK, Microalgae SPK and Jatropha SPK by quantifying their carbon intensity based on their life processes, from a “cradle-grave” perspective. Cradle-Grave, a term commonly encountered in LCA studies, encompasses process/ product based activities from the point of raw material generation (Cradle) to final product consumption (grave) [Figure 3-1]. The carbon footprint of these advanced biofuels will be weighed against that of the reference fuel, Conv.Jet fuel.

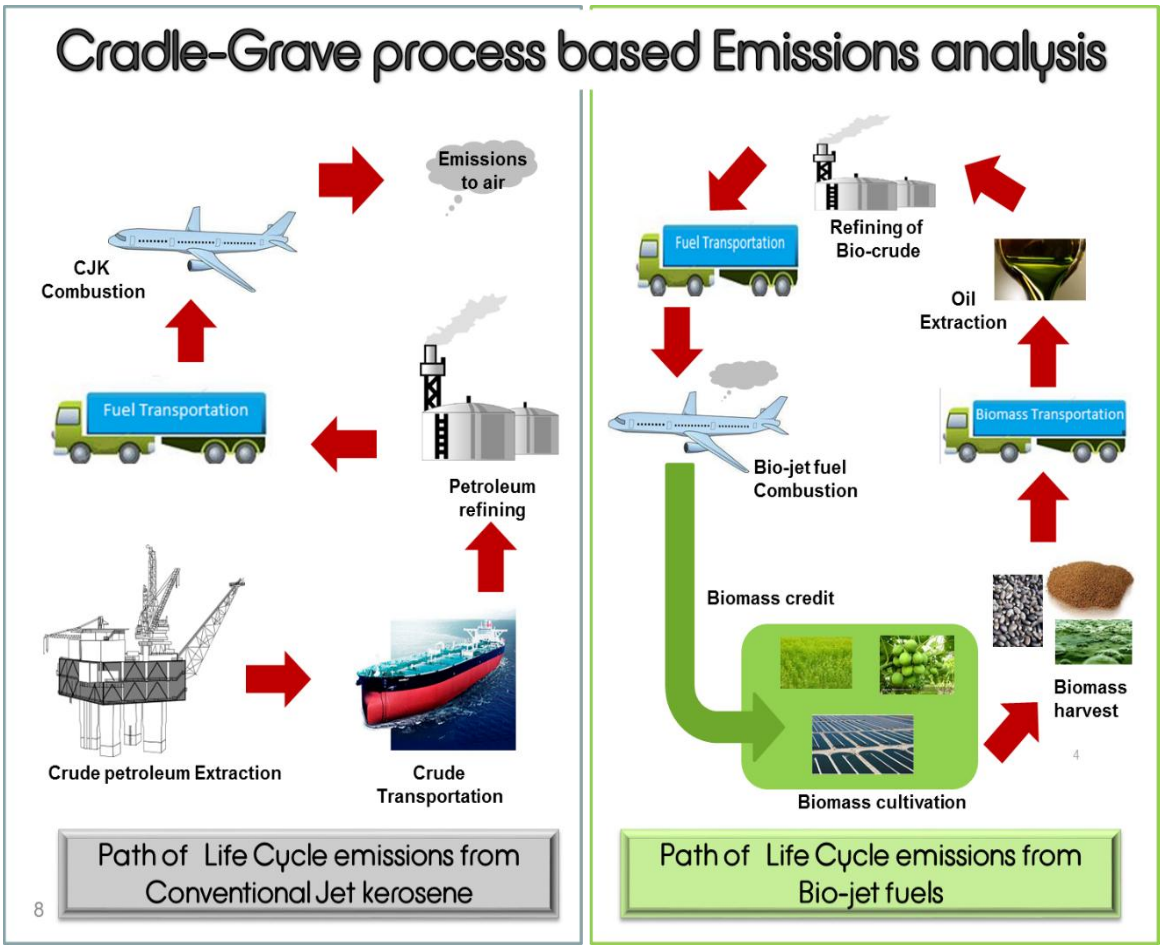


Figure 3-1: Life Cycle processes of the Conventional Jet fuel and Bio-SPKs

The objective of this environmental module was achieved through development of a holistic life cycle model called ALCEmB (**A**ssessment of **L**ife **C**ycle **Em**issions of **B**iofuels) which captures the carbon intensity of the Bio-SPKs from the point of raw material generation (cradle) to the point of fuel combustion (grave). The biojet fuels chosen for this analysis are Camelina SPK, Jatropha SPK and Microalgae SPK, collectively called as Bio-SPKs. Bio-Synthetic Paraffinic Kerosene (Bio-SPK) is plant derived lipid which is thermochemically tailored by hydroprocessing to compositions similar to Conv.Jet fuel and subsequently enable compatibility with existing engine scheme. Hence these advanced biofuels are claimed "drop-in" by nature. The chosen advanced biofuels offer broader coverage of processing techniques which is dictated by their morphological characteristics and cultivated geographical locations. In addition to the quantifications of Life Cycle Emissions (LCE), this study reports the energy intensity from processing the biofuels through Net Energy Ratio (NER) evaluation. Net energy ratio (NER) is defined as the ratio of total energy produced to total energy consumed, thus defining the technical feasibility and energy intensity of a given product.

Owing to the uncommercial nature of the biofuel candidates, such life cycle studies are bound by uncertainties. These uncertainties have been resolved with carefully considered assumptions suggested by earlier studies and industry experts. Besides process based emissions, this environmental module aims to summarise the overall life cycle emissions by including combustion emissions through use of numerically modelled engine/ aircraft systems and computational simulation of a medium-range mission with the model aircraft, operated on candidate fuels.

3.2 LITERATURE REVIEW

Life cycle assessments on the Camelina SPK [18], [21], [60] and [119] Microalgae SPK [21], [29], [55], [58], [60], [77], [120] and [121] and Jatropha SPK [1], [15], [21], [29], [49] and [111] have been conducted earlier. These studies were elaborately focussed on quantifying the life cycle GHG emissions of biofuels (renewable diesel and Hydrotreated renewable jet fuel). However, these studies were regionally isolated and specialism specific. ALCEmB aims to standardize life cycle stages (production metrics for life processes and integration of system level emission prediction), unlike earlier studies, where the adopted combustion emissions were simply assumed figures.

Biomass credit is the measure of carbon savings delivered by the biofuel plantations through natural carbon fixation (photosynthesis) and is also an important feature exclusive to biofuels. The biomass credit is generally assumed to be equivalent to the amount of CO_2 wake emissions as observed in a number of studies [15], [29], [58], [60] and [119]. Careful quantification of feedstock-specific biomass credit is crucial to ranking the biofuels based on their carbon intensity. Unlike earlier studies where assumptions were adopted, ALCEmB has attempted to quantify the biomass credit attributable to each of the biofuel plantation through incorporation of hydrocarbon chemistry and tracking the carbon cycle within the life processes.

Carbon intensity of freshwater consumption (a key criterion similar to land use) is generally overlooked in most LCA studies owing to the lack of data or use of LCA software which may innately calculate this parameter [15], [18], [29], [77] and [119]. GHG emissions attributable to water supply are assumed to be energy-demand dependent (with the type of fossil fuel used, in particular, to lift ground water to surface). In addition to the above mentioned, ALCEmB predicts carbon footprint attributable to the water consumptions unlike earlier studies. Further details have been elaborated in the sub section 3.3.2.1.

The uncommercial nature of the biojet fuel types (Bio-SPKs) required the earlier studies assume combustion emission figures attributable to the well-known, Conv.Jet fuel. For instance, most studies have assumed transportation (biomass/fuel product) based emissions for the Bio-SPKs similar to that of Conv.Jet fuel [15], [18], [29], [60], [77] and [119]. The reason for such an assumption is the consideration of a biofuel management and its logistics to be similar to that of conv. jet fuel. In accordance to the Aviation Fuel Life Cycle Assessment Working Group, [12] and a functional unit of this analysis, gCO_2e/MJ, will be used to measure the effect of fuel specific life cycle processes. This unit enables one to weigh the CO_2 emission per unit energy content for a specific fuel. However, when the functional unit of the study is gCO_2e/MJ of fuel, adoption of standardised emission figures neglects the fuel's energy factor. ALCEmB aims to use fuel-specific composition and properties to predict LCE through underpinning life-process and engine/aircraft system based investigations.

3.3 METHODS

3.3.1 Estimation of Bio-SPK composition

A fundamental pre-requisite to any fuel-centred analysis is the identification of appropriate fuel composition. The empirical composition and the molecular mass for each of the Bio-SPKs were numerically estimated from the carbon distribution data available in the open domain [94] and [107] [Figure 3-2]. The pure composition of Bio-SPKs is composed of paraffin (n & iso) (99% by mass), cyclo-paraffin (0.9% by mass) and aromatics (0.2% mass). This composition was predicted through gas chromatography (GCxGC) in accordance to ASTM D6379 of fuel testing standards, by the parent company. In general, the hydrocarbon construct of a paraffinic carbon species in a fuel is represented as

$$=a+ (2b+2) \qquad \textbf{Eq 2}$$

where, $\boldsymbol{a}$ = *no of carbon atoms in a paraffinic species and*

$\boldsymbol{b}$ = *no of hydrogen atoms in the paraffinic species*

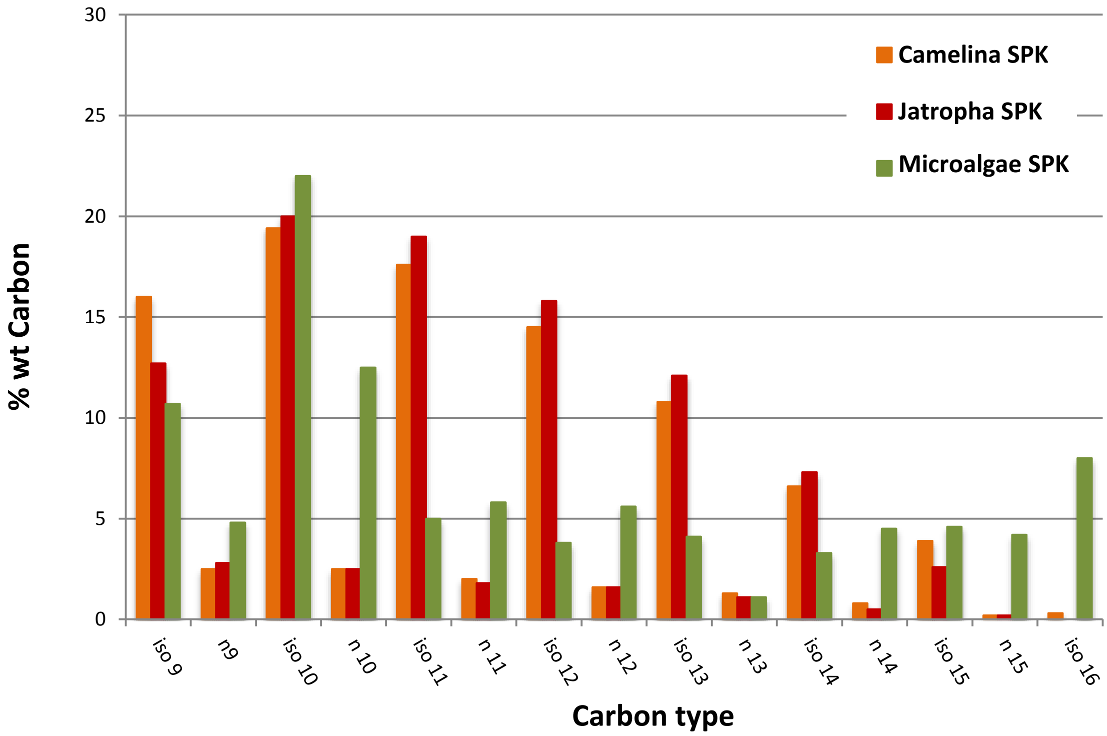


Figure 3-2: Carbon Distribution data of advanced biojet fuels [73]

The total paraffinic weight and eventually the molecular mass of each of the Bio-SPK can be calculated from their carbon spectra using the following method. The molar mass of each of the Bio-SPK is calculated from the following equations

$$\boldsymbol{d} = [\boldsymbol{c} \times \boldsymbol{a}] \quad \textbf{Eq 3}$$

$$\boldsymbol{e} = [\boldsymbol{c} \times \boldsymbol{b}] \quad \textbf{Eq 4}$$

where, *c = mass fraction of the specific paraffinic species, g*

d = Carbon component of a specific paraffinic species

e = Hydrogen Component of a specific paraffinic species

To calculate the empirical formula (C_xH_y) of the each of the Bio-SPKs

$$\textbf{\textit{Carbon no. (x)}} = \sum(\boldsymbol{c} \times \boldsymbol{a}) \quad \textbf{Eq 5}$$

$$\textbf{\textit{Hydrogen no. (y)}} = \sum(\boldsymbol{c} \times \boldsymbol{b}) \quad \textbf{Eq 6}$$

Molar mass (g/mol) of each of the Bio-SPKs can be calculated using the approach provided in Eq 7

$$\textbf{\textit{Mm = [12.01 (x) + 1.008 (y)]}} \quad \textbf{Eq 7}$$

where, Mm = Molar mass per mole of the fuel (g/mol)

[Note: 12.01 g corresponds to the atomic mass of Carbon and 1.008 g corresponds to the atomic mass of Hydrogen]

The calculations have been elaborated in Appendix A of the supplementary section. Precise estimation of hydrocarbon composition of Camelina SPK, Jatropha SPK and Microalgae SPK is crucial to the upcoming technical assessments. This data defines the performance properties of a given fuel and its resulting impact on a numerically modelled and validated engine, providing a deeper insight into their thermodynamic influence on an aero-engine performance and emission characteristics [78], [116], [137] & [142]. The empirical data and key performance properties of each of the 100% Bio-SPKs has been presented in the results and discussion section. Combustion characteristics including stoichiometric fuel/air ratio and adiabatic flame temperatures, essential for fuel combustion and subsequent emission studies were also determined using methods stated by Goodger & Ogaji, (2012), which however, demands the knowledge of fuel's empirical formula [54].

3.3.2 Life Cycle processes of Bio-SPKs

Life cycle assessment is an effective tool which was implemented to study the carbon/ energy intensity and the production cost of the biofuels from a stage-stage perspective. LCE of Bio-SPKs will be assessed through use of ALCEmB and weighed against the fossil derived reference counterpart, Jet-A1. However, the four elements of a life cycle assessment must firstly be defined.

Goal and Scope: The system boundary for this LCE analysis has been defined in Figure 3-3. The environmental module of this TERA study is devoted to analysing and quantifying the carbon intensity of the renewable biojet fuel alone and excludes renewable diesel. This paper aims to provide a more comprehensive evaluation through standardization of life cycle processes among the candidate fuels to improve the lucidity of the life cycle processes. The scope of this study also includes the product consumption (fuel combustion) which is usually accounted as avoided emissions and a relevant figure is assumed.

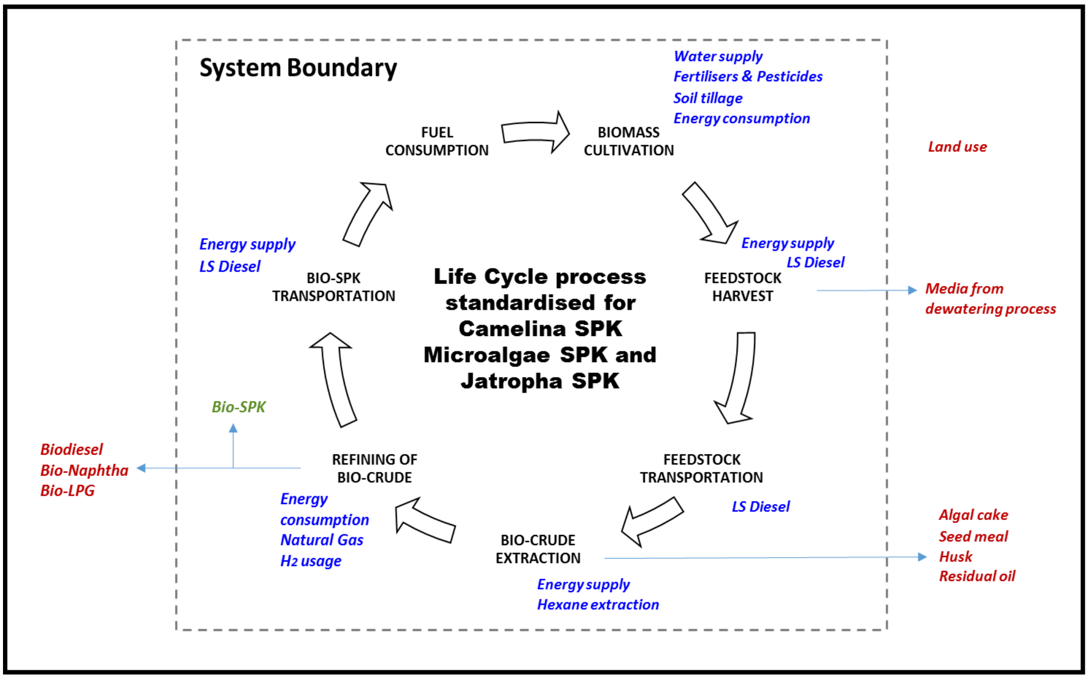


Figure 3-3: System boundary for life cycle assessment of candidate fuels

An elaborate account of a representative engine/aircraft performance operated with 100% Bio-SPKs will form a part of this environmental impact analysis. CO_2 emissions from systems operation (fuel combustion phase) will be interpreted from the performance based fuel consumption data. This technical investigation is facilitated through use of an engine/ aircraft performance simulation code operating on FORTRAN platform. This analysis will be elaborated in further detail in Chapter 5

Inventory Analysis: Quantified material inputs (fertilizer, water and nutrient), energy inputs (fossil derived energy) associated with the production of Bio-SPKs have been integrated into this life cycle study. The material and energy input have been evaluated with the energy specification of the each of the Bio-SPKs and provided in Table 3-1. Owing to the non-commercial nature of Bio-SPKs, uncertainties have been identified and dealt with the use of appropriate assumptions. Energy demands of Bio-SPKs synthesis have been documented for each of the life cycle stages.

Inventory	GHG emissions (gCO_2e/unit)	Units	References
Fertiliser		kg	[2], [15], [29], [34], [49], [55] & [74]
Urea	1845	kg	
Potassium sulphate	345.7	kg	
Phosphorus	210.0	kg	
Tillage	5800	ha	[2], [15], [21] & [23]
Electricity	780	kWh	[21], [29], [58], & [60]
Natural gas	66.3	MJ	[21], [29] & [60]
LPG	76.9	MJ	[15], [58]
Water supply	0.18-0.66	kg	[98] & [112]
Low sulphur diesel	2680	L	[29], [60]
Hexane	21	L	[2], [21] & [34]

Table 3-1: GHG equivalent emission factor of process based material/ energy inputs

Impact assessment: The anthropogenic GHGs incur a direct irreversible impact on the environment through the greenhouse effect. A method of quantifying this greenhouse gas effect and the resulting environmental impact is therefore crucial. In accordance to the Aviation Fuel Life Cycle Assessment Working Group, [12] and a functional unit of this analysis, gCO_2e/MJ, will be used to measure the effect of fuel specific life cycle processes. This unit enables one to weigh the CO_2 emission per unit energy content for a specific fuel. The CO_2 equivalent metrics have been calculated using the global warming potential factors for each of the CO_2, CH_4 and NOx which are 1, 25 and 298 respectively [19] [Eq 8]. It is essential to note that this study primarily focuses on the fuel product and the by-products have been neglected for the purpose of simplicity.

$$LCE\ \ (gCO_2\ e/MJ) = CO_2 + \left(N_2O \times GWP_{N_2O}\right) + \left(CH_4 \times GWP_{CH_4}\right) + CO_{2_{wake}} \qquad \textbf{Eq 8}$$

Interpretation of results: Predicted "cradle-grave" emissions of Bio-SPK will be weighed against the reference fuel, Jet-A1 to identify any environmental benefits / concerns associated with them.

Co-product Allocation: Systems boundary of ALCEmB begins from biomass cultivation (cradle) to wake emissions (grave) and follows energy based emission allocation as the baseline scenario. Mass based emission allocation has been undertaken and presented in section 3.4.11. Due to the uncommercial nature of the biofuels dealt in this analysis and lack of information on supply capacity, market based and displacement allocation has been omitted from this analysis.

3.3.2.1 Biomass Cultivation

Camelina: Camelina is assumed to be sustainably grown through crop rotation with Winter Wheat in Montana, USA, owing to practice of continuous Camelina crop improvement and expansion close to a million acres [97]. Besides resistance to winter season, Camelina, with its lessened need for nutrients, additionally improves the soil quality towards the next batch of winter wheat cultivation [119]. Camelina utilizes reduced amounts of soil moisture for its growth thereby decreasing its need for water supply and subsequent emissions. However, energy and water intensity of activities including soil tilling and fertiliser application have been carefully quantified through consultation of earlier literature and advice from industry experts. Energy consumption is contributed by the use of diesel in equipment for land preparation, and electricity costs towards operation of facilities standardised for a hectare of land. The energy intensity of water supply by pumping ground water to surface is measured as water supply emissions. NER (Net Energy Ratio), which is simply the ratio of energy fed into a process/product to the energy deliverable by the process/product, has been predicted for each of the life cycle process pertaining to respective biomass and production scenarios in order to quantify their energy efficiency over the annual production process.

Microalgae: Microalgal biomass was assumed to be cultivated in raceway ponds owing to their simplicity in operations and cost. The site of production is assumed to be in Southern India owing to a number of well-balanced factors including humidity, temperature cycles, availability of vast areas of non-arable land and ever-increasing interest in algae derived alternative energy. The algal culture will be constantly circulated through use of electrically operated paddle wheel. The algal strain which can serve as potential biofuel feedstock include *Botryococcus sp, Chlorella sp and Chlamydomonas sp*. A continuous supply of nutrients is supplied to the culture and with CO_2 bubbled into the medium in the form of gas mixture (e.g. 3% CO_2 and 97% Air rather than 100% air) [90]. An average requirement of CO_2 supply for algae ranges from 2.18 kg/kg of dry algae grown as reported by some studies [29], [35] and [94].

Parameters	Assumptions	Camelina	Microalgae	Jatropha	Units
Biomass Characteristics	**Seed/Biomass Bio-crude Content**	34	60	35	%
	Bio-crude density	0.906	0.918	0.91	kg/L
	Bio-crude Calorific value [a]	42.2	38.3	37.5	MJ/kg
	CO_2 fixation rate [b]	3050	100000	4050	kg/ha.yield
	Biomass productivity	-	0.7	-	g/L.day
Cultivation based Characteristics	**Area of Cultivation**	1	1	1	ha
	Cultivation capacity	1000	500	1000	ha
	Harvestable Area of Pond	-	50	-	%
	Water Supply	300	1200	500	m^3/yield
	Total Seed/ biomass yield	1700	50000	2500	kg/ha.yield
	Bio-Crude Extraction Efficiency	90	60	85	%
	Total Oil Yield	578	18000	744	kg/ha.yield
	Total Seed/ Biomass meal	1122	32000	1756	kg/ha.yield
	Production rate (per ha)	404.6	12600	520.62	kg SPK /yr
	Annual Plant capacity	404600	6300000	520620	kg SPK /yr

Note:

[a] Data on specific energy of the Bio-crude from *Camelina sativa*, Microalgae and *Jatropha curcas* were adapted from [120], [2] & [90] respectively

[b] Data on CO_2 fixation rate for *Camelina sativa*, Microalgae and *Jatropha curcas* were adapted from [148], [90] & [49] respectively

Table 3-2: Key Cultivation and Yield based assumption for each of the Bio-SPKs

Jatropha: *Jatropha curcas* is assumed to be cultivated in India due to its indigenous nature, present commercial implementation and existing plantations covering 9000 ha of wasteland. The soil type chosen for cultivation is assumed to be of average quality to reduce the plantation's impact on land usage. GHG emissions from use of Urea were adopted from earlier studies [74] and [79].

Cultivation based assumptions and production metrics have been listed in Table 3-2. Assumptions on biomass cultivations and related productivity were adopted after careful consideration from earlier published literature [76] & [143]

A method of predicting the water supply emissions based on the fossil energy source used and degree of energy demand has also be included in this study. According to Nelson et al [98] and Rothausen and Conway [112], lifting of 1 kg of water (assuming water density to be 1000L m^3) to 1m at an efficiency of 100% using diesel as the power source produces 0.665 gCO_2e. These above-mentioned specifications with the use of coal generated electricity produces 3.873 gCO_2e. The method of calculating energy consumption and emissions attributable to water supply has been presented in Equation 9 and 10.

$$\boldsymbol{Energy\ required\ (kWh)} = \frac{\mathbf{9.8}\ (\boldsymbol{m/s^2}) \times \boldsymbol{lift_{water}(m)} \times \boldsymbol{mass_{water}(kg)}}{\mathbf{3.6} \times \mathbf{10^6} \times \left(\frac{\boldsymbol{efficiency}\ (\%)}{\mathbf{100}}\right)} \qquad \textbf{Eq 9}$$

$$\boldsymbol{Net\ emissions} = \frac{[\boldsymbol{FDE\ (kWh)} \times \boldsymbol{Emissions_{FDE}}\ (\boldsymbol{gCO_2eq}\ \mathbf{kW/hr})] \times \mathbf{1}}{\boldsymbol{LHV\ of\ Bio{-}SPK\ obtainable\ from\ 1ha\ (MJ)}} \qquad \textbf{Eq 10}$$

3.3.2.2 Biomass Harvest

Camelina: Camelina seeds are assumed to be harvested mechanically using low sulphur (LS) diesel operated equipment. The harvested seeds are assumed to be transported to the refining site which is integrated with bio-crude extraction facility. Harvest capacity of each of the biomass was calculated from their region specific actual production averages reported by earlier literature and the bio-crude density presented in Table 3-2. It is essential to note that this principle of assumption on production capacity applies to the different biomass dealt in this study.

Microalgae: The algal biomass is assumed to be auto-flocculated through CO_2 starvation and concentrated by use of disc centrifuge which are considered as harvest techniques suitable for baseline allocation [29], [58] and [90]. The dewatering process of algal biomass is predominantly complex, energy intensive and depends on the structural morphology of the feedstock. FDE (Fossil-derived Energy) used to generate electricity to facilitate feedstock harvest was assumed to be natural gas and subsequent emissions have been appropriately calculated.

Jatropha: At the end of the maturation period (end of 2^{nd} year), the oil bearing seeds are assumed to be manually collected [15] & [143] and transported to the refining facility for further processing.

3.3.2.3 Feedstock Transportation

Seeds/ biomass harvested are transported to the oil extraction and refining facility which is assumed to be located at a distance of 150km. The feedstock is transported through heavy truck freight with a vehicle mileage of 6 km/L and a freight capacity of 4 tonnes.

3.3.2.4 Bio-crude Extraction

Camelina: The harvested seeds are crushed by mechanical means at the initial stage. The crushed mix of seed and oil is subjected to hexane extraction in order to separate and degum the bio-crude. The carbon intensity of hexane is 21 gCO_2e/L. This result from vent losses encountered during the meal processing and solvent recovery process [74] & [117]. According to Shonnard et al [119], the quantity of hexane used for oil extraction was 0.00125 L/ kg of seeds harvested. On the other hand, mechanical press method of bio-crude extraction is also employed. However the extraction efficiency of this process ranges between 70-80% depending upon energy demand and capacity of the press used [89]. The Lipids extracted from the biomass is called Bio-crude. The by-product of this stage, Camelina Seed cake can potentially be used as fertilizers or cattle feed. The energy requirement for this process was assumed to be 0.073 kWh/kg seeds.

Microalgae: The lipid content and composition are variable with the algal strain chosen for analysis. Therefore, the downstream procedures will have to be customised to enable high-efficiency lipid extraction. On the overall, microalgal feedstock is energy intensive at downstream processes due to their microscopic morphology. The harvested biomass is sun-dried and subjected to chemical lysis with the lipid content harvested by hexane extraction. The extracted algal bio-crude, at this instance, contains hydrocarbons, lipids, fatty acids, alcohol, aldehydes and other trace elements. The energy and hexane use to boost extraction efficiency were assumed to be 0.02 kWh/ kg and 0.016 kg/ kg of biomass respectively.

Jatropha: Jatropha seeds which are sundried, crushed and pressed through a screw press extruder is assumed to consume electricity by about 0.06 kWh/kg of seeds. The seeds were additionally subjected to hexane-based oil extraction similar to the biomass discussed earlier to improve extraction efficiency to 90%. A standard equation for the estimating total amount of bio-crude extracted from the biomass per yield per year has been presented in Equation 11.

$$\boldsymbol{Bio\ crude\ yield\ (kg)} = \left[\frac{\left(\frac{\boldsymbol{Seed\ Yield\ (kg)}\times \boldsymbol{Seed\ oil\ content}\ (\%)}{\mathbf{100}}\right)\times \boldsymbol{Extract.efficiency}\ (\%)}{\mathbf{100}}\right] \quad \textbf{Eq 11}$$

$$\boldsymbol{Total\ SPK\ yield\ (kg)} = \left[\frac{\boldsymbol{Total\ Oil\ yield\ (kg)}\times \boldsymbol{Conversion\ efficiency}_{\boldsymbol{Refining}}(\%)}{\mathbf{100}}\right] \quad \textbf{Eq 12}$$

3.3.2.5 Hydrotreatment

Hydrotreatment is a refining process where the bio-crude is converted to biojet fuel and other lighter fractions through a series of reactions in the presence of excess hydrogen at variably high temperatures and pressures [Table 3-3] in a presence of a suitable catalyst.

Hydrotreatement stages	Reaction Specifications	Values	Units
Hydrogenation	Catalyst to Bio-derived crude	15	g/L
	Catalyst	Multifunctional*	
	Temperature	590	K
	Pressure	200	kPa
Deoxygenation	Catalyst	Multifunctional*	-
	Temperature	603.15	K
	Pressure	1380	kPa
Hydrocracking	Catalyst	Multifunctional*	-
	Temperature	663.15	°C
	Pressure	7580	kPa
Isomerization	Catalyst	Multifunctional*	-
	Temperature	528.15	K
	Pressure	3275	kPa
Total Hydrogen supply	Jet fuel	3727.4	kPa/L
Jet fuel Fraction	-	70	%
Other fraction	-	30	%

Table 3-3: Temperature, Pressure and other material specifications of Bio-crude refining [90] & [94]

Degummed/ partially refined crude obtained is subjected to further refinement. Hydrotreatment of the bio-derived crude requires large amounts of hydrogen. Hydrogen requirement, in this study, is assumed to be synthesized through steam reformation of methane (40%) (Natural gas) or by naphtha to gasoline reformation (60%); routinely carried out in a petroleum refinery. Hydrotreatment comprises Hydrogenation, Deoxygenation (Decarboxylation, Decarbonylation and Hydro-Deoxygenation), Selective hydrocracking and isomerization of bio-crude. The steps involved in Hydrotreatment of the bio-crude have been obtained from industrial patents [90] & [94]. The resulting products of this reaction will be renewable jet fuel (70%) and renewable diesel (15%) and the remaining fraction being made of naphtha with other lighter fractions derived from a sustainable biological source. Further details on the hydrogenation process have been elaborated in Appendix B. The Hydrotreatment process is assumed to source electricity generated from natural gas.

3.3.2.6 Bio-SPK transportation

The Bio-SPK is transported to the storage facility or destination of product consumption from the refining site, which is assumed to be located at a distance of 150 km. Owing to the uncommercial nature of the Bio-SPKs, earlier workers have adopted the transportation emission for conventional jet fuel for the alternative fuels [15], [29], [60] and [119] which contradicts the consideration of energy dependent functional unit (gCO_2 e/MJ of fuel product) and addressed by ALCEmB in this analysis.

3.3.2.7 Fuel Combustion

Wake emissions resulting from combustion of a given fuel contributes to 70% of total LCE of each of the fuel candidates. Careful prediction of combustion based emissions is, therefore, crucial to the ranking the fuel candidates. This research, unlike earlier studies which use assumed figures for combustion emissions [15], [21], [29] [58] and [119] aims to predict the two main system based GHGs (CO_2 and NOx) from their elemental compositions. CO_2 and H_2O are direct products of any hydrocarbon combustion and thus, their quantifications are straight forward. The combustion temperatures for each of the Bio-SPKs were predicted using respective composition assuming that the hydrocarbons undergo complete combustion with air as the oxidant [Equation 13].

$$C_xH_y + m_s\,(O_2 + 3.76N_2) \rightarrow xCO_2 + \frac{y}{2}H_2O + (3.76.m_s)N_2 \qquad \textbf{Eq 13}$$

where, m_s= Stoichiometric moles of air (Oxidant)

Fuel composition, fuel use for engine performance and aircraft operations over the medium-range trajectory, determined from earlier analyses were incorporated to determine the system level CO_2 emissions of each of the fuel candidate. The outcome of this assessment has been presented in results and discussion section

$$CO_{2_{wake}} = \frac{CC_{fuel}}{LHV_{fuel}} \times \frac{Mm_{CO_2}}{Mm_C} \qquad \textbf{Eq 14}$$

where , $CO_{2_{wake}}$= CO_2 emissions from the wake of an aircraft (gCO_2e/MJ of fuel)

CC_{fuel} = Carbon Content of the fuel (mole fractions)

LHV_{fuel}= Lower Heating Value of the fuel (MJ/g)

Mm_{CO_2} = Molecular mass of CO_2 (g/mol)

Mm_C = Molecular mass of Carbon (g/mol)

As mentioned earlier, CO_2 emissions are assumed to be stoichiometric products of combustion (fuel's carbon content dependent). NOx emissions are, however, influenced by a multitude of parameters including fuel composition, combustor inlet conditions, combustor architecture and operating conditions. NOx prediction therefore demands the use of a robust emission prediction model that enables numerical modelling of a conventional combustor, numerical simulation and quantification of engine emission index.

The study conducted and presented in Chapter 4, entails prediction and analysis of the thermodynamic properties of each of the fuel candidates leading to their implementation into a chosen engine performance evaluation. This analysis is further extended into a user-defined medium-range mission level assessment and attributable mission level emission prediction. The performance of engine/aircraft performance is measured in terms of fuel burn which in turn will lead to the ultimate purpose of wake emission prediction (towards the "grave" phase LCE). This study has been elaborated in greater details with the associated assumptions in Chapter 5.

3.3.3 Life Cycle processes of Conventional Jet fuel

The Life cycle processes and emissions of conventional Jet-A1 have been adopted from earlier studies [60], [75] and [85]. However, the life cycle inventory was reconstructed and the emissions have been recalculated through incorporation of technology efficiency improvement of 11.1%. The life cycle emissions of Jet-A1 were determined to be 105.0 gCO_2e/MJ of Jet-A1. Further details on the assumptions and the life cycle process of Jet-A1 can be obtained from Appendix C.

3.4 RESULTS AND DISCUSSION

3.4.1 Chemical composition of Bio-SPKs

The chemical characteristics of the fuel candidates are essential in order to determine their consumption based carbon footprint. This information also aids the deduction of biomass credit obtainable from their respective biomass cultivation process. The molecular data for each of the fuel candidates has been presented in Table 3-4.

Hydrocarbon	Molar mass (g/mol)	Molecular formula
Jet-A1	174.4	$C_{12.5}$ $H_{24.4}$
Camelina SPK	159	$C_{11.2}$ $H_{24.4}$
Micralgae SPK	164	$C_{11.5}$ H_{25}
Jatropha SPK	160	$C_{11.3}$ $H_{24.5}$

Table 3-4: Molecular mass of analysed hydrocarbons

The H/C ratio has been determined to be relatively higher than that of JetA-1 facilitating a 3% reduction in GHG emissions upon fuel combustion as tabulated in Table 3-5. Molar mass of the fuel candidates was essential in order to determine the carbon and hydrogen content of the fuel. The higher hydrogen content of the Bio-SPKs is reflected in their lower heating value. The increased hydrogen content of Bio-SPK is environmentally favourable in terms of relatively higher fuel burn and lower soot formation upon combustion. Certain other thermochemical and physical characteristics exhibited by the Bio-SPKs in close resemblance with conventional Jet fuel have been tabulated in Table 3-5

Hydrocarbon	Carbon content	Hydrogen content	H/C ratio	Lower Heating Value (MJ/kg)
Jet-A1	0.86	0.14	1.95	42.8
Camelina SPK	0.85	0.15	2.18	44.1
Microalgae SPK	0.85	0.15	2.17	43.2
Jatropha SPK	0.85	0.15	2.19	44.3

Table 3-5: Molecular formula estimation of analysed bio-hydrocarbons

The chemical composition of the Bio-SPKs predicted above shows discrepancies relative to that of Conv.Jet fuel. This observation theoretically hints that Bio-SPKs are likely to exhibit varying thermodynamic impact and subsequently varying fuel performance properties relative to Jet-A1. Fuel compatibility in existing systems becomes significant with aero-engine as it dictates the airline industry's sensitivity to the two main factors: techno-economical and passenger safety considerations. It is essential that any new fuel is completely compatible with the existing engine/ aircraft configurations in order to ensure technical reliability, passenger safety and thus profitability to the airline operator (eliminating the need for engine upgrade) and passenger safety (storage and handling properties ideal through variable phase of operation).

A clear insight into the Bio-SPKs compatibility with the existing aero-engine is understandable only through an elaborate experimental set-up (bench, rig and flight test). This study, on the other hand, has attempted to qualitatively analyse the behaviour of the Bio-SPKS within an engine fuel system which stems from their underpinning elemental composition. This analysis has been presented in greater detail in chapter 6.

3.4.2 Direct and Indirect Land use change

Land use change (LUC) is one of the emission contributing factors associated with biofuels and is also a hotly debated uncertainty for consideration. Emissions from land use change are scaled based on the area of land used and its fertility factor. However, in many studies, this analysis feedstock have been determined to perform well in marginal land [15], [18], [77], [29], [119], [120] & [149] and thus eliminate the risk of "food vs. fuel" conflict.

Camelina sativa, in this study, have been assumed to be crop rotated with Winter wheat which can be expected to contribute to indirect Land use change (iLUC). However, the iLUC emissions have been excluded in this study owing to the biofuel crop's ability to improve soil quality over its life time. Cultivation of microalgae is independent of arable land requirement as a result of which LUC emissions are eliminated in this scenario. Cultivation of *Jatropha curcas* on non-arable land has been demonstrated to reclaim waste land. Bailis and Baka, [15], have assumed this scenario to contribute to emissions from indirect land use change. However, these emissions have been omitted since it is outside the scope of this TERA study.

3.4.3 Biomass cultivation

Emissions related to biomass cultivation arise from use of fertilizers and nutrients. Kindred et al, (1998), reported that nitrogen based fertilizers contribute the highest GHG emissions due to N_2O emissions emanating from mineralization of nitrogen in the soil. Besides urea, emissions linked to other fertilisers have been adopted from Lal,R (2004) [79]. GHG emissions associated with quantified fertiliser input were calculated as prescribed by IPCC.

Bio-source	**Parameters**		**Values**	
			Quantity (kg/kg feedstock)[d]	**Emissions (gCO_2 /kg feedstock) [b, d]**
Camelina	Fertilizer inputs [a]	Urea	0.07	119.1
		Phosphorus pentoxide	0.03	4.5
		Potassium sulphate	0.04	11.6
		Water supply	17.64	3.2
		Diesel (Tillage)	0.04	3.4
	Fertilizer induced emissions	Total Emissions		138.4
		Net Emissions (gCO_2e/MJ)		**9.9**
Jatropha	Fertilizer inputs [a, c]	Urea	0.09	161.9
		Phosphorus pentoxide	0.02	3.8
		Potassium sulphate	0.04	13.6
		Water supply	24	16.0
		Diesel (Tillage)	0.04	2.3
	Fertilizer induced emissions	Total Emissions		197.6
		Net Emissions (gCO_2e/MJ)		**21.6**
Microalgae	Fertilizer inputs [a]	Urea	0.07	124.4
		Phosphorus pentoxide	0.04	8.56
		Potassium sulphate	-0.07	-25.0
		Water supply	20	13.3
		Energy supply (kWh kg^{-1} seed)		3.51
	Fertilizer induced emissions	Total Emissions		125.0
		Net Emissions (gCO_2e/MJ)		**16.7**

Note:

[a] Data obtained from [15], [29], [77] & [143]

[b] Total emissions were calculated using fertilizer relevant emission data from [79]

[c] Potassium sulphate incurs a negative emissions flow since the algal cakes obtained at the end of the extraction process is used as source of potassium [29], [89]

[d] Feedstock refers to Camelina seeds, Jatropha Fruit, and Microalgal biomass respectively.

Table 3-6: GHG emissions from resource inputs into Biomass Cultivation

Biomass cultivation was observed to be the second highest emissions contributor to the overall life cycle of Bio-SPKs. To improve the specificity of this finding, emissions related to water supply were observed to be significant [Table 3-6]. With the realisation of depletion of fresh-water resources, careful selection of feedstock with lower demands for irrigation is equally significant as land use emissions. *Camelina sativa*, owing to its lesser demand for irrigation, produced the lowest of water supply emissions. However, the productivity attributable to *Jatropha curcas* was observed to be biased to water supply. Abou Kheira and Atta, (2010), observed that Jatropha trees with increased water supply performed well, in terms of seed quality and oil content [1].

3.4.4 Biomass Credit

Biofuel plantations perform natural carbon sequestration through photosynthesis. Biomass derived carbon deficit is allocated to a product or a process depending upon its capacity to sequester CO_2 (atmospheric / anthropogenic) during its life cycle. The resulting CO_2 is also expressed as gCO_2 e/MJ of fuel product.

Zhang et al, (2012) have reported that *Camelina sativa* CO_2 has a carbon fixation rate of an average of 3.1MT/ ha.yr [148]. This data was interpolated into this analysis and the carbon credit apportioned to Camelina SPK was determined to be 70gCO_2/ MJ fuel. Carter et al, 2012, stated that microalgal biomass requires a CO_2 supply of twice its dry cell weight. An average of 1200 ppmv of CO_2 supply has been recorded to be sufficient to improve biomass productivity [29]. Thus, the biomass credit allocated to Microalgae SPK was determined to be 71.5 gCO_2/MJ of fuel. With respect to *Jatropha curcas,* Firdaus et al, (2010) and Romijn H.A, 2011, have experimentally determined the capacity of a 3 year old plantation to sequester an average of 13 tons CO_2/ha per annum [49] & [111]. This data led to the allocation of a carbon credit of 70.0 g CO_2/MJ for Jatropha SPK.

3.4.5 Biomass Harvest

The emissions associated with Camelina seed harvest results from use of LS diesel for harvesting. Microalgal biomass, owing to its microscopic structure, has to be centrifuged thoroughly during the dewatering process. The energy intensity of biomass harvest is variable with the morphology of the feedstock microalga. Carter et al, (2010), have assumed an electric electricity supply of an average of 1.07 kWh/kg biomass for baseline scenario which has been adopted for this study [29]. Jatropha seeds are harvested manually and therefore do not incur any CO_2 emissions.

3.4.6 Feedstock Transportation

The assumptions considered earlier resulted in standard transportation based emissions of 0.067kgCO_2/kg of LS diesel. Initially, the emissions related to transportation of each feedstock type have been calculated using the lower heating value (LHV) of total SPK obtainable from one hectare of land.

3.4.7 Bio-crude Extraction

The lipid content within the biomass is extracted using the solvent n-Hexane. Emissions from n-Hexane occur through vent losses upon reaction of the solvent with crushed mix of lipids and seeds/biomass. The by-products generated at this stage include seed/biomass cake. The seed cake and husk meal generated from Jatropha are poisonous and can potentially be used as biomass for direct combustion. Emissions related to hexane use were fairly equal with each of the feedstock because these emissions depended upon the degree of biomass yield and total obtainable SPK energy obtainable from the same. These emissions fell in the range of 0.45-0.5 gCO_2 e/MJ.

3.4.8 Hydrotreatment

Bio-SPK is synthesised through Hydrotreatment process which results in the production of different distillates including renewable jet fuel (Bio-SPK) and renewable diesel. From the knowledge of the Hydrotreatment process illustrated, it is evident that air emissions released from the process include CO_2 from decarboxylation and NOx emissions from the hydrogenation step. However, the amount of GHG released at each stage is unknown due to lack of information in open literature. The final products of Hydrotreatment comprises 70% of renewable jet fuel, 15% of renewable diesel and the rest of the fraction is made of lighter liquid and gaseous products. The net GHG emissions arising from Hydrotreatment to produce individual Bio-SPK types was therefore is assumed to be 10.3 gCO_2e/MJ of the fuel product similar to earlier life cycle analysis [2], [15], & [29]. It is also essential to note that the Hydrotreatment is an energy intensive process and therefore electricity generated using Natural gas was assumed to power this life stage.

3.4.9 Bio-SPK transportation

The product of analysis (Bio-SPK) derived from the Hydrotreatment process is transported through truck freight to storage facilities which are assumed to be located at a distance of 150 km. The vehicle mileage was assumed to be 6 km/L of diesel. The CO_2 emission for LS diesel is 2.68 $kgCO_2/kg$ of fuel. The calculated Bio-SPK transportation emissions have been determined to be higher than the values adopted in previous work. The reasons for dissimilarities in fuel transportation based emissions values between this study and that of previous workers can be due to assumptions of similarities in fuel properties between Bio-SPK and the standard fuel. Therefore the strategy of earlier studies was to bridge this gap was to adopt Jet-A1 transportation emissions into the LCA of biofuels.

3.4.10 Bio-SPKs combustion

Fuel Combustion is the phase which contributes the highest GHG emissions in this "Cradle-Grave" emission assessment. Therefore, it is imperative to predict this phase with utmost accuracy. The route of fuel utilisation, combustion and release of wake emissions have been undertaken through computation modelling and numerical simulation to best imitate an experimental setup. The model developed has been cross-checked and validated with existing commercial benchmark model (Twin shaft turbofan engine- CFM56-5B/2; Airframe- A321; Medium-range missions London, Heathrow to Quebec, Canada). Further details on the method of analysis and outcome have been presented in section 5.4. However, emissions attributable to the fuel combustion, in this module, were predicted through a simplified empirical method listed in the section 3.3.2.7 and the "cradle-grave" life cycle emissions of the candidate fuels have been tabulated in Table 3-7. A schematic presentation of the same has been included in Figure 3-4 for better visualisation of the effect of biomass credit on LCE reduction.

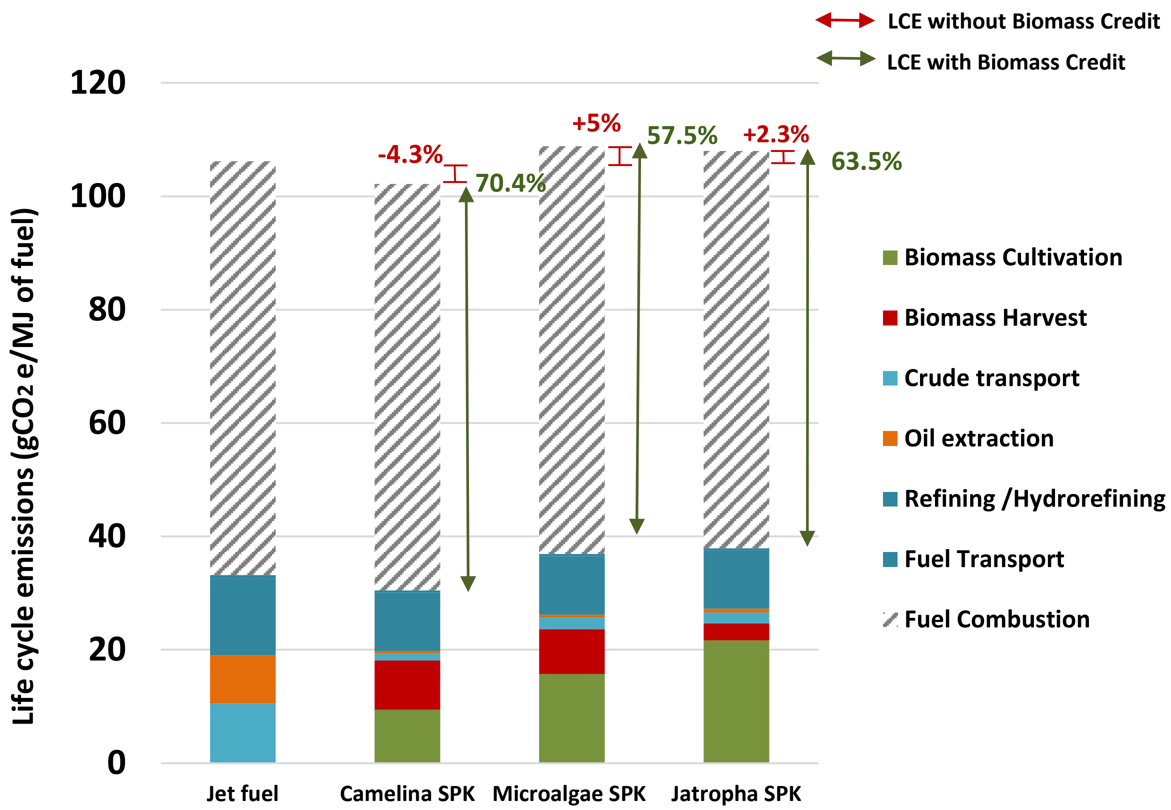


Figure 3-4: Diagrammatic representation of LCEs and its offset through Biomass credit

Life Cycle stages	Emissions (gCO_2e/MJ of fuel)						
		Camelina SPK		Microalgae SPK		Jatropha SPK	
	Jet –A1	ALCEmB	[18], [119]	ALCEmB	[123], [143]	ALCEmB	[15], [143]
Biomass Cultivation	-	**9.9**	15.1	**16.6**	22.5	**21.6**	24
Biomass Credit	-	**-70.0**	-70.2	**-71.5**	-70.5	**-70.0**	-72.0
Feedstock Harvest	-	**8.2**	-	**9.5**	-	**3.0**	0.0
Feedstock Transportation	10.5	**1.2**	1.7	**2.3**	1.5	**1.9**	1.5
Oil Extraction	8.5	**0.5**	-	**0.6**	-	**0.7**	-
Refining/ Hydrotreatement [a]	13.5	**10.3**	10.3	**10.3**	10.3	**10.3**	11
Fuel transport	0.6	**0.4**	0.6	**0.39**	0.6	**0.38**	0.6
Fuel Combustion	73	**71**	70.4	**72**	70.4	**70.6**	70.4
Total emissions without carbon credit	106.1	**101.5**	-	**112.0**	-	**108.5**	-
Total emissions with carbon credit	106.1	**31.4[b]**	34.2	**40.1[b]**	42	**38.0[b]**	39.7
% Reduction	0	**70.4**	76	**57.5**	59	**63.7**	71

Note:

[a] The GHG emissions average for Hydrotreatment of bio-crude was adopted from [90] & [94] due to the proprietary nature of this process

[b] Total emissions may not add up to indicated figures due to round off of decimals

[c] Mass allocation considers 70% SPK synthesis from Jet fuel production process

Table 3-7: Life Cycle Emissions of candidate fuels predicted using LCE model ALCEmB

3.1.1 Life Cycle Emissions of Candidate fuels

The overall life cycle emission of Bio-SPKs relative to that of Conv.Jet fuel has been predicted using the life cycle emission prediction model, ALCEmB. Biomass credit, a feature unique to the Bio-SPKs (from photosynthesis of biomass plantation) is capable of reducing their life cycle emissions by about 70-72g. The Life cycle emissions of Camelina SPK, Microalgae SPK and Jatropha SPK were determined to be 31.4g, 40.1g and 38g respectively, relative to that of Conv. Jet fuel (106.1g). Major discrepancies in emissions where observed in the following life cycle stages: biomass cultivation and feedstock harvest. Among the three biofuel candidates, Jatropha cultivation was observed to have the highest emissions owing to the increased quantities of water and fertiliser input relative to the quantity of Bio-SPKs generated from 1 hectare of land. On the other hand, Camelina requires relatively lower quantities of water and fertilisers and is crop-rotated with winter wheat which in turn reduces its overall cultivation based footprint. In terms of feedstock harvest, Microalgae SPK was determined to possess higher carbon footprint since this third-generation biofuel feedstock requires high end technology for downstream processing. Mature Jatropha fruits, on the other hand, are hand-picked. The harvest emissions of 3 g attributable to Jatropha SPK are from transportation of seeds across the plantation.

3.4.11 Co-Product Allocation & Net energy ratio

Mass allocation (ISO 14044) enables excess allocation of emissions to the comparatively higher number of co-products generated in the process of all the three feedstock. Mass based allocation reduces the overall life cycle emissions of Camelina SPK, Microalgae SPK and Jatropha SPK to 24, 29, 29.5 gCO_2e/ MJ of fuel, respectively. The reduction in LCE obtained with mass based allocation in comparison with energy based allocation for Camelina SPK, Microalgae SPK and Jatropha SPK was determined to be -11.7%, -18.3% and -17.3% respectively. Microalgae SPK benefited the most from mass based allocation due to its considerably higher biomass output and subsequent increase in carbon fixation rate.

NER (Net Energy Ratio), which is simply the ratio of energy fed into a process/product to the energy deliverable by the process/product, has been predicted for each of the life cycle process pertaining to respective biomass and production scenarios in order to quantify their energy efficiency over the annual production process. According to ISO 14000, life cycle energy analysis of nuclear energy, photovoltaic and high energy petroleum products has been conducted. A similar approach was used to predict the energy efficiency of the existing technology for Bio-SPK processing. The net energy ratio of Camelina SPK, Microalgae SPK and Jatropha SPK was determined to be 1.158, 1.135 and 1.164 as presented in Figure 3-5. The pattern of energy use between the Bio-SPKs has been fairly constant in all the life cycle stages except that of biomass harvest. The energy intensity of the harvest process varies with the morphology of biofuel feedstock. Microscopic morphology of algal biomass thus demands high end harvest equipment (disc centrifuge) which was determined to consume 1.62$\pm$0.5 kWh/ kg algal biomass. An increase in electricity consumed at this stage, relative to that spent on other feedstock, has led to drop in NER with Microalgae SPK. However, on an overall, all processes with were observed to be energy efficient (NER>1) with microalgae SPK and the other candidate biofuels as well. The reason

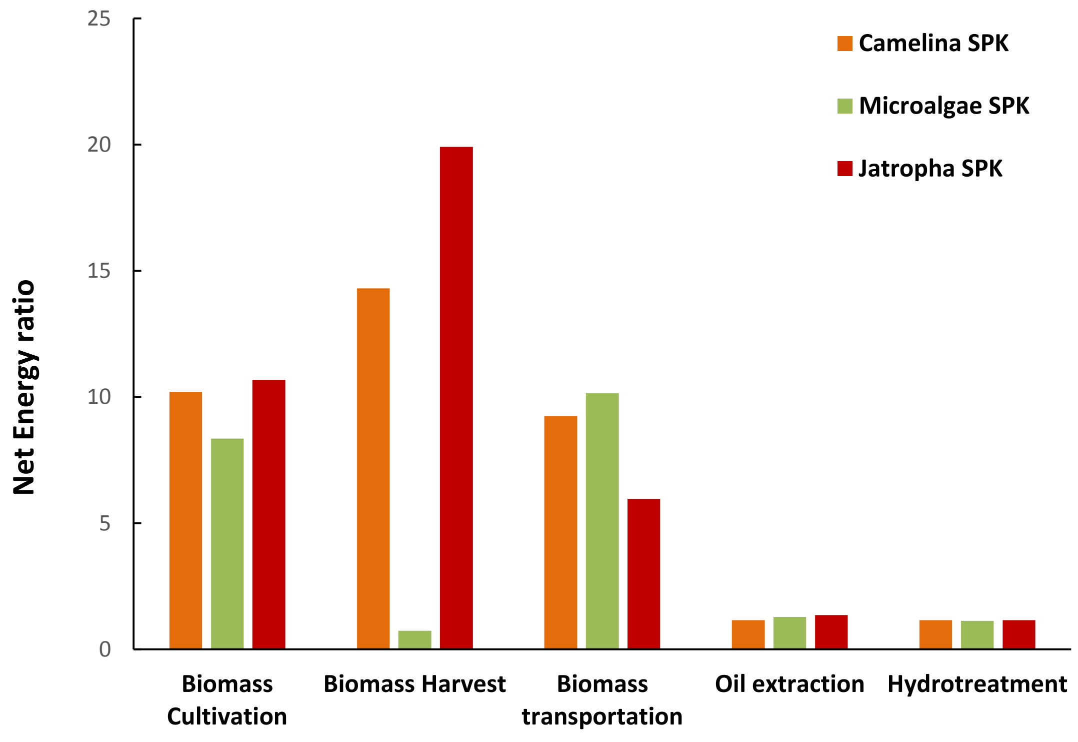


Figure 3-5: Net Energy Ratio vs. life cycle processes of the Bio-SPKs

3.5 CONCLUSION

ALCEmB is a “Cradle-Grave” GHG emission prediction model devoted to advanced biofuels. Life cycle carbon savings delivered by 100% blends of Camelina SPK, Microalgae SPK and Jatropha SPK with respect to Jet-A1, were determined to be 70%, 58% and 64% respectively. The GHG emissions of each of the Bio-SPKs were calculated through ALCEmB by accounting region-specific feedstock-carbon intensity (e.g. fertiliser, water, fossil fuels) as opposed to standardised figures used in earlier literature [15], [18], [21], [58] [60] & [143]. The Bio-SPKs were able to clearly demonstrate their environmental competence at process level and system level against the reference fuel, Conv.Jet fuel. Among the Bio-SPKs, Camelina SPK was determined to possess the lowest carbon intensity among the biofuel candidates. Camelina feedstock may appear to be more environmentally viable option. However, the natural carbon sequestration and waste land reclamation capabilities of Microalgae and Jatropha can have an equally significant positive impact coupled with improvement of social-economic conditions and energy independence of developing nations. Further reductions in life cycle emissions may be achievable through

- Use of organic fertilizers and pesticides derived from Bio-crude production process
- Improvements in Plant/ strain yield characteristics.
- Further developments in management of biofuel plantations and Bio-crude extraction processes.
- Use of potential fuel type by-products of Bio-SPK production process.

However, upon grading the Bio-SPKs based on their “Cradle-grave” emissions, ALCEmB reports Camelina SPK has a relatively lower carbon intensity relative to the other two biofuel candidates.

Secondly, the rate of carbon sequestration is proportional to the carbon content of Bio-crude and subsequently Bio-SPKs, provided the mass and energy balance across the hydrotreatment process (for all the three types of bio-crudes) is maintained constant. The higher the capacity of biomass to fix CO_2, the higher will be the carbon content of Bio-SPK. Recent strain development efforts which include higher CO_2 fixation rate is expected to have a marked effect on the chemical composition of resultant biojet fuel [148]. However, there is a probability for UOP’s

Renewable jet process to find a solution to this issue through techno-economic improvements to the existing hydrocracking process; resulting in Bio-SPKs of standard compositions. Bio-SPKs, on an overall scale of study, have been determined to be a valuable asset in terms of following benefits associated with it besides sustainable method of energy generation. They include

- Afforestation,
- Waste land reclamation,
- Community uplift in developing countries

These benefits are likely to outweigh the drawbacks associated with life cycle emissions. However, this can be demonstrated only through long term life cycle assessment. The combustion emissions reported in this study, through theoretical calculations, will be required to be verified through simulation techniques to get a clearer portrait of Bio-SPKs combustion emissions within in aircraft engine. This study, however contributes to knowledge through a holistic environmental analysis of the carbon emissions allied with processes of each of the Bio-SPKs synthesis and the potential of these “Drop-in” biofuels in the aviation industry.

4 DETERMINATION OF THERMODYANAMIC FLUID PROPERTIES OF BIO-SPKS

(Technical Module)

4.1 INTRODUCTION

ALCEmB (Assessment of Life Cycle Emissions of Bio-SPKs) has not only demonstrated the environmental competence of the advanced biofuels but has also provided a valid motive to extend the analysis of biofuels to system level evaluation. The technical assessment of Bio-SPKs is expected to establish the engine based thermodynamic impact imparted by Camelina SPK, Microalgae SPK and Jatropha SPK through a virtual and representative gas turbine performance simulation.

4.2 LITERATURE REVIEW

The significance of an accurate gas model for engine level performance has been acknowledged in many studies. Studies of reference [10], [134] & [142] carried out a technical quantitative assessment on Fatty Acid Methyl Esters (FAME- 1st generation biofuels) and FT-SPK blends that operated a turboprop and turbofan engine. References [134] & [142] were virtual experiments in nature, similar to this study. However, these studies failed to report any analysis on the thermodynamic fluid properties of the alternative fuels assessed except study of reference [134] which predicted the fluid property model for 1st generation biofuels (FAME). The technical module of this TERA study is initiated with the development and analysis of a dedicated gas model (for the development of fuel-specific thermodynamic fluid library) and use of the gas model towards rigorous engine performance estimation. Uncommercial nature of the biofuels in question resulted in a rare recovery of studies from the open domain, most of which had adopted hypothetical fuel compositions besides other studies which undertook elaborate laboratory based rig and flight test programs [28] and [29]. These studies reported the outcome of rig-based experiments and flight tests but failed to detail the effect of fuel properties on the performance of engine/airframe configuration. The technical module of this TERA study aims to bridge this gap in literature by incorporating numerically predicted chemical composition of Camelina SPK, Microalgae SPK and Jatropha SPK, unlike assumed compositions used in earlier studies. This is followed by the development of a robust thermodynamic model for the prediction of Bio-SPK based post-combustion fluid properties which are of significance to jet engine performance simulation. The fluid properties were predicted as a function of temperature (T), pressure (P) and fuel-air ratio (FAR). Rigorous engine performance analysis is a means of non-linear computational simulation which, unlike linear numerical simulations, assumes the working fluid to behave like partially real gas. This assumption also indicates that the fluid properties which include enthalpy, entropy, gamma property, density, and isobaric specific heat, will be influenced by temperature (T) and pressure (P) conditions that vary at the different stations of an operating jet engine.

Before proceeding further, a brief look into the thermodynamic definitions of engine cycle calculations built within TURBOMATCH is essential. A fully rigorous engine cycle simulation demands the definition of governing thermodynamic principles. However, for the purpose of basic introduction, simplified definitions adopted from Walsh and Fletcher (2004), [139], has been presented below.

$$\boldsymbol{h = H0 + \int Cp.dT} \qquad \textbf{Eq 15}$$

where, *h = Specific Enthalpy (kJ/kg)*

H0= Energy per kilogram of gas relative to a stipulated zero datum

Cp = Specific heat at constant pressure (kJ/kg.K)

dT = change in temperature (K)

(**Note**: for fully rigorous method of engine cycle estimation, *Cp.dT* becomes a function of temperature, pressure and FAR and is generated using a polynomial specific to temperature difference. The change in enthalpy is a rather preferred measure than the absolute enthalpy itself in an engine performance simulation).

Similarly, entropy is fundamentally defined as follows

$$\boldsymbol{S_2 - S_1 = \int \frac{Cp}{T} dT - R \times ln(\frac{P_2}{P_1})} \qquad \textbf{Eq 16}$$

where, S = change in Entropy (J/kg.K)

P_1 = Inlet pressure condition (kPa)

P_2 = Outlet pressure condition (kPa)

R = Gas constant (J/kg.K)

(Note: in fully rigorous method of engine cycle estimation, *Cp/T.dT* becomes a function of temperature, pressure and FAR and is generated using a polynomial specific to temperature difference)

Some studies of reference, [78] & [137] have appreciated the precision achieved with fully rigorous engine cycle estimation and also indicate that its inaccuracies are influenced by the quality of ideal gas assumptions and thermodynamic models. The current version of TURBOMATCH employs thermodynamic definitions from Walsh and Fletcher (2004), [139], for rigorous engine-cycle calculation. The authors of these definitions have also indicated that these polynomials are only suitable for non-dissociated combustion-gas modelling up to temperatures of just 2000K [139]. From Eq 15 & 16, the significance of predicting Cp with the best achievable accuracy is evident. Similarly, studies of reference [27] have brought to light that most thermodynamic models do not capture the translational, rotational and vibrational energies of the particles (sensitive to temperature changes) in a fluid system which contributes precise estimation of Cp. This study, in addition to predicting the fluid properties of the Bio-SPK, aims to develop and implement a valid thermodynamic model which accounts for variations in temperature/ pressure and equilibrium combustion products, unlike the existing model employed in the current version of TURBOMATCH.

4.2.1 Thermodynamic Fluid model

The thermodynamic properties of fluids (air, fuel/ air mixture and combustion gases) are dependent on the operating parameters across the engine. The fuel, upon combustion, is destined to undergo dissociation where combustion products other than CO_2, H_2O and N_2 will be found in the exhaust gases. The kinetic energy of the combustion gases influence the turbine performance which in turn feeds into a continuous engine cycle defining the requirement of a robust gas model. The method through which the above mentioned was achieved is as follows

1. Construction of a thermodynamic fluid library for Camelina SPK, Microalgae SPK and Jatropha SPK as a function of T,P and FAR with the following fluid properties
    - Enthalpy (h)
    - Entropy (s)
    - Gas Constant (R)
    - Specific Heat at Constant Pressure (Cp)
    - Dynamic Viscosity (μ)
    - Adiabatic Index (γ)

2. The influence of the three variables, listed below, on the gas properties has been assessed. Previous studies [44] & [116] have adopted a rigorous method of fluid property estimation through linear interpolation using the listed variables in addition to Water Air Ratio (WAR). They are

   - Temperature (200-3000K)
   - Pressure (0.5, 5 and 50 atm)
   - Fuel Air Ratio (0.02, 0.04, 0.06 and Stoichiometric)

3. Detailed account of the resulting combustion products from an equilibrium reaction which include

   - Nitrogen
   - Oxygen
   - Argon
   - Neon
   - Water vapour
   - Carbon di-oxide
   - Carbon monoxide
   - Sulphur-dioxide

4.2.2 Kinetics of Dissociated Combustion

Dissociated combustion is an endothermic chemical reaction which takes place at temperatures >1750K and at low pressure conditions. A chemical equilibrium reaction results in combustion products including CO, NO, NO_2, SO_2, with monoatomic species which include O, N, OH, and H (variable with fuel composition). Other negligible constituents, as indicated in [92] & [116] include C_2H_2, CH_2CO, $O(CH)_2O$, $HO(CO)_2OH$, C_2H_3, CH_3CN, CH_3CO, C_2H_4, C_2H_4O, CH_3CHO, CH_3COOH, $OHCH_2COOH$, C_2H_5, C_2H_6, $CH_3N_2CH_3$, C_2H_5OH, CH_3OCH_3, $CH_3O_2CH_3$, CCN, CNC, OCCN, C_2N_2, C_2O, C_3, C_3H_3, C_3H_4, C_3H_5, C_3H_6, C_3H_6O, C_3H_7, C_3H_8, CNCOCN, C_3O_2, C_4, C_4H_2, C_4H_4, C_4H_6, C_4H_8, $(CH_3COOH)_2$, C_4H_9, C_4H_{10}, C_4N_2, C_5, C_5H_6, C_5H_8, C_5H_{10}, C_5H_{11}, C_5H_{12}, $CH_3C(CH_3)_2CH_3$, C_6H_2, C_6H_5, C_6H_5O, C_6H_6, C_6H_5OH, C_6H_{10}, C_6H_{12}, C_6H_{13}, C_6H_{14}, C_7H_7, C_7H_8, C_7H_8O, C_7H_{14}, C_7H_{15}, C_7H_{16}, C_8H_8, C_8H_{10}, C_8H_{16}, C_8H_{17}, C_8H_{18}, C_9H_{19}, $C_{10}H_8$, $C_{10}H_{21}$, $C_{12}H_9$, $C_{12}H_{10}$, HCN, HCO, HCCN, HCCO, HNC, HNCO, HNO, HNO_2, HNO_3, HCHO, HCOOH, H_2O_2, $(HCOOH)_2$, N, NCO, NH, NH_2, NH_3, NH_2OH, NO_3, NCN, N_2H_2, NH_2NO_2, N_2H_4, N_2O_3, N_2O_4, N_2O_5, N_3, N_3H and O_3.

When adiabatic flame reaches peak temperatures >1800K, the sufficiently stable species such as H_20 and CO_2 can also be dissociated to mono-unstable species like CO, O, OH. NOx emissions can be quoted as examples of this behaviour where the N_2 atoms from air are dissociated to N atoms and bonded with atmospheric oxygen atoms to form NO and NO_2.

$$CO_2 \rightleftharpoons CO + \frac{1}{2}\, O_2 \qquad \textbf{Eq 17}$$

$$H_2O \rightleftharpoons H_2 + \frac{1}{2}\, O_2 \qquad \textbf{Eq 18}$$

$$H_2O \rightleftharpoons OH + \frac{1}{2}\, H_2 \qquad \textbf{Eq 19}$$

$$\frac{1}{2} O_2 \rightleftharpoons O \qquad \textbf{Eq 20}$$

$$\frac{1}{2} H_2 \rightleftharpoons H \qquad \textbf{Eq 21}$$

$$\frac{1}{2} N_2 + O_2 \rightleftharpoons NO + \frac{1}{2}\, O_2 \qquad \textbf{Eq 22}$$

The level of dissociation is temperature and pressure dependant. Higher combustion temperature favours the bond breaking and, therefore, the temperatures of dissociated products are relative higher. Higher temperature favours higher levels of dissociation. It is essential to note that pressure is directly proportional to the number of moles. From the above reactions, it is evident that the dissociation process is favoured by low pressures. This confirms that the behaviour of dissociated species is based on Le-Chatelier's Principle which states that *when a system in equilibrium experiences a change in temperature, pressure, volume or concentration, the system will shift to a new equilibrium to counter the effects of the change.* In the equation17-22, the increased temperature or low pressure can be seen as a scenario on the reactant side which is corrected by the system to a new equilibrium through dissociation [54]. Dissociation results in low energy dissociated species with lower specific heat capacity. Therefore, there is a steep drop encountered in the heat transfer and density of the gas mixture. In order to reduce dissociation (reduction of non-CO_2 emissions) increasing pressure/ decreasing combustion temperatures can bring about a chemical rebound. This behaviour will influence the turbine performance by increasing the nozzle pressure ratio improving the jet-stream characteristics (improved enthalpy release, denser fluid) thus increasing the thrust output. Knowledge of the effects of the variables (T, P and FAR) on dissociation and its subsequent impact on engine component behaviour is crucial to comprehend of the performance properties of a given fuel on gas turbine engine performance.

4.3 METHODOLOGY

4.3.1 Bio-SPK Composition

The chemical composition of the fuels in question is the underpinning element towards the prediction of their caloric and transport property. Their compositions (presented in Table 3-4 and Table 3-5) were numerically estimated from their basic carbon distribution data and the method of numerical prediction has been established in Appendix A.

4.3.2 NASA CEA (Chemical Equilibrium with Applications)

Fluid property tables were developed using a FORTRAN based computational code called CEA (Chemical Equilibrium with Applications) developed by Sanford Gordon and Bonnie McBride in 1994 at NASA Glenn research centre, Ohio, US. A number of chemical equilibrium software available for the determination of thermodynamic properties include CANTERA, GASEQ, MINTEQ and Kineticus. However, NASA CEA was chosen for this study owing to its established industrial level accuracy [27]. NASA CEA is a thermodynamic program which estimates and holds thermodynamic data for over 2000 chemical species at chemical equilibrium condition. These fluid characteristics are estimated using a 9-constant co-efficients through iterative algorithm specific to temperatures between 200 K -20000 K. The key feature of CEA is its ability to accurately estimate temperature dependant properties (*Isobaric Specific heat capacity, Enthalpy and Entropy*) with reliable precision despite the effects of higher thermodynamic temperatures at a relatively shorter computational time. The CEA code is continually updated with newer chemical species and more robust co-efficients to boost its accuracy e.g. the older version of 4^{th} order polynomial was replaced by seven-term functions in the newer version which has been further elaborated in the associated literature [92] and provided in the following section between equation 22-24. The input specifications and variables required to create a query and predict thermodynamic library using the industrially accepted Chemical equilibrium software called NASA CEA (NASA Chemical Equilibrium with Applications) has been illustrated in Appendix D and associated literature [92] & [93].

4.3.3 Empirical Equations for Fluid property estimation

A characteristics exhaust gas is composed of the following components which are as follows

- Carbon-dioxide

- Oxygen
- Nitrogen
- Water vapour
- Argon
- Carbon monoxide
- Neon
- Sulphur-dioxide

Caloric properties of the gas mixture is dictated by the caloric properties and the concentration if individual species from the exhaust gases. NASA CEA uses seven-term functions with integration constant that has been determined to be more accurate among the various thermodynamic models analysed, as stated by studies of reference [27], [78] and [137]. The empirical equation for enthalpy, entropy and isobaric specific heat capacity (properties dependant on temperature) where predicted through least square fit in order to minimise discrepancies arising from higher thermodynamic temperatures [92]. The thermodynamic definitions related to NASA CEA have been presented in equations 23-25.

Isobaric Heat Capacity:

$$\frac{Cp}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \quad \textbf{Eq 23}$$

Enthalpy:

$$\frac{H^0\,(T)}{RT} = -a_1T^{-2} + a_2T^{-1} + lnT + a_3 + a_4\frac{T}{2} + a_5\frac{T^2}{3} + a_6\frac{T^3}{4} + a_7\frac{T^4}{5} + \frac{b_1}{T} \quad \textbf{Eq 24}$$

Entropy:

$$\frac{S^0\,(T)}{R} = -a_1\frac{T^{-2}}{2} + a_2T^{-1} + a_3lnT + a_4T + a_5\frac{T^2}{2} + a_6\frac{T^3}{3} + a_7\frac{T^4}{4} + b_2 \quad \textbf{Eq 25}$$

where, *a = substance-specific least square co-efficient*

T = Temperature (K)

b_1 & b_2 = integration constants

4.4 RESULTS & DISCUSSION

Fluid property tables were generated for each of the bio-SPKs and the reference fuel (Jet-A1) using the NASA CEA code. This analysis was undertaken to comprehend the impact of variation in temperature and pressure on the thermodynamic fluid properties. The effects of these parameters on fuel types which are variable from one another has been schematically represented and discussed below.

4.4.1 Specific Enthalpy

Specific enthalpy (h) corresponds to the amount of available useful work per unit mass (kJ/kg) of a given fuel at isobaric conditions. Enthalpy is a function of temperature and gas composition.

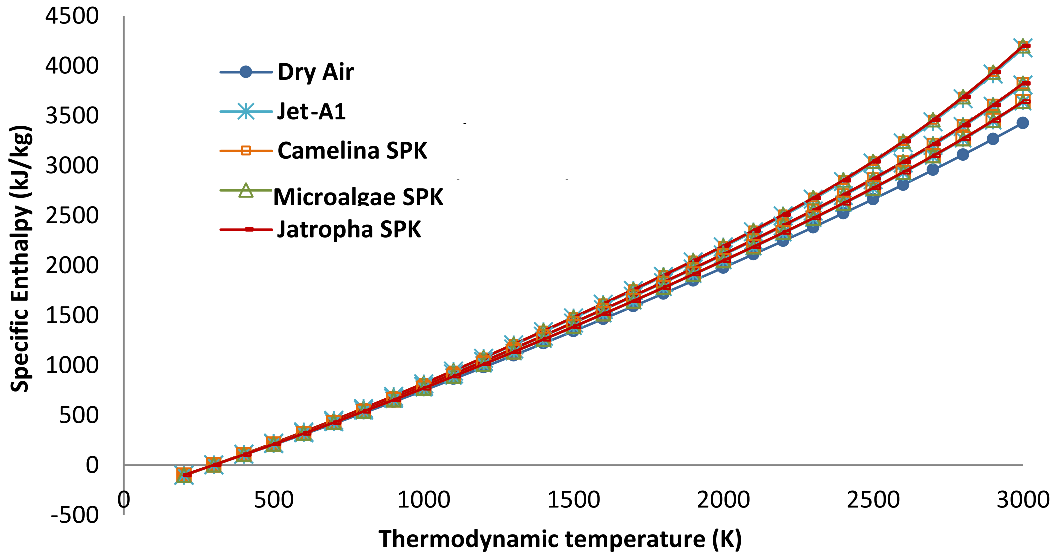


Figure 4-1: Effect of Temperature and FAR on Specific enthalpy (h)

Specific Enthalpy is used to denote the enthalpy change of system and not the absolute value itself. This change corresponds to the amount of fuel/heat added to a system at constant pressures (50 atm). It is equal to the change in internal energy and the work done on expansion of the gas.

$$\Delta \boldsymbol{H} = \Delta \boldsymbol{E} + \boldsymbol{P} \Delta \boldsymbol{V} \qquad \textbf{Eq 26}$$

where, ΔH = *Change in enthalpy*

ΔE = *change in internal energy*

P = *constant pressure, kPa*

ΔV = *change in working volume of the system*

4.4.1.1 Effect of Pressure

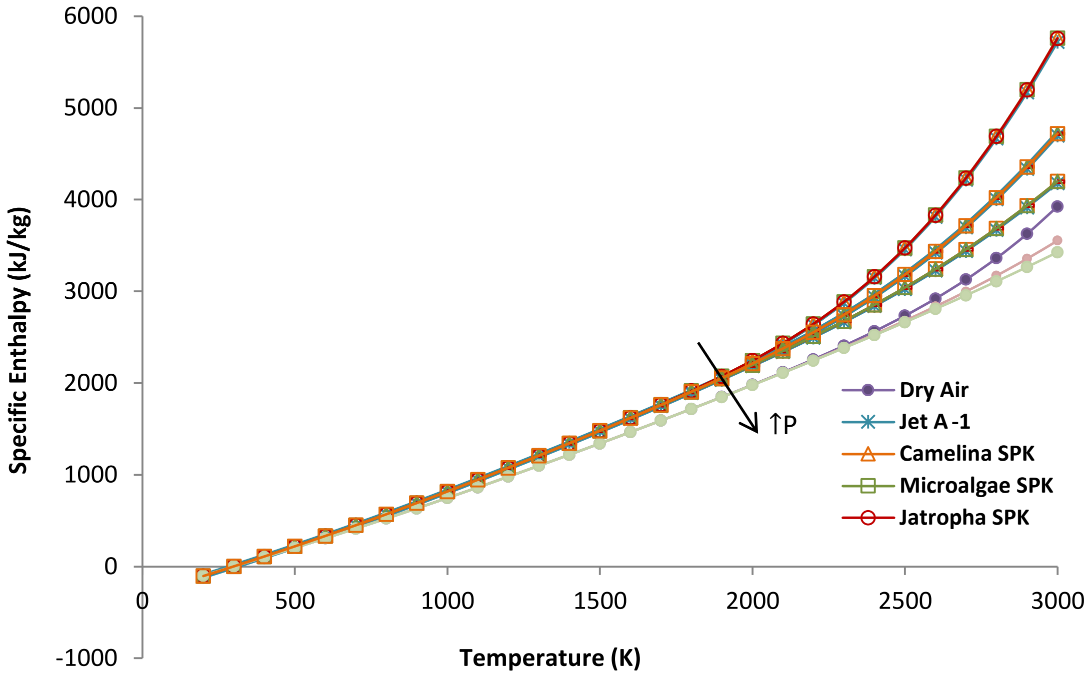


Figure 4-2: Effect of pressure on Specific Enthalpy (h) of combustion products

Enthalpy change, in real gas, is influenced by low pressure conditions. This behaviour operates on Le Chatelier's law, where a gradual increase in enthalpy is observed with drop in pressure. As mentioned earlier, dissociation is a result of an external influence, which in this case is low pressure. The system adjusts to this change by shifting itself to a new equilibrium through dissociation. Dissociated species result in lower enthalpy relative to non-dissociated species. Dissociated species possess lower internal energy (from loss to energy through dissociation) and therefore lower enthalpy of formation. This phenomenon occurs due to their ability to overcome bond energies using energy from increasing temperature of the environment. Therefore, enthalpy decreases with drop in pressure as presented in Figure 4-2.

4.4.2 Entropy

Specific Entropy (s) is a measure of losses encountered (disorder) in the system. It is a result of adiabatic compression or expansion of an air-gas mixture in a system and is represented as entropy per unit mass of the system. Similar to the previous scenario, entropy is a function of FAR and temperature. A measure of change in entropy is crucial to performance calculation to quantify the kinetic losses encountered within the engine from adiabatic compression and expansion of the working fluid.

4.4.2.1 **Effect of Temperature and FAR**

An increase in temperature increases the disorder (losses) of a system (gas mixture) through excitation of monatomic and diatomic molecules of the dissociated combustion gases. This is exhibited by an increase in entropy and this phenomenon is observable with an increase in FAR of the gas mixture as well [Figure 4-3]. Further to our analysis, the enthalpy of an isobaric system is equal to the amount of heat added. Therefore, increase in entropy is linear with that of enthalpy.

$$\Delta \boldsymbol{H} = \Delta \boldsymbol{Q} \quad \textbf{Eq 27}$$

$$\Delta \boldsymbol{S} = \frac{\Delta \boldsymbol{Q}}{\Delta \boldsymbol{T}} \quad \textbf{Eq 28}$$

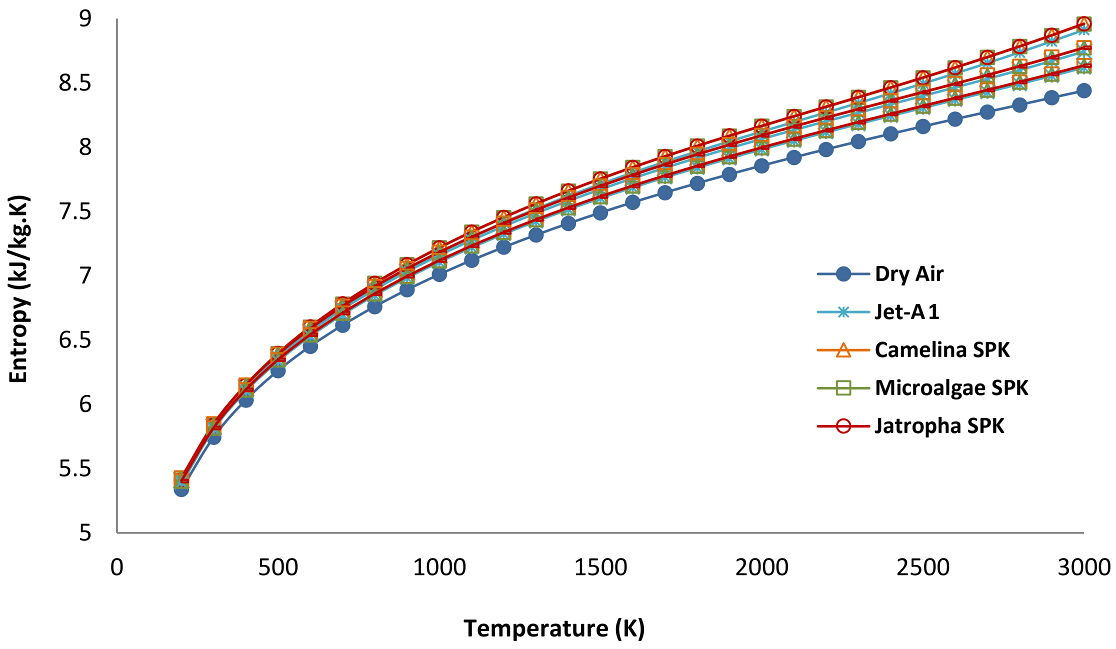


Figure 4-3: Effect of Temperature and FAR on entropy of combustion products

4.4.2.2 **Effect of Pressure**

At high pressure, the space available for molecular excitation is reduced thereby reducing the disorder created in the system. The Figure 4-4 demonstrates drop in entropy with increase in pressure.

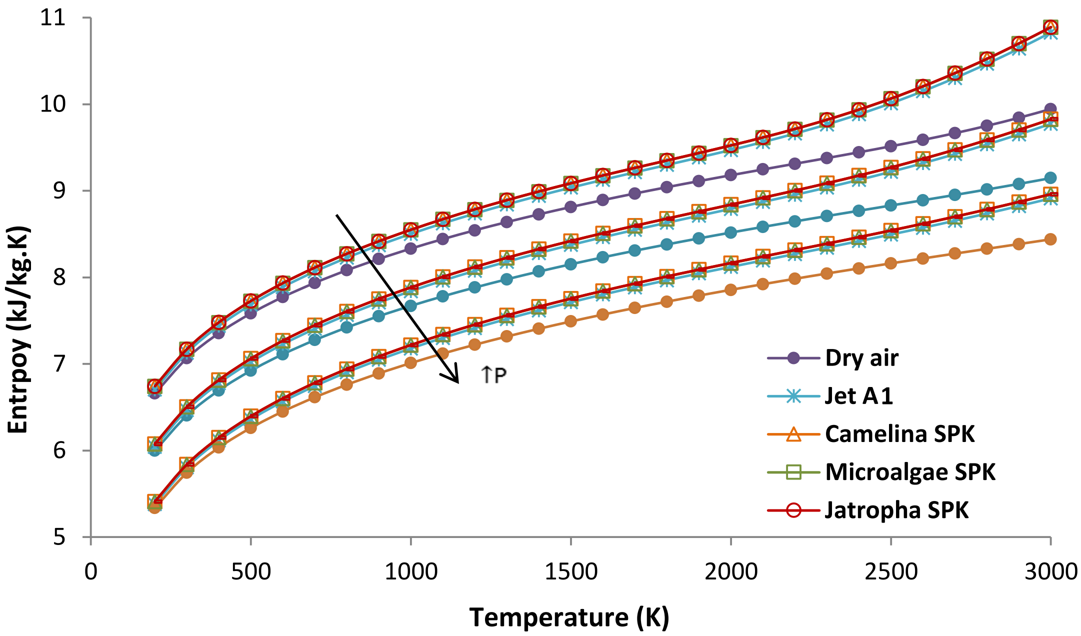


Figure 4-4: Effect of pressure on entropy (s) of combustion products

4.4.3 Specific Heat capacity

Specific Heat capacity (Cp) of the substance is the amount of energy required to raise the temperature per unit mass of a system by 1°C at constant pressure. This study specifically considers specific heat at constant pressure rather than at constant volume (C_v) owing to the steady flow of gas within a gas turbine. The unit of Specific Heat capacity at constant pressure chosen for this study is J/Kg/K. Accurate estimation of Cp is crucial to estimate work and energy balance across the shafts in an operational gas turbine engine. Hand calculations entail the use of constant value of Cp was used for gas turbine performance calculations e.g. Hot gas Cp = *1156.9 J/kg.K;* Cold gas Cp =*1004.7 J/kg.K.* However, this method was inaccurate resulting in errors up to 5% [139]. It is essential to estimate Cp with high levels of accuracy, specifically for rigorous method of engine performance estimation, at temperature below 1600K. At higher temperatures where the dissociation of combustion products is significant, Cp becomes s function of pressure as well. Therefore, Cp values corresponding to varying temperature ranges are to be included to improve the accuracy of performance calculation.

$$C_p = \frac{\Delta H}{\Delta T} \qquad \textbf{Eq 29}$$

where *Cp = Specific Heat capacity at constant pressure, kJ/mol.K*

ΔH= Enthalpy change

ΔT = Temperature change

4.4.3.1 Effect of Temperature and FAR

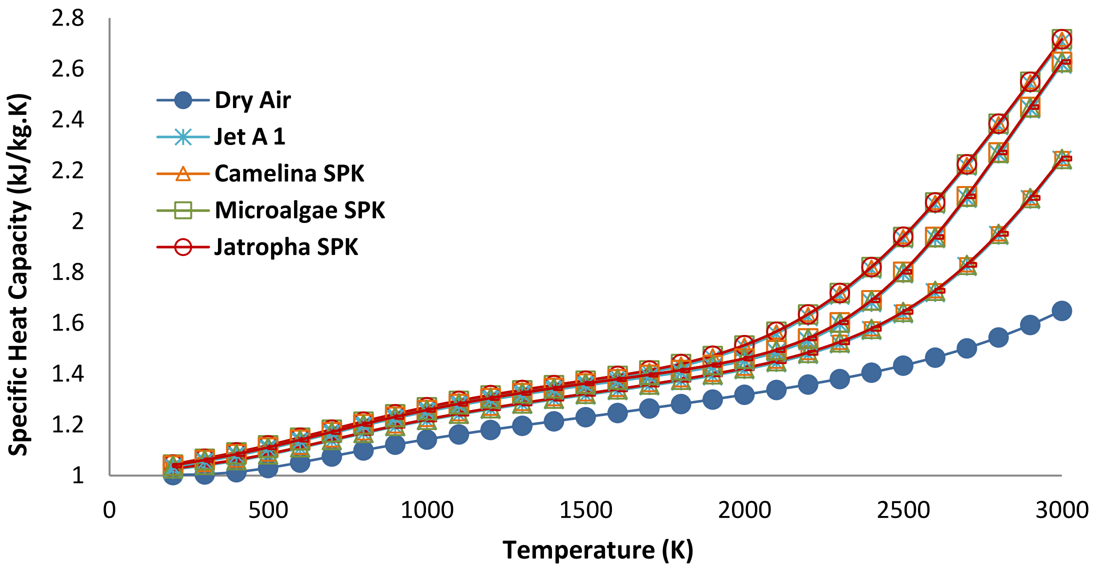


Figure 4-5: Effect of temperature and FAR on Isobaric specific heat

Isobaric Specific heat (like Specific Enthalpy) increases linearly with temperature and FAR. A sharp increase in specific heat is notable from roughly 1800K onwards with the commencement of dissociation. The sensitivity of Cp to the H/C ratio of the gas mixtures is more pronounced when shifting from lean mixture to stoichiometric fuel air mixture. Therefore, temperature has its influence on this caloric property [Figure 4-5].

4.4.3.2 Effect of Pressure

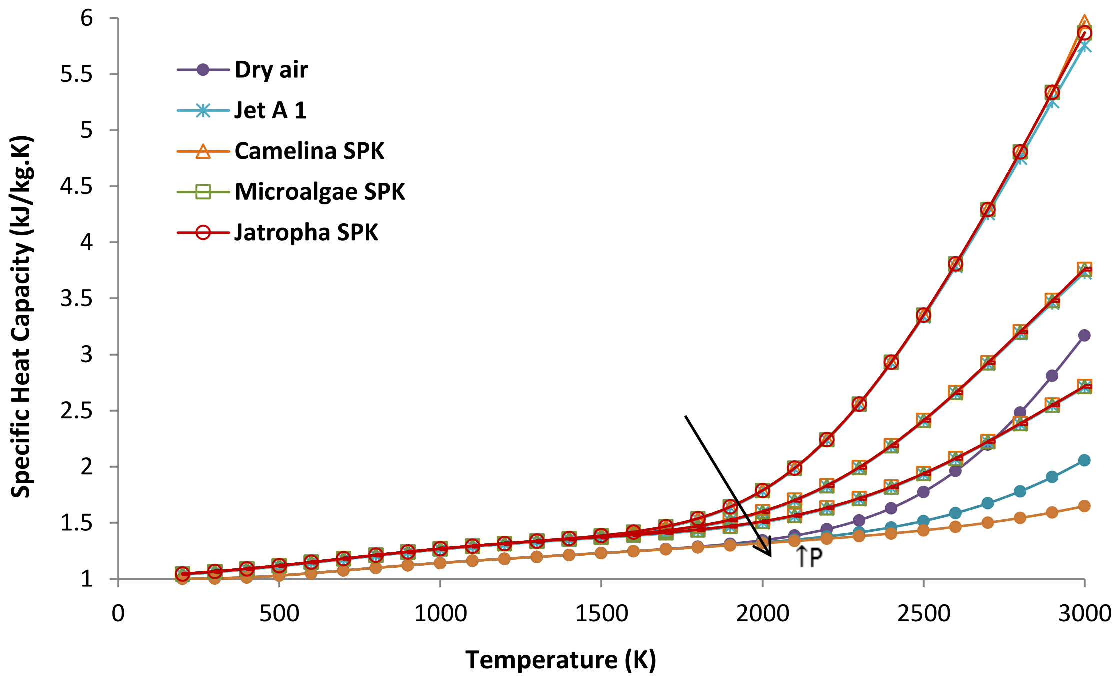


Figure 4-6: Effect of Pressure on Isobaric specific heat

The amount of heat required to raise the temperature of a system at high pressure is relatively lower than that required for a system at low pressure. This phenomenon is evident from dissociation temperatures (>1700K) where a sharp rise in Cp is observed to balance the dissociation (heat loss) effect of the combustion species [Figure 4-6].

4.4.4 Isentropic Co-efficient

Isentropic Co-efficient or Gamma (γ) is defined as the ratio of specific heat capacity of the mixture at constant pressure to the specific heat capacity at constant volume. γ is a function of temperature and gas composition.

$$\gamma = \frac{C_p}{C_v} = \frac{C_p}{C_p - R} \qquad \textbf{Eq 30}$$

where, *Cp = Specific heat capacity at constant pressure, kJ/mol.K*

Cv = Specific heat capacity at constant volume, kJ/mol.K

R = Gas constant, kJ/mol.K

Gamma property (similar to Cp, during hand calculations) under ideal gas conditions is assumed as standard values 1.4 and 1.33 for cold gas and hot gas respectively. However, when considering real gases (in rigorous simulation of jet engine performance), gamma values become T, P and FAR (even WAR) dependent which demands real-time modelling of equilibrium kinetics to improve the robustness of engine performance simulations. Gamma is significantly used in the determination of efficiencies, temperature and pressure changes in gas turbine components. E.g. Temperature changes and pressure changes across the stations of an operating gas turbine are determined using equation 31 and 32 respectively.

$$T_2 = T_1 \left[1 + \frac{\left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} - 1}{\eta_c} \right] \qquad \textbf{Eq 31}$$

$$P_4 = P_3 \left[1 - \frac{1 - \left(\frac{T_4}{T_3}\right)^{\frac{\gamma}{\gamma-1}}}{\eta_T} \right] \qquad \textbf{Eq 32}$$

where, $\eta_c = Isentropic\ Compressor\ efficiency$

T_1 & T_2 $= Station\ temperatures\ across\ a\ compressor,\ K$

$\eta_T = Isentropic\ Turbine\ efficiency$

P_3 & P_4 $= Station\ pressures\ across\ a\ turbine\ component,\ kPa$

4.4.4.1 **Effect of Temperature and FAR**

Increase in temperature is detrimental to the gamma property of the gas mixture. This behaviour can be explained through the concept of degrees of freedom (DOFs)

$$\gamma = \frac{DOF+3}{DOF} \quad \textbf{Eq 33}$$

DOFs provide an insight into the state of a given system by defining the independent co-ordinates of movement of a gas molecule in excited state. For a gas molecule, the mathematical Cartesian co-ordinates (x,y and z) have been adopted for definition and this includes translational, rotational and vibrations motion. In general, monoatomic species are expected to have 3 DOFs (Degrees of Freedom) (3 translational) and diatomic species contain 5 DOFs (3 translation and 2 rotational) at standard conditions. However, the number of DOFs may increase with increase in temperature resulting in a drop in gamma property. The drop in adiabatic index becomes non-linear with increasing FAR. This is can be due to varying concentration of monatomic and diatomic combustion species released as a result of the fuel combustion.

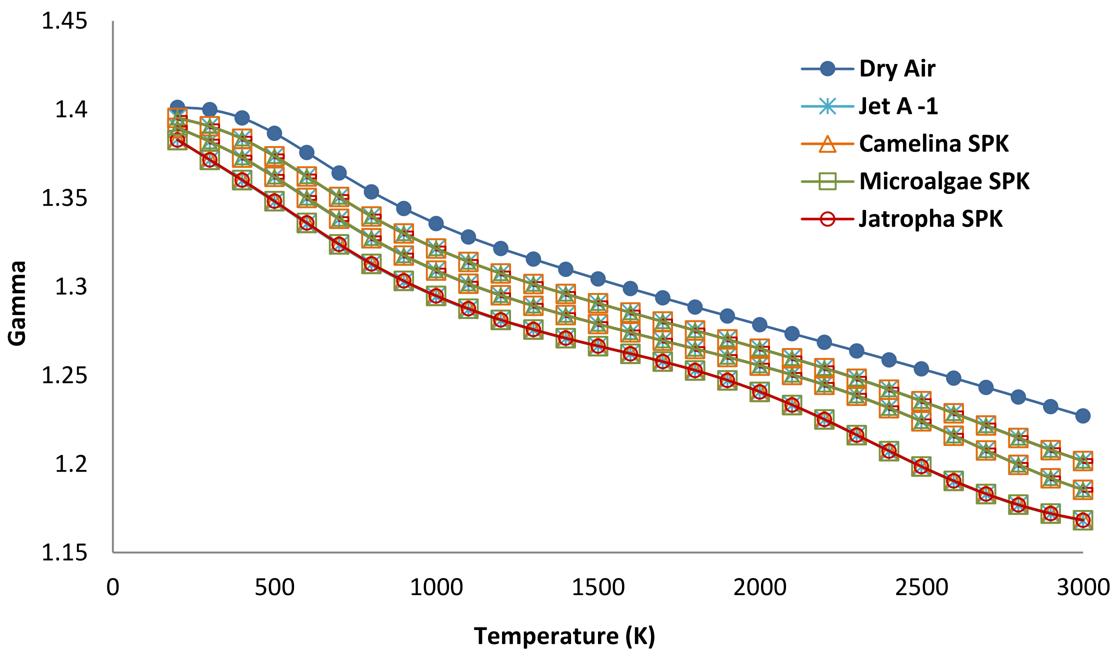


Figure 4-7: Effect of Temperature and FAR on gamma

4.4.4.2 **Effect of Pressure**

As the legends indicate in Figure 4-8, the drop in isentropic co-efficient is inversely related with ascending pressures. However, a deviance from linearity is observed upon reaching dissociation temperatures (<1500K).

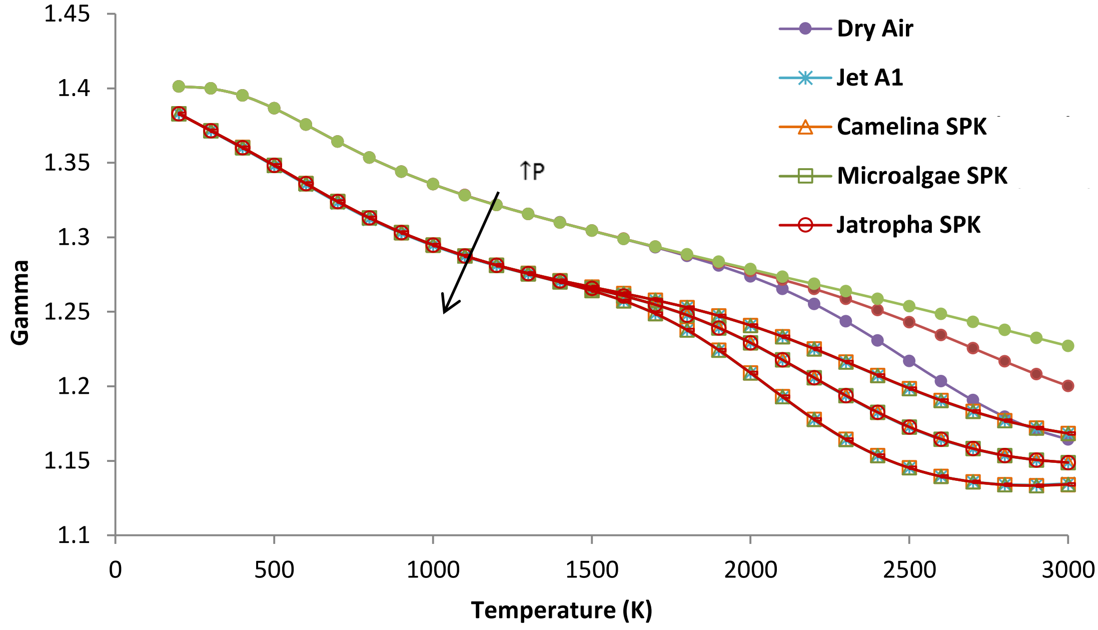


Figure 4-8: Effect of pressure on gamma

This behaviour can be illustrated with the DOFs (Degrees of Freedom) theory. Dissociations are primarily favoured by low pressure conditions thereby resulting in the formation of higher concentrations of monatomic species (like for e.g. OH, O, N, H). These monatomic species with higher DOFs result in relatively lower gamma values (gas mixture at 0.5 atm). Thus with higher pressure conditions, gamma values are higher.

4.4.5 Gas constant

Gas constant (R) of a given mixture is the ratio of universal gas constant to the molecular mass of the products of combustion and is expressed as kJ/kg.K in this study.

$$R = \frac{R_{universal}}{Mm} \qquad \text{Eq 34}$$

where, $R_{universal}$ = *Universal gas constant, J/K.mol*

Mm = *molar mass of gas mixture, kg/mol*

4.4.5.1 Effect of Temperature

Gas constant is independent of temperature until dissociation temperatures (>1500K) are reached [Figure 4-9]. Changes in the molecular mass of the gas composition result from the dissociation of combustion products to monoatomic species. This drop in the molecular mass of the real gas mixture consequently increases the specific gas constant of the same. With respect to the effect of FAR on the transport properties of the gas, dissociation effects encountered with higher FARs, (Stoichiometric FAR in this case) concludes that specific gas constants increase with FAR of the gas mixture.

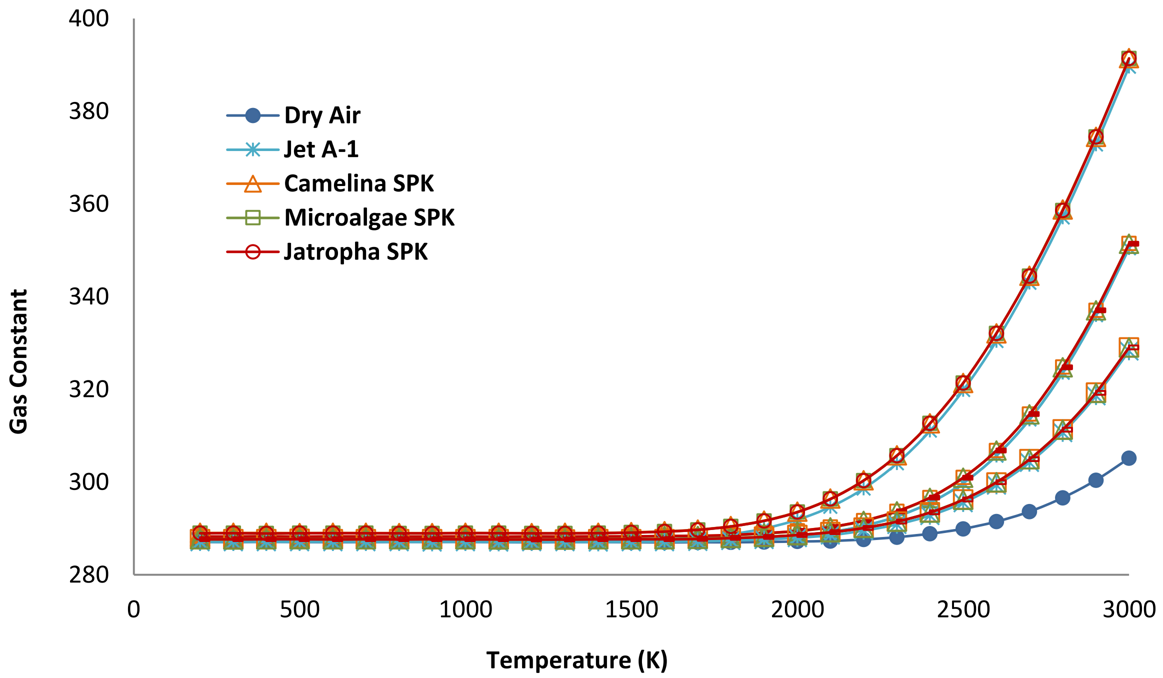


Figure 4-9: Effect of temperature and FAR on gas constant

Gas constant is independent of variation in pressure conditions.

4.4.6 Caloric properties of Bio-SPKs

The effects of variables encountered by the thermodynamic fluid system in an operational engine (temperature, pressure and FAR) have been discussed in the earlier section.

Gas Property	Fuel Type	% Diff from Jet-A1
Specific Enthalpy (h) (kJ/kg)	Camelina SPK	0.51
	Microalgae SPK	0.49
	Jatropha SPK	0.52
Entropy (s) (kJ/kg.K)	Camelina SPK	0.53
	Microalgae SPK	0.5
	Jatropha SPK	0.55
Isobaric Specific heat (Cp) (kJ/kg.K)	Camelina SPK	0.59
	Microalgae SPK	0.58
	Jatropha SPK	0.60
Gamma (γ)	Camelina SPK	0.48
	Microalgae SPK	0.47
	Jatropha SPK	0.49
Gas constant (R) (J/kg.K)	Camelina SPK	0.56
	Microalgae SPK	0.54
	Jatropha SPK	0.57

Table 4-1: % Difference in Fluid Thermodynamic Properties between the Bio-SPKs and Jet-A1

Bio-SPKs have 13% higher hydrogen content relative to the baseline. This particular variation has an impact on the enthalpy released upon combustion because in hydrocarbon fuels, H_2 contains 4 times higher enthalpy relative to C. Similarly, from the perspective of an important gas property, Cp, which finds application in the seven term function of other caloric properties, combustion by-product H_2O has 2 times the Cp of CO_2 / CO. The more comprehensive table containing the caloric properties of Bio-SPKs has been provided in Appendix D. These differences were evaluated by calculating average value of each of the property at three temperature ranges (<1800K, 1800K and >1800K) and deriving an average % difference among the values determined. It is clearly evident from the analysis undertaken above that the Bio-SPKs are not identical to that of conventional Jet fuel [Table 4-1].

4.4.7 Bio-SPK Fluid Model for Engine Performance Simulation

The fluid models developed above for each of the Bio-SPKs are expected to be implemented into TURBOMATCH - Ver 2.0; an in-house developed gas turbine performance simulation software. It is essential to appreciate the fundamental principle of TURBOMATCH before proceeding to the method of implementation.

Studies of reference [25], [27] & [243] have established that the discrepancies in fluid properties result from very low (<400K) and very high (>2300K) thermodynamic temperatures owing to the complications in calculating unknown parameters. For instance, isobaric specific heat capacity is estimated from the different modes of energy (vibrational, rotation and translational). Very low temperatures contribute through higher rotational energy and higher temperatures may contribute through electron excitation and vibrational energy. The contribution of energy release from each mode is thus, temperature dependant. Consideration of mutual interactions among these energies is expected to deliver precision in estimating Cp. However, attention to such intricacies complicates the technical model and escalates uncertainties in the results.

4.5 TURBOMATCH-legacy version

The legacy version of TURBOMATCH is the predecessor of its version 2.0. A brief account of the TURBOMATCH will be given in the next chapter. With respect to thermodynamic property calculation, the legacy TURBOMATCH operated on Walsh and Fletcher polynomials [139] (W&F polynomials), 8th order polynomials effective within the ranges of 200-2000K which have been presented below

4.5.1 Walsh & Fletcher (W&F) Polynomials

The 8th order polynomials have been provided for the key caloric properties in Equation 35-38

For **Specific Heat Capacity** at constant pressure (kJ/kg.K)

$$\boldsymbol{Cp = A0 + A1 * Tz + A2 * Tz^2 + A3 * Tz^3 + A4 * Tz^4 + A5 * Tz^5 + A6 * Tz^6 + A7 * Tz^7 + A8 * Tz^8} \quad \textbf{Eq 35}$$

where $A_{0\text{-}10}$ = *substance specific constants [139]*

Tz = Ts/1000

Ts = Static temperature (K)

➢ For **Specific Enthalpy** (kJ/kg)

$$\boldsymbol{H = A0 * Tz + \frac{A1}{2} * Tz^2 + \frac{A2}{3} * Tz^3 + \frac{A3}{4} * Tz^4 + \frac{A4}{5} * Tz^5 + \frac{A5}{6} * Tz^6 + \frac{A6}{7} * Tz^7 + \frac{A7}{8} * Tz^8 + \frac{A8}{9} * Tz^9 + A9} \quad \textbf{Eq 36}$$

➢ For **Entropy (J/kg.K),** Cp/T.dT must be calculated for which the difference in temperatures can be generated using

$$\boldsymbol{fT_2 = A0 * ln(TS2) + A1 * T2Z + \frac{A2}{2} * T2Z^2 + \frac{A3}{3} * T2Z^3 + \frac{A4}{4} * T2Z^4 + \frac{A5}{5} * T2Z^5 + \frac{A6}{6} * T2Z^6 + \frac{A7}{7} * T2Z^7 + \frac{A8}{8} * T2Z^8 + A10} \quad \textbf{Eq 37}$$

$$\boldsymbol{fT_1 = A0 * ln(TS1) + A1 * T1Z + \frac{A2}{2} * T1Z^2 + \frac{A3}{3} * T1Z^3 + \frac{A4}{4} * T1Z^4 + \frac{A5}{5} * T1Z^5 + \frac{A6}{6} * T1Z^6 + \frac{A7}{7} * T1Z^7 + \frac{A8}{8} * T1Z^8 + A10} \quad \textbf{Eq 38}$$

Where, *T_2Z and T_1Z = TS_2/1000 and TS_1/1000 respectively.*

[NOTE: the substance specific constants [139] are available only for products resulting from non-dissociated combustion (N_2, O_2, CO_2 and H_2O).]

4.6 TURBOMATCH Ver 2.0

A robust thermodynamic model was integrated into the TURBOMATCH legacy version for sound and reliable air/gas property prediction. The renewed version is now called TURBOMATCH ver 2.0.There are other methods by which the thermodynamic fluid data can be calculated on TURBOMATCH

- Use of established polynomials
- Use of thermodynamic property tables
- Implementation of dedicated combustion kinetics software
- last but least desirable- work with the assumption of ideal gas mixture

In general, care must be taken to ensure that the thermodynamic data generated from any combustion kinetic software is accurately incorporated or calculated by the engine performance software for precise engine cycle prediction.

Use of property tables can be beneficial in terms of saving computational time. However, the accuracy of the data is dependent on the volume of tables available. NASA CEA generates huge libraries of thermodynamic property which has to be manually handled and errors become imminent in such procedures. This study has opted for the use of established technical equations which are reliable in terms of accuracy over the range of thermodynamic temperatures (200-3000K). Higher temperatures (>1800K) are least encountered in commercial jet turbines for clean emissions, engine life, reliability and safety considerations. However, it is essential to ensure that the thermodynamic data are accurately predicted accounting for dissociation species as well.

BSW equations (named after *Bücker* et al (2003), [27] for this study), were adopted for the calculation of caloric properties into TURBOMATCH owing to their reliable accuracy relative to the caloric properties determined from Chemical Equilibrium with Application software by NASA. According to a study [27], isobaric specific heat determined using their BSW equation was in close association with that derived from the seven-term functions of the CEA code (Deviation$\pm 0.05\%$). Empirical polynomials for the prediction of essential caloric property for each of the combustion products have been provided below

4.6.1 BSW Equations

The BSW equations employed in TURBOMATCH for cycle-thermodynamic data estimation are as follows in equation 39-41.

- For **Specific Heat Capacity** at Constant Pressure

$$C_{p,k}^{0} = \sum_{i=1}^{10} a_{k,i} \left(\frac{T}{T_0}\right)^{b_i} \qquad \textbf{Eq 39}$$

where k = *specific combustion species*

T_0 = *static temperature (273.15 K)*

T = *Thermodynamic temperature (K)*

b_i = *optimization exponent*

- For **Enthalpy** of the components

$$h_k^0 = a_{k,I} + \sum_{i=1}^{10} a_{k,i} \frac{T_0}{b_i+1} \left(\frac{T}{T_0}\right)^{b_i+1} \qquad \textbf{Eq 40}$$

- For **Entropy**

$$s_k^0 = a_{k,II} - R_m \, ln \frac{p}{p_0} + a_{k,1} \, ln \frac{T}{T_0} + \sum_{i=2}^{10} \frac{a_{k,i}}{b_i} \left(\frac{T}{T_0}\right)^{b_i} \qquad \textbf{Eq 41}$$

These equations have been determined to predict the caloric properties of equilibrium combustion products with highest accuracy up to a temperature range of 3000K (in spite of the fact that aero-engine do not operate beyond 1800K).

4.6.1.1 VALIDATION OF BSW POLYNOMIALS – A COMPARATIVE ASSESSMENT

The robustness of the BSW thermodynamic model was compared with that of Walsh and Fletcher polynomials in terms of Cp estimation attributable to the standard combustion gases water vapour, oxygen, nitrogen and carbon-di-oxide. This assessment was carried out over a range of temperatures from 273.15 K-2800.15 K at a pressure of 1 atm. Isobaric specific heat (*Cp*) was used to validate between the two models.

[**NOTE**: the above method has been carried out for the estimation of Isobaric specific heat only with coefficient available for each combustion species in both W&F and BSW polynomials.]

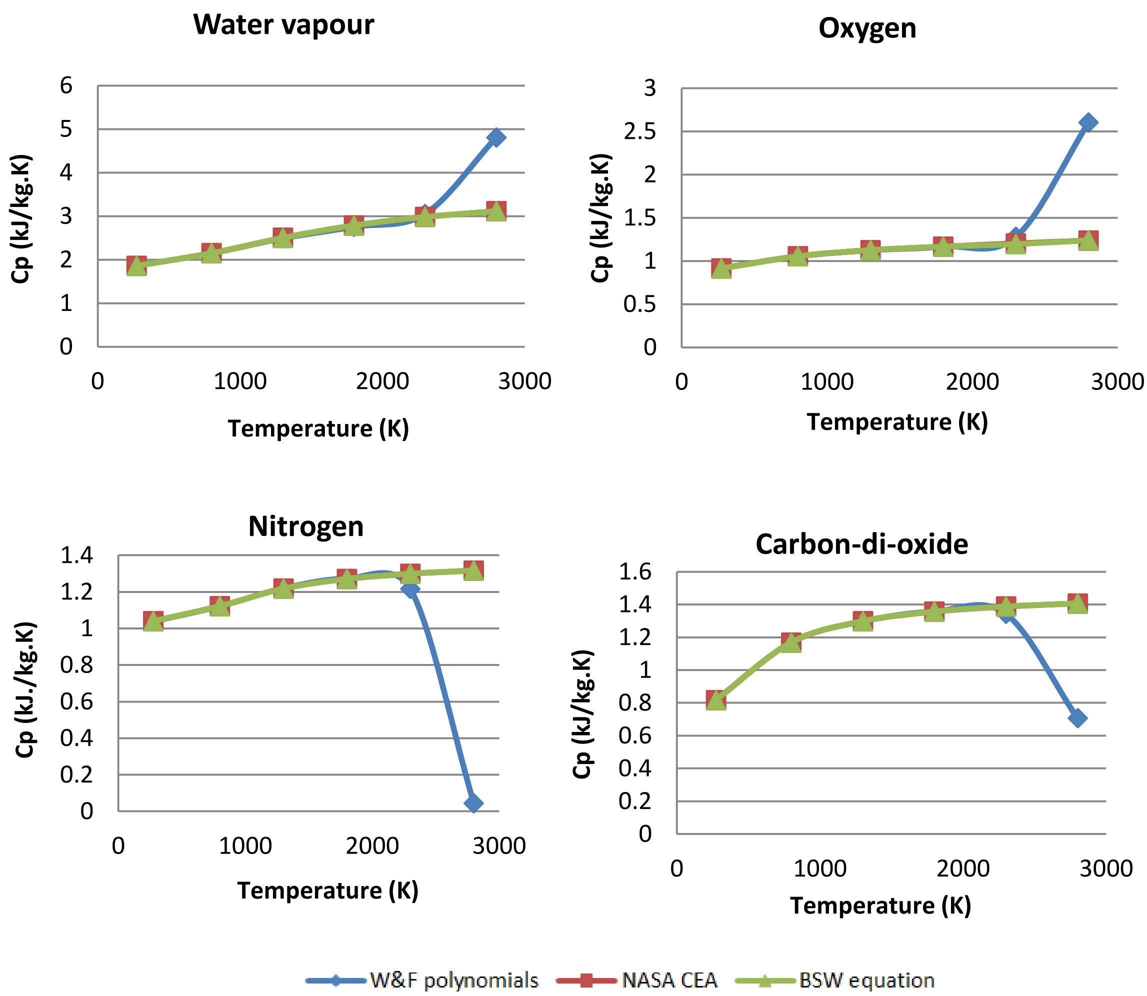


Figure 4-10: Comparison of estimated isobaric specific heat between W&F model and BSW model against that of standard NASA CEA

1.1.1 Discussion

As clearly visible from the above figures, estimation of Cp for individual combustion gases using BSW is accurately close to the reference method (NASA CEA). The deviations visible in the W&F polynomial generated Cp is due to the fact that the polynomials do not account for dissociation effects which are imminent from higher temperatures (>1800K). Secondly the % deviation between BSW and NASA CEA models were determined to estimate the significance of variation. The % deviation was calculated as follows

$$\%\ \boldsymbol{deviation} = \frac{Cp - Cp_{ref}}{Cp_{ref}} \qquad \textbf{Eq 42}$$

Upon comparison of Cp data derived from NASA CEA model and TURBOMATCH ver.2.0 based model (BSW equations), the percentage deviation of Cp among individual combustion products were determined to <±0.001%. An average deviation of -0.001% was encountered when considering Cp of gas mixtures.

T (K)	**% deviations**							
	N_2	**O_2**	**Ar**	**Ne**	**H_20**	**CO_2**	**CO**	**SO_2**
273.15	-0.0002	-0.0019	0.0003	-0.0002	-0.0010	0.0004	0.0003	0.0002
800.15	0.0005	-0.0005	0.0003	-0.0002	0.0000	0.0001	0.0001	0.0000
1300.15	-0.0008	-0.0003	0.0003	-0.0002	-0.0002	0.0005	0.0004	-0.0001
1800.15	0.0005	0.0001	0.0003	-0.0002	0.0001	0.0006	0.0000	0.0001
2300.15	0.0005	0.0022	0.0003	-0.0002	0.0000	0.0004	0.0003	0.0000
2800.15	0.0005	0.0025	0.0003	-0.0002	-0.0001	0.0006	0.0002	-0.0001

Table 4-2: % Deviation in Isobaric Specific heat (Cp) between BSW equation and NASA CEA

1.2 Integration of Data for Bio-SPKs into TURBOMATCH

Estimation of the caloric properties of each of the combustion species is essential to predict engine cycle operations with highest accuracy, as mentioned earlier. The data required for the integration of Bio-SPK into TURBOMATCH ver 2.0, apart from the above mentioned caloric and transport properties include the following.

- Concentrations (mass fractions) of combustion products for each of the Bio-SPKs
  - Nitrogen
  - Oxygen
  - Argon
  - Neon
  - Water vapour
  - Carbon di-oxide
  - Carbon monoxide
  - Sulphur-dioxide
- Fuel composition (C_xH_y)
- Stoichiometric FAR
- Stoichiometric AFR
- Lower heating values of each of the bio-SPKs (kcal/kg)

The following data for each of the Bio-SPKs (Camelina SPK, Microalgae SPK and Jatropha SPK were fed into the fuel sub-routine of the TURBOMATCH ver2.0 source code, in the form of the following array.

```
"STOICFUEL(1,1:10)=(/66.61957041_RK,0._RK,0.793496420_RK,0.001706444_RK,11.75
_RK,12.02559666_RK,0._RK,0._RK,0.067911485_RK,85.3221957_RK/)"
```

Where, RK refers to a variable declaration in FORTRAN. Further information on choosing a fuel type for a specific engine performance simulation can be found in the next chapter.

1.3 LIMITATIONS

1.3.1 NASA CEA

A user may not be able to run the CEA program over a range of 200-2000K in one go due to in-built lack of space for users definition of temperature ranges. This may result in an increase in computing time for the user and possibility of errors during exporting bulky results. The thermodynamic library can be updated with additional species and chemical mixtures. For instance, the universally used Jet-A1 which has a varied chemical composition compared to Jet-A1 fuel is not available in the thermodynamic library. Current version of the CEAgui does not provide the option to export data on the molar fraction of combustion products (data required for implementation of new fuels into TURBOMATCH). These restrictions make handling of data from NASA CEA more tedious.

1.3.2 BSW Equation

BSW equation is reasonably accurate in the estimation of thermodynamic data using just two variables i.e. temperature and pressure, resulting in two dimensional gas property determination. The above mentioned equations were formulated considering the gas mixture to be of ideal nature. However, Bucker et al, (2003), were able to determine that at low temperatures and high pressure, the resulting gas mixtures deviate significantly from Ideal gas behaviour [27]. This effect is more profoundly observed in the estimation of Caloric properties for moist air. The adoption of this equation despite such a limitation can only be reasoned with the fact that there are no real gas thermodynamic models available and the property tables for the fuel were generated without the consideration of WAR (Water to Air ratio).

1.4 CONCLUSION

Elaborate gas profile for Camelina SPK, Microalgae SPK, Jatropha SPK and the reference fuel (Jet-A1) was developed using a robust/ validated thermodynamic fluid model. This exhaustive fluid model delivers an insight into the behaviour of partially ideal gases that have attained equilibrium upon combustion of a given fuel. This study infers that the combustion gases attributable to the Bio-SPKs behave almost similar to that of our Conv.Jet fuel. This behaviour is favourable in term of satisfying compatibility with an engine of existing scheme and configurations. However, the minor disparities were observed between the reference fuel and Bio-SPKs. The effect of these disparities on a representative engine/ aircraft performance has to be further investigated. For instance, the lower heating value of Bio-SPKs is higher than our reference by 2%. Intuitively, some difference in the performance of jet engine when using Bio-SPKs can be anticipated. In order to further investigate the thermodynamic effects on engine performance, this technical module has opted for virtual experimentation which has been presented in greater detail in the Chapter 5

5 BIO-SPK OPERATED ENGINE/ AIRCRAFT LEVEL PERFORMANCE AND EMISSIONS EVALUATION

(Technical Module)

5.1 INTRODUCTION

A robust gas model required to generate a thermodynamic gas profile for the Bio-SPKs, as a function of temperature, pressure and FAR is in place. The thermodynamic influences of these advanced biofuels are required to be investigated through a representative virtual experiment. This experiment entails rigorous numerical simulation of user-modelled and validated engine/ airframe configuration. The outcome of this study is the quantification of the jet engine performance characteristics imparted by the thermodynamic fluid profile attributable to Camelina SPK, Microalgae SPK and Jatropha SPK relative to that of Conv.Jet-A1. Additionally, emissions that are numerically quantified through virtual modelling and simulations of fuel combustion and significant to this TERA study are CO_2 and NOx.

5.2 LITERATURE REVIEW

The performance of 100% biofuel-operated jet engine has been evaluated by very limited numbers of studies. For instance, studies of reference [73] carried out an extensive experimental investigation on varying blends of UOPs Bio-SPKs, FT-SPK, and GTL from Sasol, Syntroleum and Shell (25%, 50% with JP-8 and 100% pure). In this analysis, influence of blended biofuels alone was assessed with insufficient information on fuel composition or have the implications of fuel properties on hardware and material performance been established. Similarly virtual studies, of reference [39] and [142], went onto assess the behaviour of pure Bio-SPKs through virtual experiments. However, any analysis into the fuel-specific thermodynamic properties and its effect on jet engine performance have seldom been reported.

Evaluation from fuel-property viewpoint enables one to appreciate and dedicatedly decide the most technically viable alternative fuel for their choice of aircraft, trajectory and mission-range. This segment of technical module (engine performance) aims to evaluate and establish the effects of the “performance” properties of 100% Bio-SPKs (Camelina SPK, Microalgae SPK and Jatropha SPK) on a chosen civil turbofan engine. The performance characteristics imparted by the candidate biofuels, on an operational jet engine, is measured as specific fuel consumption (SFC) at fixed thrust. The quantified engine fuel consumption will be zoomed into a representative mission level performance assessment with all the three Bio-SPKs. The goal of this assessment is to precisely quantify combustion based emissions from use of Camelina SPK, Microalgae SPK, Jatropha SPK relative to Conv. Jet fuel. The outcome of this assessment feeds into the ALCEmB towards the “fuel combustion” phase. It is essential to predict these emissions with utmost precision as this phase is the highest LCE contributor (≈70%). Wolters et al, 2012, went onto assess the potential system level emissions of Bio-SPKs at different biofuel blend concentrations (50% and 100%). However, they were able to report only CO_2 emissions for an assumed fuel weight carried on short and long range mission of subsonic aircraft. Besides mission level CO_2, this technical module aims to predict NOx emission resulting from combustion of Camelina SPK, Microalgae SPK and Jatropha SPK, in a conventional combustor, in line with the ICAO’s LTO specifications for emission measurement (power setting).

Secondly, this module is expected to deliver a deeper insight into the systemic-thermodynamic variations or similarities anticipated from the engine operated with the Bio-SPKs and a qualitative comprehension of the effect of fuel’s “performance” properties on a turbofan engine of present day configurations.

A number of methods [[10], [28], [29] and [39]] for NOx emission prediction exist ranging from simplified empirical techniques to computationally intensive and high fidelity fluid dynamics simulations. P_3-T_3 method of NOx emission estimation is the most commonly employed empirical method. In spite of P_3-T_3 method being the most popular method for emissions estimation, physics based stirred reactor approach was adopted to study the emission indices of Bio-SPKs. P_3-T_3 method is suitable only for estimation of NOx emission (except EICO) from combustors of fixed dimensions operating on conventional fuel types [33]. Additionally, this model cannot account for variations in combustor geometry and air-fuel mixture based homogeneity characteristics specific to alternative fuels [11]. Most importantly, the gas composition is expected to vary with the three difference types of Bio-SPKs subjected to emission evaluation. This analysis has still adopted P_3-T_3 method (towards Conv.Jet fuel) [33] of

NOx estimation, in addition to the stirred reactor model, to validate the modelled reactor. This universality of P_3-T_3 in empirical estimation of EINOx stems from the use of constant pressure exponents (*m* & *n*) which, however, takes a toll on the accuracy of the prediction. The P_3-T_3 method of emission estimation is presented in Eq 43.

$$\boldsymbol{EINOx_{FL} = EINOx_{SL}\left(\frac{P_{3FL}}{P_{3SL}}\right)^{n}\left(\frac{FAR_{FL}}{FAR_{SL}}\right)^{m} exp(H)} \qquad \textbf{Eq 43}$$

where, FL = *Flight condition*

SL = *Sea level static*

n = *pressure exponent*

m = *FAR exponent*

H = *Humidity correction factor*

The exponents, n and m, were assumed to be 0.4 and 0.0 as suggested by studies of reference [33] to be ideal when engine specific exponents are unavailable.

This technical module has opted for a simplified physics based model which estimated the emission index of a given engine operating with the given fuel as a function of the following

- P_3-T_3 specifications (Combustor inlet parameters also defined by ambient conditions)
- Mass flow and fuel flow specifications
- Segmentation of the reactor – Flame Front, Primary, Intermediate and Dilution zone.
- Fuel/ Fuel-Air mixture specifications
    - I. Thermo-physical properties - Stoichiometric flame temperature, caloric properties (Cp, γ, h, s, η), fuel density, bulk modulus, viscosity, flash point, boiling point, thermal conductivity, vapour pressure
    - II. Chemical – Thermal stability, LHV, aromatics, sulphur and nitrogen content.
    - III. Degree of homogeneity and zonal equivalence ratio

It is also essential to note that the influence of fuel composition and specifications was not reported by any other studies except that of Rahmes et al, (2009) [107]. This study has taken this effort further to study the subsequent impact of candidate fuels from fuel specification viewpoint of analysis. Medium-range mission level emissions for CO_2 and NOx have been calculated for an integrated engine-airframe combination, which is also a common inadequacy, encountered in emissions studies.

5.3 METHODOLOGY

The study was carried out sequentially as indicated below

- Development of a numerical engine model
- Matching the modelled engine with an existing baseline through comparison of publicly available performance data. Required data unavailable from public domain was deduced through reverse-iteration of cycle parameters at design point and off-design (e.g. W, SFC, PR, F_n) and the model will be validated
- Development of a numerical airframe model from an appropriate baseline airframe by matching aircraft range, weight and airframe geometry specifications.
- Integration of modelled engine and airframe towards mission level performance assessment of Bio-SPKs over a user-defined medium-range flight trajectory.
- Identify, report and discuss the performance similarities/ variation imparted by the Bio-SPKs at mission level performance, relative to that of Conv.Jet A-1.

The engine model developed for virtual performance simulation will be denoted as “CU-Jet” (Cranfield University Jet) throughout this study. An appropriate airframe to accommodate the two CU-Jet-engines will have to be modelled and matched with an existing airframe [A321-112]. The modelled aircraft will be called “LokAir” and airframe matching procedures will also follows a similar approach of iteration, matching and validation methodology adopted for virtual engine model development. The modelled engine/ aircraft operated with the candidate fuels will be denoted as presented in Table 5-1.

Modelled component	Fuel types	Designation
CU-Jet (engine)	Conv. Jet fuel	CU-Jet-K
	Camelina SPK	CU-Jet-C
	Microalgae SPK	CU-Jet-M
	Jatropha SPK	CU-Jet-J
LokAir (aircraft)	Conv. Jet fuel	LokAir-K
	Camelina SPK	LokAir-C
	Microalgae SPK	LokAir-M
	Jatropha SPK	LokAir-J

Table 5-1: Designations for an engine/ aircraft when operated with the different fuel candidates

5.3.1 Jet Engine Performance Analysis

An experimental gas turbine rig test has been determined to cost in the range of thousands of pounds per run, excluding any damage to the equipment and additional costs incurred from use of sensors including other specialist equipment. The reason for the choice of a virtual experiment is, therefore, evident from time and cost considerations. The extents of simulation vary between simplified models with multitude of assumptions to fully-rigorous models with limited number of assumptions. Fully-rigorous simulation of jet engine performance desirably requires the consideration of real working fluids (where the gas properties are dependent on T, P FAR and WAR). A new set of empirical thermodynamic models, incorporated into TURBOMATCH, enables treatment of working fluids as partly-ideal since the fluid properties are considered a function of temperature and gas composition (FAR) only. This evaluation has opted for fully rigorous simulation of engine performance where the performance parameters across the engine stations are variable with the associated cycle parameters (T, P and FAR). To begin with, the method of numerically modelling the gas turbine engine in the virtual environment has been presented in section 5.3.1.1.

5.3.1.1 Virtual Model of CU-Jet

The key design parameters required to construct the engine CU-Jet with reliable precision were available from open literature and manufacturer specification [32] and [57]. Familiarity with the performance threshold for off-design performance analysis (Take-off and Top-of climb conditions) aided closer matching of the modelled engine with the baseline, through reverse iteration approach.

Virtual modelling of CU-Jet engine required the following data.

- Compressor pressure ratio (calculated from overall pressure ratio specifications)
- Bypass ratio, Fan pressure ratio and fan efficiency are required
- General arrangement (GA) of the engine.

CU-Jet was modelled to contain the following components. A schematic of the engine modelled from its baseline CFM56-5B/2 provided in Figure 5-2.

- A single stage fan

- A Bypass duct leading to cold nozzle
- Booster (4-stages) and a high pressure compressor (9-stages)
- Combustor
- High pressure (HP) turbine driving the high pressure compressor through HP shaft
- Low pressure (LP) turbine driving the booster and the fan through LP shaft.
- Hot nozzle section continuing from LP turbine.

A brief description on the nature and the method of operation of TURBOMATCH has been presented in Appendix F. Detailed data on the governing principles of engine performance simulation and program capabilities can be obtained from literature of reference [37].

5.3.1.2 Design Point Simulation

Any gas turbine is primarily designed to operate at purpose/ condition specific engine configurations, component efficiencies and other thermodynamic cycle parameters. A given engine spends most of its operating time at its design point. Moreover, an engine's design point is pivotal to determining its operating threshold which is termed as Off-design performance. This study is based on the performance analysis of CU-Jet operating at Cruise (DP), Take-off (OD) and top of climb (OD) modes coupled with the investigation of variation in performance when using Bio-SPKs.

a. **CFM56-5B/2 – The Parent Engine**

CFM56-5B/2, presented in Figure 5-1, is a two-shaft high bypass engine, jointly manufactured by General Electric and Snecma belonging to the CFM56 family finding application in A321 type Airbus aircraft. It is essential that the hypothetical model is designed in close agreement with the baseline engine to enhance the level of confidence on the performance results of the former.

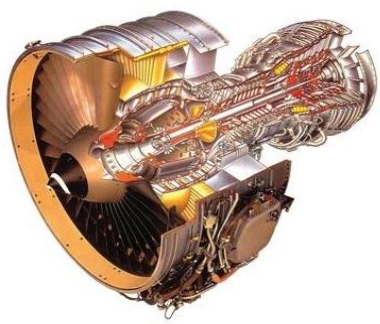


Figure 5-1: A cutaway image of CFM56-5B/2 [32]

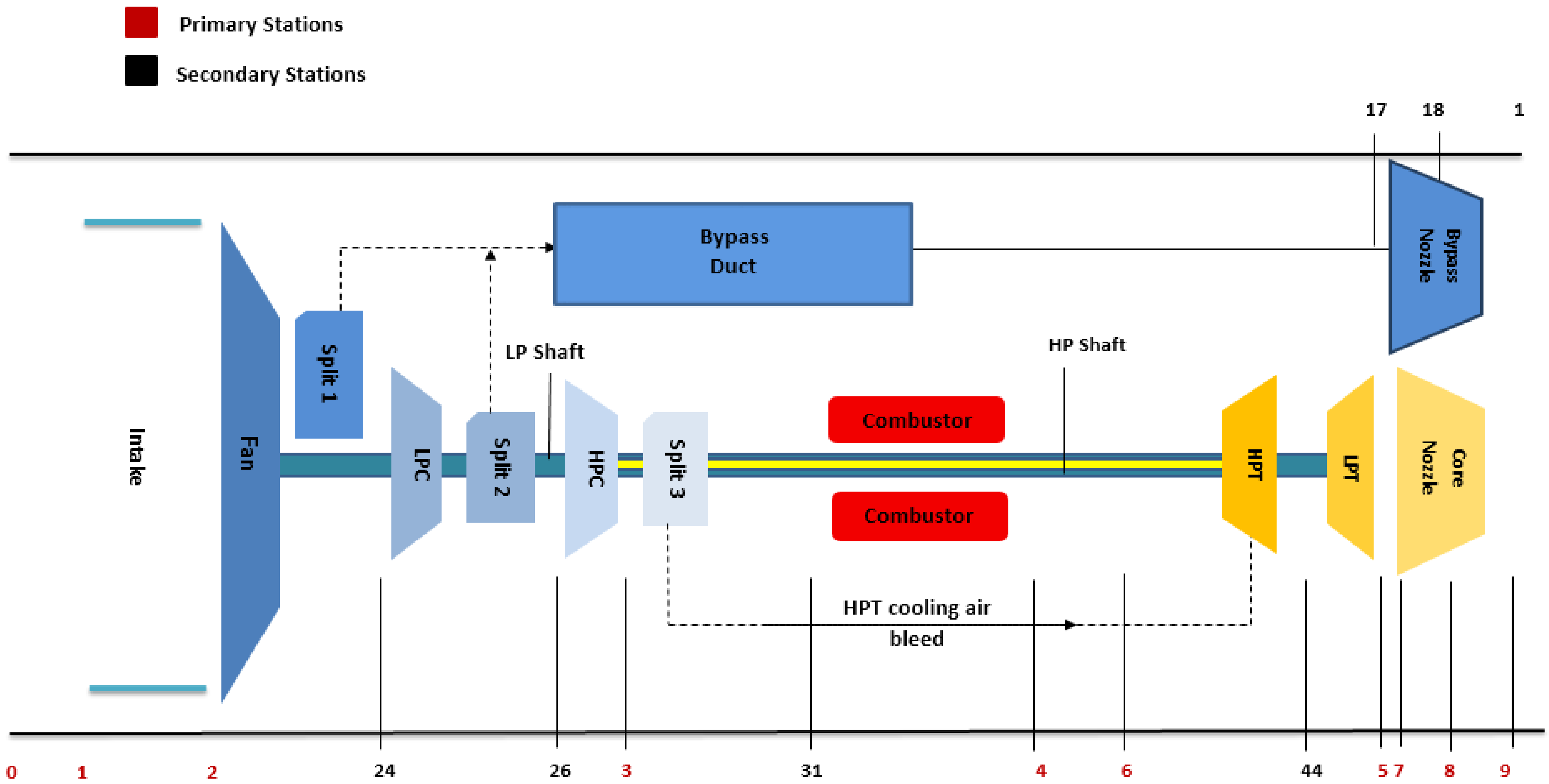


Figure 5-2: A general schematic of CU-Jet engine

(Note: Stations numbered according to ARP-755A nomenclature for turbofan engines [139])

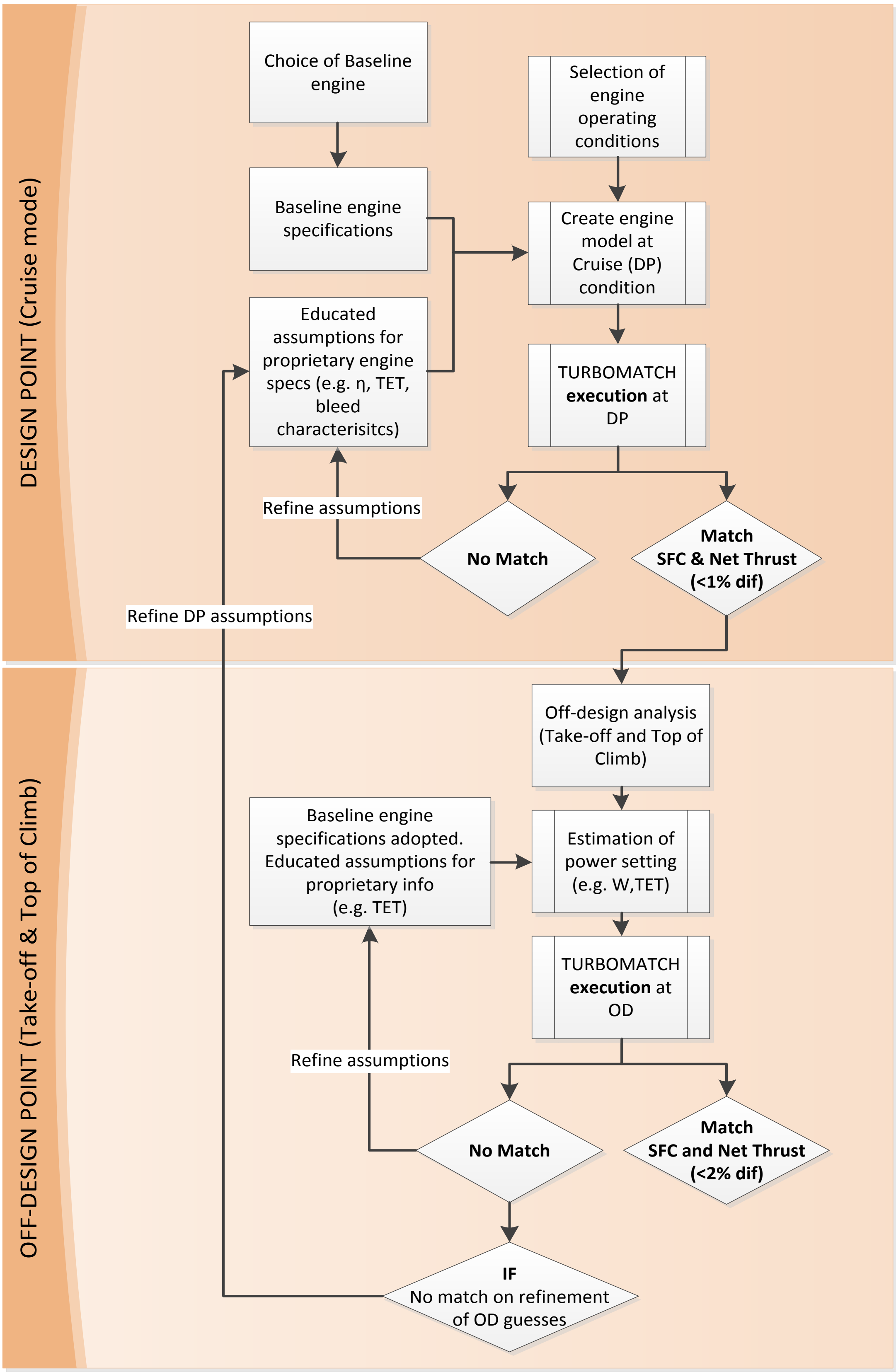


Figure 5-3: Matching procedure for design and off-design conditions between CU-Jet with baseline engine

The essential engine data and cycle parameters for CFM56-5B/2 have been provided Table 5-2.

Parameters	Values			Units
	Cruise	Top of Climb	Take-Off	
Net Thrust	26	28.5	138	kN
Mass flow	-	-	433.6	kg/s
Specific Fuel Consumption	15.4	-	9.8	g/kN.s
BPR	-	-	5.5	
OPR	-	35.9	-	
Red line EGT		1220		K
Fan speed		5200		rpm
Core speed		15183		rpm
Fan Stages		1		
Low Pressure compressor stages		4		
High pressure compressor stages		9		
High pressure turbine stages		1		
Low pressure turbine stages		4		
Engine Weight		2381		kg
Application		A321-112		

Table 5-2: CFM56-5B/2 engine performance data [32] and [57]

5.3.1.3 Off Design Performance Simulation

Take-off (TO) and Top of climb (TOC) modes have been chosen as the off design conditions owing to the requirement of the engine to operate outside the design point (Cruise). Some of the key cycle parameters such as the bypass ratio (BPR), mass flow (W) and specific fuel consumption (SFC) were determined from manufacturer’s specifications [57]. The variable which was iterated here to match the off-design engine performance data obtained from public domain was the turbine entry temperature (TET). A flowchart describing the method of model development has been presented in Figure 5-3. The assumptions that were used in the simulation of CU-Jet at design point and off-design conditions have been provided in Table 5-3.

Off-design analysis of CU-Jet-K at varying altitudes and ambient temperature conditions was also performed. This procedure was undertaken in order to assess the operating threshold of the engine model in a virtual environment and the parameters adopted for off-design performance have been provided as follows.

- Effect of Altitude at cruise mode – TET (handle:1200-1800K); Constant Mach no (0.8)

- Effect of Altitude at cruise mode- Mach no (handle: 0.0-0.8); TET constant (1355K)
- Effect of Ambient temperature at Take-off mode- TET (handle: 1200-1800K), Mach no constant (0.0). The outcome of this analysis has been elaborated in Appendix G.

5.3.1.4 Assumptions

A. Thermodynamic

- The Fuel used for design point and off-design analysis of CU-Jet is Conv. Jet fuel
- The working fluid in the cold section (intake to combustor inlet) is assumed to behave like atmospheric air
- Gas properties vary with operating conditions. They are accurately calculated and incorporated into cycle performance prediction. Therefore, the gas mixture is assumed to behave like a partially ideal gas

B. Design

Parameters	Values	Units
FPR	1.75	-
Booster PR	1.75	-
HPC pressure ratio	11.65	-
$\eta_{is\ fan}$	90	
$\eta_{is\ booster}$ and $\eta_{is\ HPC}$	87.5	
$\eta_{is\ LPT}$	91	
$\eta_{is\ HPT}$	89	%
Combustor pressure loss	5	
η_{comb}	99.9	
Mechanical transmission	100	
Cruise (DP) altitude	10668	m
Take-off (OD) altitude	0	m
Cruise Mach no	0.8	-
Take-off Mach no	0.0	-
Deviation from T_{amb} & P_{amb}	0	˚C/atm

Table 5-3: Design based assumptions for CU-Jet

C. Parametric

- The engine is assumed to be operating at steady state conditions with choked nozzles as a result of which the non-dimensional mass flow at the inlet of the turbine is constant.
- Combustion pressure losses (5%) and component efficiencies across the engine are assumed to be constant.

5.3.2 Mission Level Performance Assessment

The performance of the CU-Jet engine was zoomed out and interpreted over a user-defined flight trajectory comprising take-off, climb, cruise, descent and landing segments. This study was undertaken to measure mission based fuel burn from use of Bio-SPKs. In order to achieve this objective, a model aircraft, (LokAir) equipped with two CU-Jet engines, was numerically developed. HERMES is a FORTRAN based flight cycle simulation program which co-operates with the engine performance code to define the mission performance characteristics over a user-defined trajectory [38]. Further data on the input specifications and nature of operation are presented in the upcoming sections.

5.3.2.1 Required Input data

The aircraft modelled for the purpose of this assessment will be called “LokAir” which comprises airframe modelled from baseline, A321-100, using manufacturer’s specification [7]. The model aircraft resulting from the combination of modelled airframe integrated with the modelled twin-shaft turbofan “CU-Jet” will be denoted as “LokAir” in the upcoming sections. The key input specifications required for this assessment have been listed below

1. Wing and fuselage geometry
2. Weight related data including max take-off weight, max payload weight, max fuel weight and max landing weight obtained from manufacturer’s specification
3. Mission related data and assumptions used for this analysis have been provided below.
   i. Taxi-in at idle and take-off conditions
   ii. Climb comprising 18 segments with top of climb reaching an altitude of 10668m
   iii. Single cruise segment at an altitude of 10668m
   iv. Single descent
   v. Landing segment is calculated by the code upon provision of landing time which was chosen to be 6 min, for this study.
   vi. 5% trip fuel was stored towards contingencies, diversion or hold

Range specifications for the baseline aircraft was obtained from its respective payload-range diagrams. Missions range has been fixed at 4675 km representing a typical medium-range flight between London Heathrow (LHR) and Bahrain International (BAH).

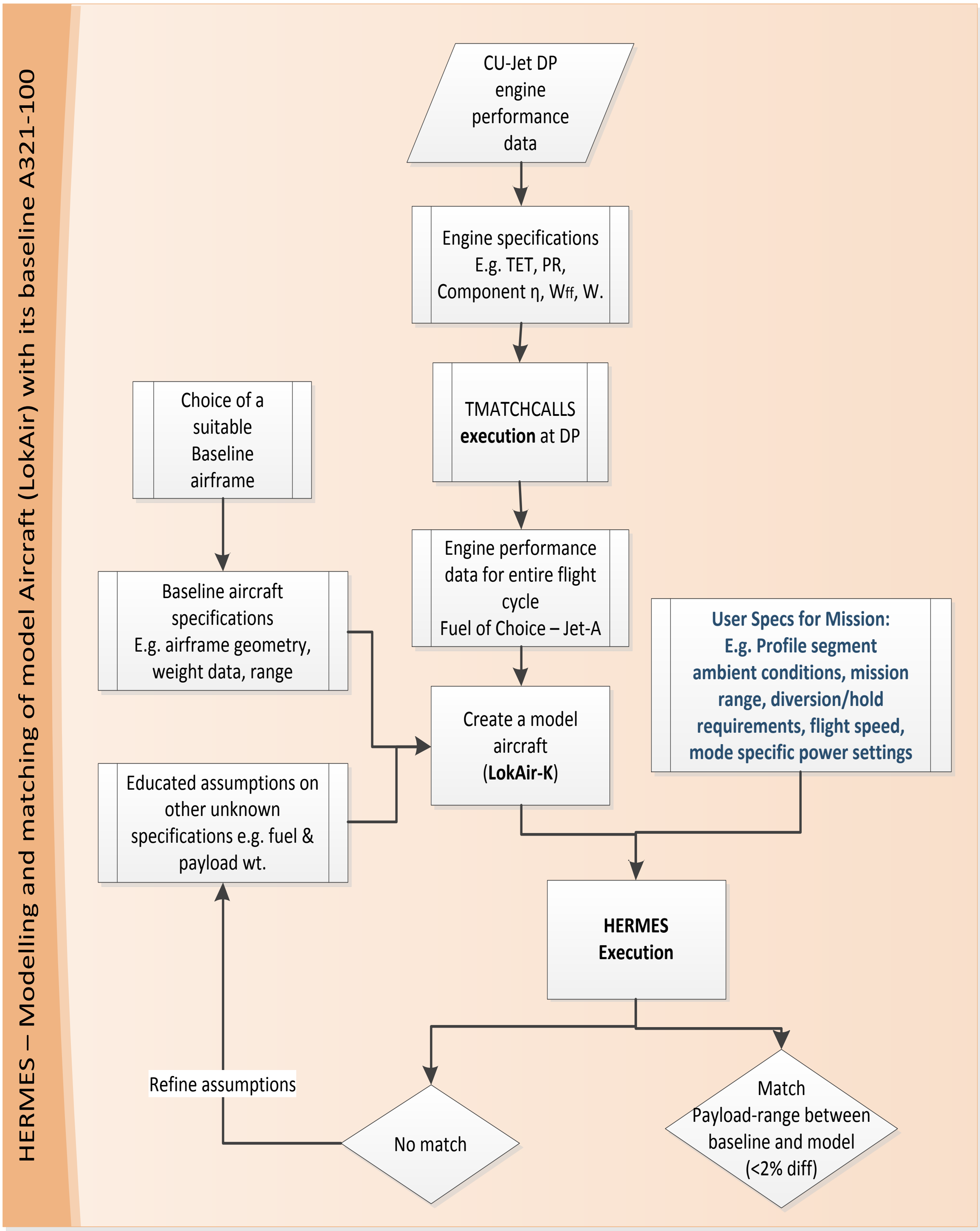


Figure 5-4: Model Aircraft matching (with baseline A321-100) procedures for through reverse iteration approach

5.3.2.2 Assumptions

The aircraft performance simulation has been carried out through point-mass based modelling. Point-mass modelling refers to determination of mission based metrics (e.g. fuel burn, range) through calculation of factors such as aircraft weight, fuel consumption and engine performance characteristics at each user-defined segments. The parameter which is fixed for this method of modelling is drag co-efficient of the aircraft (C_{D0}). Other operating variables such as induced drag coefficient (C_{D1}) and lift coefficient (C_L) are internally calculated by the model. The program was restricted to main medium-range mission with no diversions. The geometric and weight data adopted in this study were hypothetically guessed or adopted if available, from a baseline aircraft design (A321-112). A brief account on the data required and method of developing an aircraft model, validation and mission fuel burn assessment has been schematically represented in Figure 5-4. Further elaboration of the required input parameters have been provided in the Table 5-4.

5.3.2.3 Aircraft weight breakdown

A PLR (Payload-Range) diagram for the baseline aircraft (A321-100) acquired from technical data [7] was used to estimate the payload/ range (threshold) specifications towards construction of "*LokAir"*.

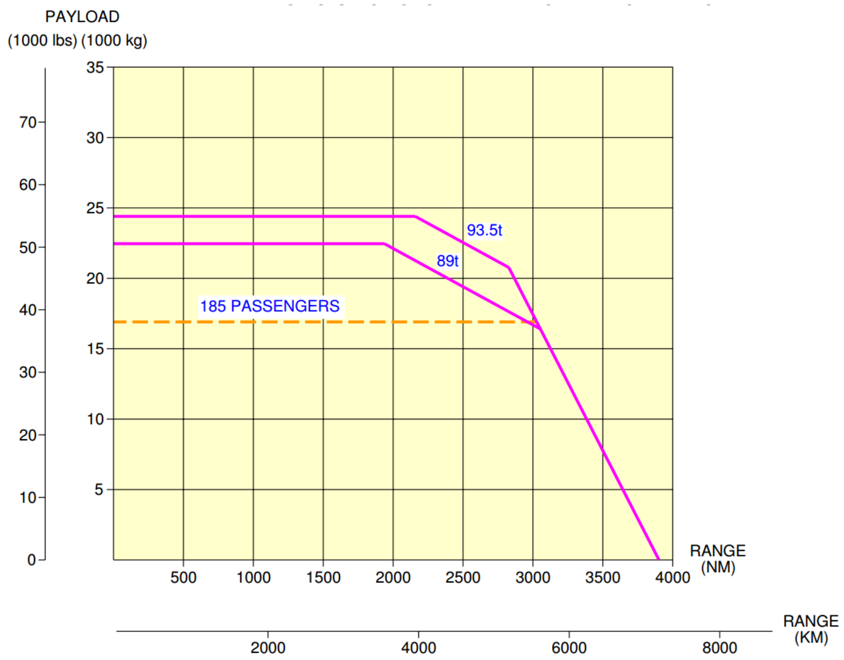


Figure 5-5: Payload-range diagram for A321-100 [7]

A PLR diagram provides information related to the potential range obtainable from maximum expendable load for a specific aircraft. This diagram is constructed using key weight data specific to a particular aircraft [Figure 5-5].

Specifications	Values	Units
Max Take-off weight	83000	
Max Payload Weight	22798	
Max landing weight	74500	kg
Max fuel weight	18806	
Aircraft weight	44357	
Max fuel range	4000	
Max ferry range	5400	km
Max payload range	7100	
Note: 199 passengers assumed; Average weight of a male: 79kgs; Average weight of a female: 58 kgs**;**		

Table 5-4 : Weight/ range specifications for model aircraft, LokAir-K [7]

A brief introduction to key weight data has been provided below

- **Operating Empty Weight (OEW)** - Weight of the aircraft [airframe weight (AW), Engine weight (EW) and Crew weight (CW)] with no fuel or payload. However, includes the weight of the crew and essential/ additional equipment required for the aircraft.

$$OEW = AW + EW + CW \qquad \textbf{Eq 44}$$

- **Maximum Take-off Weight (MTOW)**: Maximum weight at which the aircraft can take off at any weather conditions. MTOW is comprises aircraft payload (PW), fuel (FW) and operating empty weight (OEW).

$$MTOW = FW + PW + OEW \qquad \textbf{Eq 45}$$

- **Maximum Zero fuel weight (MZFW):** Maximum weight of the aircraft comprising max payload (MPW) and aircraft weight (A/C W) without fuel for engines. This weight can be determined by following

$$MZFW = OEW + MPW \qquad \textbf{Eq 46}$$

- **Maximum Payload weight (MPW)**: Maximum weight of the payload (cargo & fuel) that can be carried on an aircraft.

$$MPW = OEW - MZFW \qquad \textbf{Eq 47}$$

- **Maximum Fuel weight (MFW):** Weight of the aircraft with maximum fuel content and without payload.

The range for each of the parameters obtainable from the PLR diagram for A321-100 (Max Payload, Max fuel and Max ferry) have been determined [Figure 5-5]. It is essential for the virtual airframe to accommodate the modelled engines (CU-Jet) under the user-specified payload-range specifications. Therefore, the airframe model had to be developed through reverse iterative procedures and matched with baseline aircraft (A321-100) characteristics. Inaccuracies resulting from these modifications have been validated with the PLR diagram. The error difference between the model and baseline was strictly restricted to <2%. The method of constructing a PLR diagram has been illustrated in literature of reference [45].

5.3.2.4 Geometry Specifications

Aircraft geometry specifications required by HERMES towards the development of the model airframe, LokAir, have been specified in Table 5-5.

Specifications	Values	Units
Wing area	123	m^2
Wing span	34	m
Wing sweep	25	degrees
Aspect ratio	9.48	-
Fuselage length	44.51	m
Fuselage diameter	3.96	m
No of Engine	2	-
Engine weight	2381	kg/engine
Engine type	CFM56-5B/2	-
No of passengers	185	
Max range	4260	km

Table 5-5 : A321-112 characteristics as baseline specification for LokAir [7]

5.3.3 Fuel Combustion and Emission Evaluation

The “fuel combustion” phase contributes to the ≈70% of the total life cycle emissions. Therefore, careful prediction of combustion based CO_2 emission from each of the candidate fuels is crucial to systematically comprehend their overall life cycle emissions, unlike assumed figures encountered in earlier literature. This engine based emission quantification contributes to the overall environmental module within this TERA study. With respect to the prediction of NOx emissions, stirred reactor approach where the partitioned reactors within a combustion chamber are assumed to be partially/ perfectly stirred. The Degree of NOx formation is assumed to be influenced by fuel characteristics, reactor dimensions and power settings. Quantification of NOx emissions was undertaken at power settings prescribed by ICAO specifications for Landing-Take off (LTO) emission measurement (engine emission index (EI) determination). Additionally, emission from other throttle settings including climb, cruise and descent have also been included, for the knowledge of the readers on the NOx emissions from the entire mission profile.

5.3.3.1 Numerical Prediction of Aero-engine Emission Index

A physics based model for emission estimation is expected to capture the physics and chemistry involved in a given combustion process towards quantitative prediction of pollutants. Emission estimation was undertaken with the consideration of a conventional combustor to be a partitioned into different reactor. These reactors are in turn assumed to be partitioned into a partially stirred reactor comprising the flame front and a series of perfectly stirred reactor comprising the primary (PZ), intermediate (IZ) and dilution zones (DZ) of the combustor.

HEPHAESTUS is a FORTRAN based computation code, developed at Cranfield University for the numerical modelling and prediction of jet engine emission index under user-defined combustor and fuel specification.

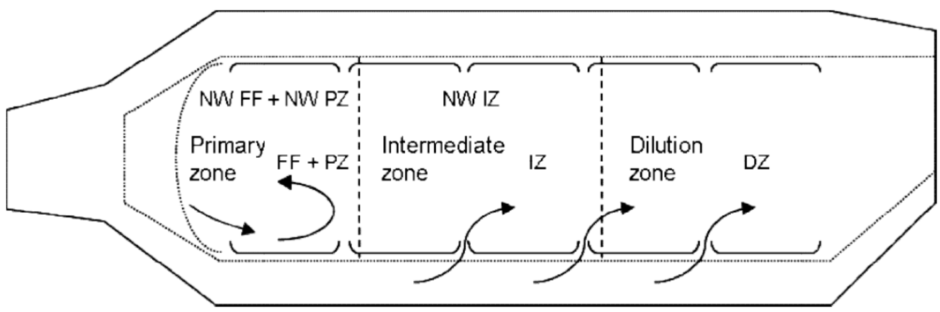


Figure 5-6: Diagrammatic representation of a conventional combustor [139]

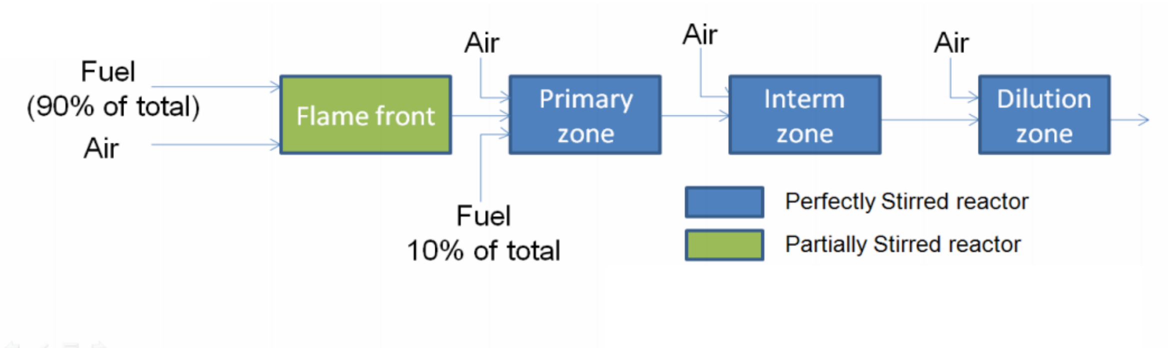


Figure 5-7: Schematic of Conventional Combustor representing the arrangement of partial and perfectly stirred reactors within HEPHAESTUS [103]

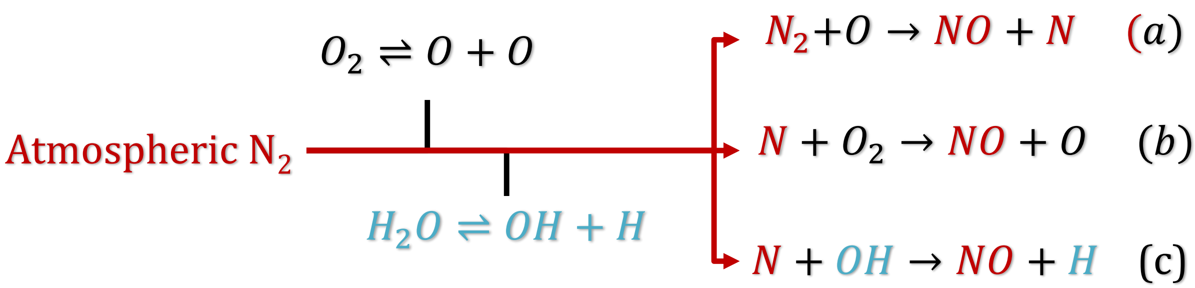
HEPHAESTUS is constructed with algorithms that enable the prediction of engine emission index of existing and novel design concepts/fuels. HEPHAESTUS aids quantification of the pollutants from the combustion process as a function of turbulent mixing in reactors. Therefore, the emission prediction model utilises a combination of a series of partially and perfectly stirred reactors. Mixture of fuel-air with recirculating hot gases is assumed to instantaneously take place in perfectly stirred reactor, thereby instantly attaining chemical equilibrium at molecular level. However, such a perfectly stirred condition does not account for mixture inhomogeneity e.g. non-uniform distribution of fuel-rich, fuel lean spots and resulting local temperature and equivalence ratios. Additionally, the rate of non-uniformity in reactor’s equivalence ratio must also be statistically quantified. It is essential to note that the above mentioned factors are essential determinants of the degree of NOx formation which now provides a rationale for the consideration of a partially-stirred reactor. It is also essential to note that HEPHAESTUS accounts for turbulent mixing through consideration of a “mixing parameter” which is a measure of the consistency of turbulent mixing between the fuel, air and hot combustion gases within the stirred reactors. The degree of NOx formation is influenced by the rate of formation of radicals from the attainment of chemical equilibrium. The kinetics of chemical equilibrium is precisely predicted with the use of NASA CEA code operating in the background of HEPHAESTUS. NASA CEA aids the determination of the concentration of equilibrium products and their fluid properties through minimisation of Gibbs free energy at constant temperature and pressure. In order to carefully quantify the concentrations of NOx emissions formed, algorithms for kinetic calculations of NOx emissions were built by the author of the model [31].

The empirical prediction of CO_2 emissions is relative straight forward since the fuel is assumed to undergo stoichiometric combustion and CO_2 emission is directly proportional to the carbon content of the fuel.

5.3.3.1.1 NOx formation mechanisms

A. Thermal NOx

Nitric Oxide (NO) resulting from oxidation of atmospheric nitrogen is called thermal NOx. Thermal NOx, formed through Zeldovich mechanism, is the dominant contributor to the overall NOx emissions and result from hotspots and post flame gases of combustion, according to studies of reference [139]. Pathways of NOx formation from Zeldovich mechanism is presented below.

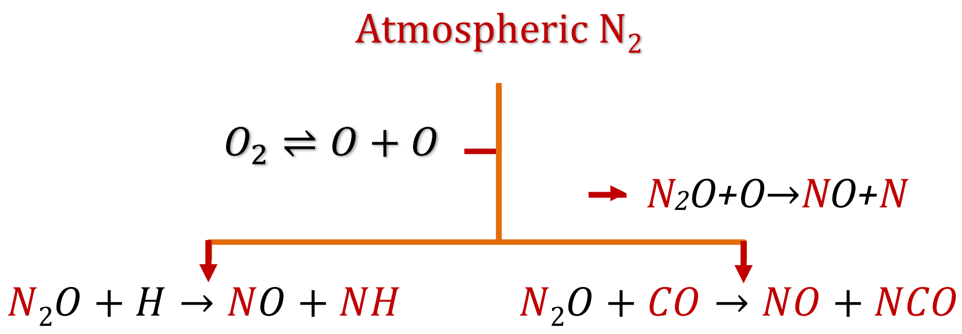


The competition for oxygen species (O) between the fuel and nitrogen at higher temperature (>1800K) and low equivalence ratios takes a shift towards the latter shooting up NO formation as expressed in (a) of the figure above. NOx emission is still released at fuel rich conditions from comparatively elevated flame temperatures through mechanism (b) which is still relatively lesser than that released from (a) [83]. The mechanism of Thermal NOx infers that NOx emissions are primary influenced by inlet temperatures, flame temperatures (a fuel dependent parameter) and residence time.

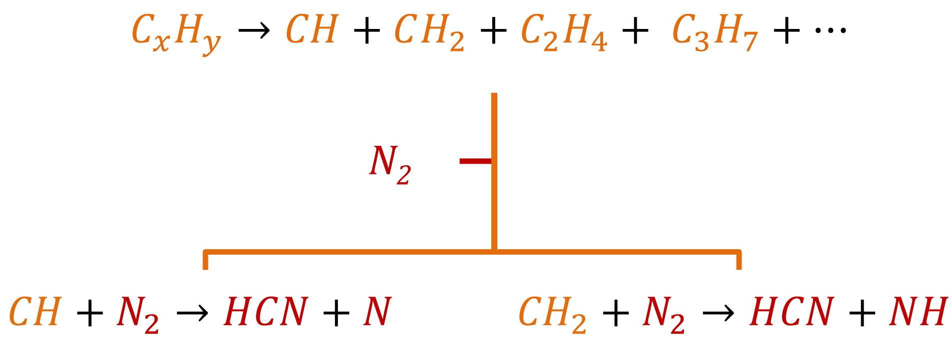
Careful calculation of equilibrium concentrations of the radicals indicated in the schematic representations (a), (b) and (c), i.e. oxygen, nitrogen, molecular oxygen/ nitrogen, hydroxyl groups is crucial to calculation of Thermal NOx. The author of HEPHAESTUS assumes that the equilibrium products and their fluid properties are predicted as a function of their local temperatures and pressures. The kinetic mechanisms of the different types of NOx formation is further elaborated by the author in the literature of reference [31] and they have not been elaborated in this study since it falls outside the scope of this study.

B. Nitrous Oxide Mechanism

N_2O contributes to the formation of NO by the following mechanism



C. Prompt NOx



Prompt NOx is generated from reaction of atmospheric nitrogen with the variety of hydrocarbon radicals available from the hydrocarbon combustion. The HCN molecules and the N atoms formed will be oxidized to NO completing the reaction. This mechanism is called as Nicol mechanism of NO formation.

D. Fuel NOx

Nitrogen content of a given fuel can contribute to overall NOx emissions which however are determined by the fuel type used. Fuel bound NOx increases with increasing flame temperature. Achieving this task requires user-definition of fuel and reactor based specifications. Further details on the underpinning principles of HEPHAESTUS and modification made to the parent code can be found in [31] & [103].

5.3.3.2 Integration of Bio-SPKs

Implementation of Bio-SPKs into the physics based model required the following modification. It is essential to note that HEPHAESTUS assumes the combustion to take place through equilibrium. Therefore, estimation of fluid properties for the fuel-air mixture and combustion products is essential for NOx estimation. This precision is achieved by coupling HEPHAESTUS with NASA CEA (Chemical Equilibrium with application).

The input data that was required for the insertion of Camelina SPK, Jatropha SPK and Microalgae SPK into the source code are as follows

- Chemical composition of the Bio-SPKs (C_xH_y)
- Molecular data and Thermo-physical properties (Molar mass, LHV and Density)

Data for input parameter was, as mentioned earlier. Each of the Bio-SPKs was assigned a Fuel type (FTYPE) number. The principle behind gas property estimation operating in NASA CEA gui was observed to be followed in HEPHAESTUS as well. The Input data required for insertion of Bio-SPKs into the source code has been tabulated in Table 5-6.

Fuel Name	Molecular formula	Molecular mass
Camelina SPK	$C_{11.2}\ H_{24.4}$	158.8
Microalgae SPK	$C_{11.5}\ H_{25}$	163
Jatropha SPK	$C_{11.2}\ H_{24.5}$	160.1

Table 5-6: Fuel specifications required for Bio-SPKs integration in HEPHAESTUS source code

Further information on the nature of the HEPAESTUS can be obtained from the works of reference [31] and [103].

5.3.3.3 Reactor Customisation

The modelled reactor had to be customised to that of an existing engine, CFM56-5B/2, through matching and must also be validated. Emission Index for CFM56-5B/2 operated with Jet-A1 provides a standard for customisation of the CU-Jet reactor. The dimensions and air mass flow fractions for each of the reactor zones have been presented in Table 5-7.

Parameters	Length (m)	Air flow fraction (%)	Flow Area (m^2)
Flame front	0.00830	28	0.20617
Primary zone	0.02025	7.3	0.20617
Intermediate zone	0.09375	6.7	0.20617
Dilution zone	0.09375	58	0.20617

Table 5-7: Customised reactor dimensions for CU-Jet emission model

Other engine parameters [fuel flow and combustor inlet parameters] indicated [Appendix H] were adopted from the engine performance prediction software, TURBOMATCH. The parameters were extracted for the four throttle settings indicated in the ICAO emission assessment for aircraft engines; Take-off (100%), Climb out (85%), Approach (30%) and Idle (7%). An example of the engine parameters required as input specifications to quantify NOx emissions through HEPHAESTUS have been presented in Table 5-8.

Flight Phase	T_{amb} (K)	Altitude (m)	W_{in} (kg/sec)	T_{in} (K)	P_{in} (kPa)	W_{ff} (kg/sec)
Take-off	288	0	64.5	886.2	37.62	1.388
Climb-out	288	475	62.6	820.8	36.56	1.1137
Approach	272	1500	25.1	700.6	12.65	0.3503
Idle	288	0	8.5	580	4.02	0.124

Table 5-8: Ambient and Combustor inlet conditions for Emission model customisation and validation

5.3.3.4 Method of Validation

The numerically modelled combustor will be matched with that of the baseline, CFM56-5B/2, by reverse iteration approach [by attempting to match just the EINOx attributable to both the engine operating at ICAO suggested LTO (Landing Take-off power settings [Figure 2-3]]. The EI NOx emission attributable to CFM56-5B/2 (operated with Jet-A1) can be found in the public domain [69]. To improve the validity of the numerical combustor model, the match in % difference in EINOx emission reported between the model and the baseline was restricted to <2%. A schematic representation of the method of combustor modelling, matching and validation procedure has been provided in Figure 5-8

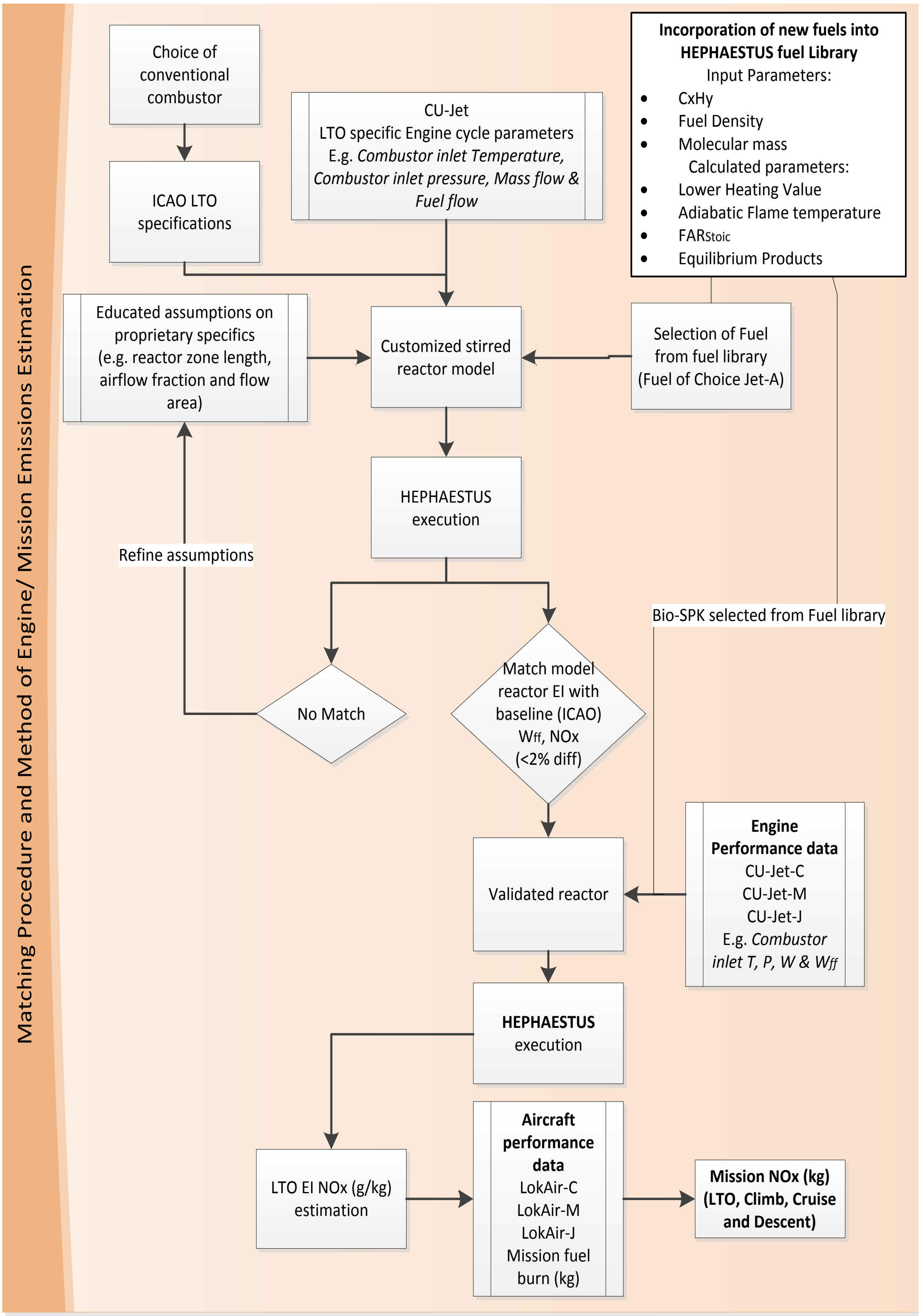


Figure 5-8: Method of reactor customisation and engine/mission level emission estimation for Bio-SPKs

5.3.4 Assumptions

Aero-engines are expected to function at a variety of operating envelope unlike stationary gas turbines. This fundamental factor has monumental influence on the number and degree of pollutants formed from fuel combustion. Therefore, the necessity for a robust model which sensitively accounts for variations in cycle parameters and other fuel based factors mentioned above becomes desirable. However, consideration of such intricate details requires engine-specific proprietary information (e.g. combustor dimensions, pressure co-efficient, pressure loss factor, spray evaporation, pattern factor) without which the level of uncertainty increases. To eliminate the need for unavailable data, HEPHAESTUS has opted for the stirred reactor approach with the below mentioned assumptions

i. The combustion chamber is assumed to be a stirred reactor. The reactor has been divided into flame front (FFZ), primary zone (PZ), intermediate zone (IZ) and dilution zone (DZ). FFZ is assumed to be a partially stirred reactor to model the inhomogeneity in fuel/air and gas mixing. The mixing in a partially stirred reactor is assumed to be incomplete at molecular level which subsequently results in the formation of eddies with different residence times. Such a characterisation of FFZ is expected to predict NOx emissions with better accuracy. The other 3 zones are considered perfectly stirred reactors where the gas and air/fuel mixtures are instantaneously mixed to chemical equilibrium. Further details on modelling assumptions have been illustrated in [31].

ii. Certain parameters including fuel injector parameters, fuel spray characteristics, pattern factor, flow recirculation and flame unsteadiness have not been considered to maintain the universality of the emission model

5.4 RESULTS & DISCUSSION

5.4.1 CU-Jet Engine performance

PARAMETERS	CRUISE (DP)	TAKE OFF (OD)	TOP OF CLIMB (OD)	UNITS
Altitude	10668	0	10668	m
Mach no	0.8	0	0.8	-
Fan Pressure ratio	1.75	1.801	1.797	-
Overall Pressure ratio	32.4	35.9	34.7	-
Fan isentropic efficiency	90	90	90	%
Booster isentropic efficiency	87.5	87.5	87.5	%
HPC isentropic efficiency	87.5	87.5	87.5	%
HPT isentropic efficiency	91	91	91	%
LPT isentropic efficiency	89	89	89	%
P_a	0.34	1.0132	0.34	kPa
T_a	243	288	243	K
TET	1355	1635	1412	K
Mass flow (W)	162.5	431	166.7	kg/s
Fuel Flow (W_f)	0.4056	1.3880	0.4543	kg/s
Net Thrust (F_n)	25.8	137.7	28.5	kN
Specific Fuel Consumption	15.6	9.75	15.82	g/kN.s

Table 5-9: Performance characteristics of CU-Jet engine model

Certain proprietary parameters including component efficiencies and pressure losses had to be refined for CU-Jet to match the performance characteristics of CFM56-5B/2. Engine performance data for CU-Jet from its design point (Cruise mode) and Off-design operations (TO and TOC) were computationally simulated with TURBOMATCH using the reference cycle parameters mentioned. The outcome of this analysis were compared and validated with our base engine CFM56-5B/2. Chosen validation parameters were Net Thrust and SFC [Table 5-10].

5.4.1.1 Engine model Validation

The parameters of validation chosen between CU-Jet and CFM56-5B/2 were net thrust (**Fn**) and Specific fuel consumption (**SFC**). As mentioned earlier, the % deviation between the model and baseline were restricted to <1% for design point condition and <2% for off-design condition.

PARAMETERS	CFM56-5B/2	CU-Jet	% Deviation
Fn $_{Cruise}$ (kN)	25.9	25.8	-0.15
SFC $_{Cruise}$ (g/kN.sec)	15.45	15.6	0.94
Fn $_{TO}$ (kN)	137.8	137.7	-0.03
SFC $_{TO}$ (g/kN.sec)	9.85	9.7	-1.54
Fn $_{TOC}$ (kN)	28.5	28.5	0.06
SFC $_{TOC}$ (g/kN.sec)	-	15.82	-

Note:
Data of parent engine for validation obtained from [32] & [57]

Table 5-10: Comparative validation of CU-Jet performance characteristics

Off-design performance evaluation of CU-Jet-K undertaken with Mach no and TET as handle at varying altitude and ambient temperature condition have been presented in Appendix G.

5.4.2 Jet Engine performance with Bio-SPKs

To evaluate the performance characteristics imparted by the Bio-SPKs on an existing aero-engine, it is essential to understand the thermo-physical behaviour of a given fuel within the gas turbine. The chemical composition of Bio-SPKs is a crucial determinant of key caloric properties which are of significance to engine performance (fuel LHV and combustion temperatures). The operating variables in this analysis include TET and fuel flow. The three Bio-SPKs were weighed against our reference fuel in terms of specific fuel consumption at a range of TET (1200-1800K), constant Mach no and altitudes and thrust output (10668m for Cruise mode and 0.0m for Take-off mode) [Figure 5-9].

5.4.2.1 Specific fuel consumption

During design (cruise) and off-design evaluation (Take-off, Climb) CU-Jet-C, CU-Jet-M and CU-Jet-J Bio-SPKs were determined to deliver fuel savings of about 1.5-2.8%, relative to CU-Jet-K. The quantified values of fuel saving achieved has been graphically presented in Figure 5-9 and Figure 5-11. The fuel savings were delivered by the Bio-SPKs due to the higher hydrogen content (9-11% higher) which in turn boosts the LHV, relative to Conv.Jet fuel. The effect of lower heating value on the fuel saving is more robustly presented in Figure 5-10 and Figure 5-12 where the energy spent to achieve the fixed net thrust has been schematically presented as Energy Specific Fuel Consumption (ESFC).

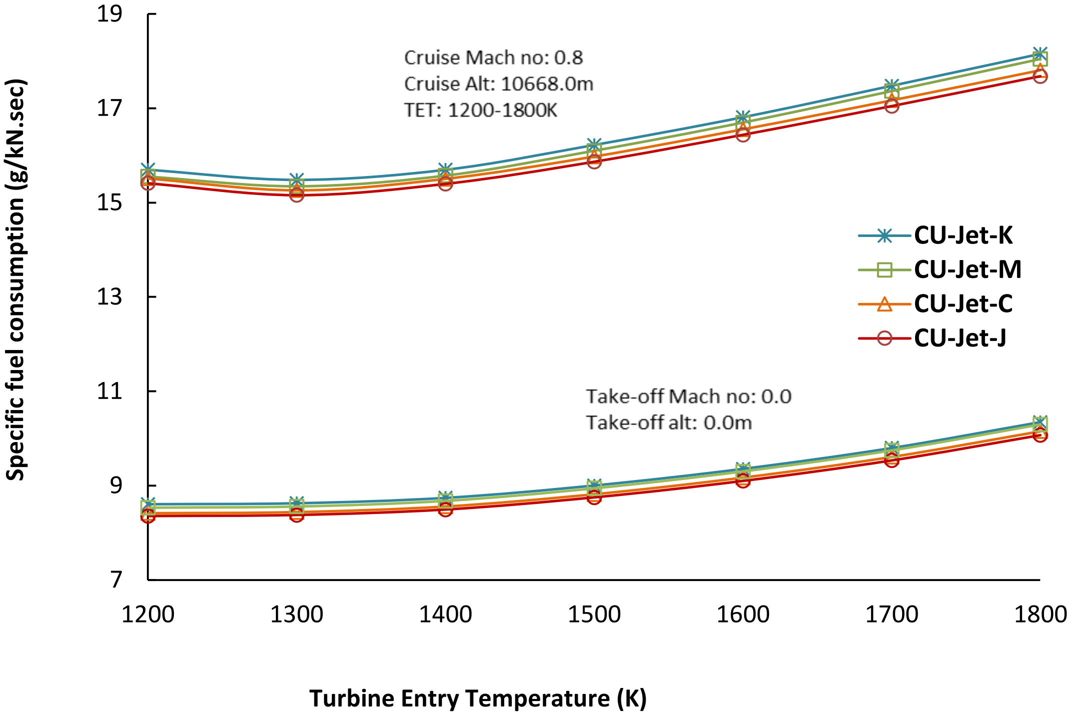


Figure 5-9: Comparison of SFC among fuel candidates at cruise and take-off mode

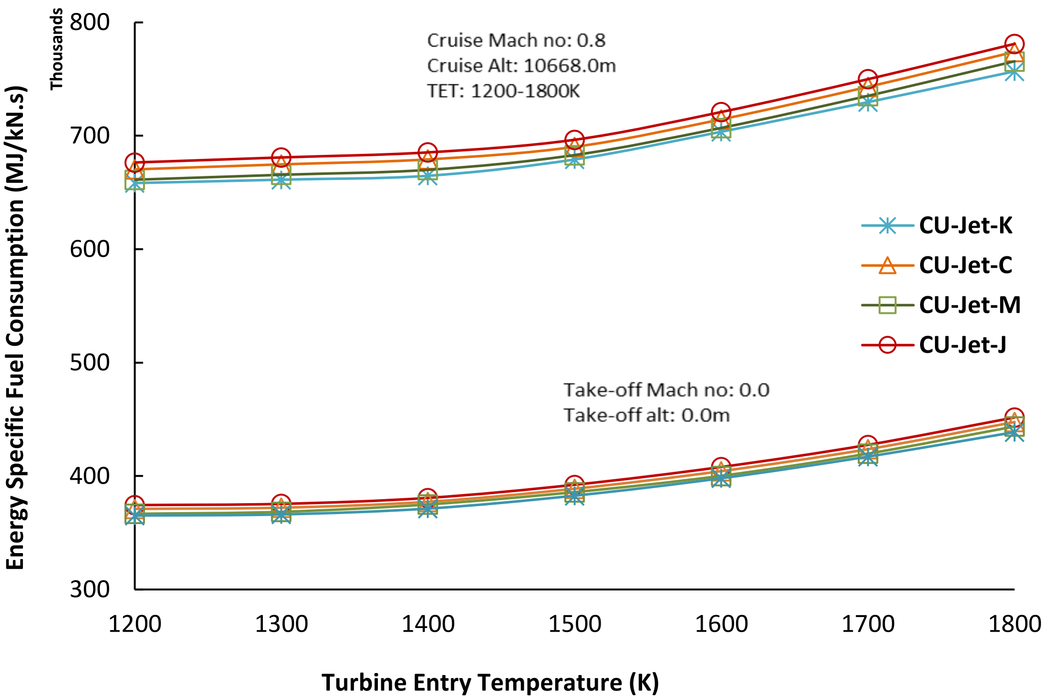


Figure 5-10: Comparison of Energy Specific Fuel Consumption among fuel candidates at cruise and take-off mode

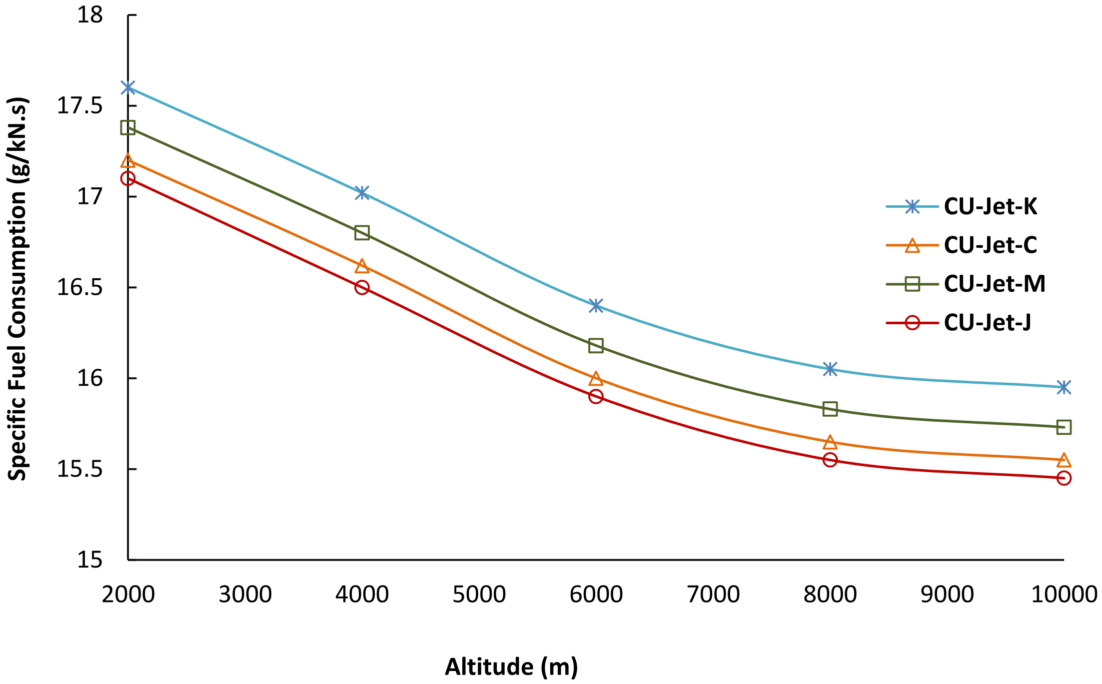


Figure 5-11: Comparison of SFC among fuel candidates during the Climb phase

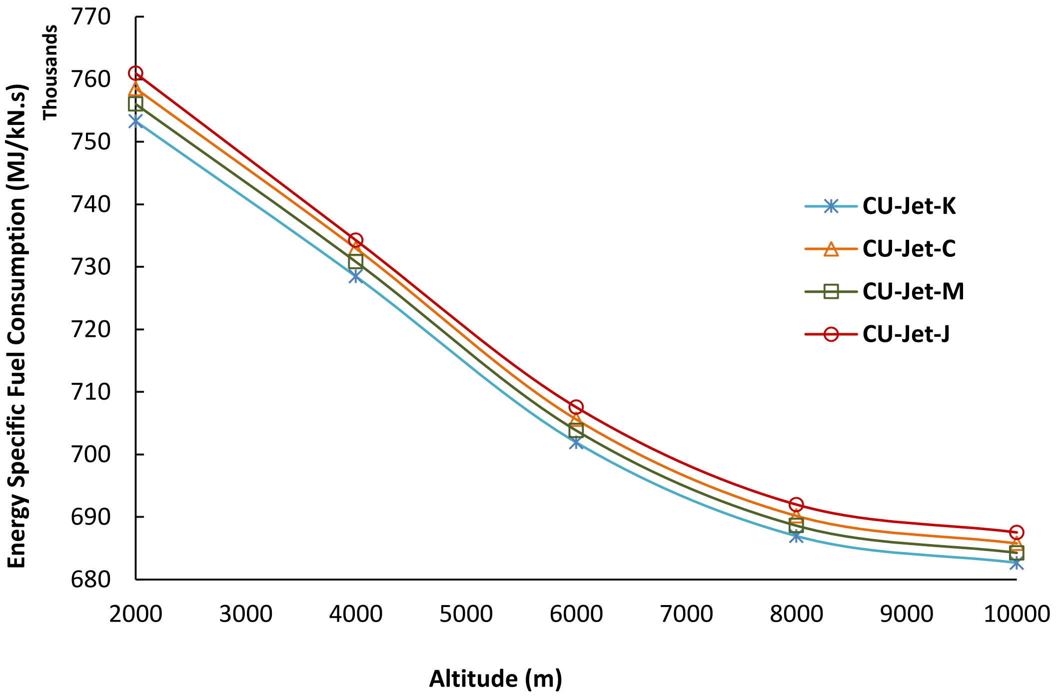


Figure 5-12: Comparison of Energy Specific Fuel Consumption among fuel candidates during the Climb phase

[Note: Operating conditions vary with the altitude TET and Thrust is maintained constant]

Energy Specific fuel consumption (ESFC) is the product of Specific fuel consumption (SFC) and lower heating value of the given fuel (LHV). The unit designated to ESFC is MJ/kN.sec. The Net thrust (Fn) appropriate for different power settings, were fixed for the biofuel operated performance evaluation. Therefore, the amount of energy required to achieve the fixed thrust is will vary with the amount of fuel flow. From the ESFC calculated for each of the candidate fuels, it is evident that a relatively lower quantity of Bio-SPK is needed to deliver the same net thrust delivered by that of conv.jet fuel, Jet-A1. The effect of fuel LHV and FAR on engine SFC has been provided in section 5.4.2.2.

Fuel	ESFC (MJ/kN.s)				LHV (MJ/kg)	% Δ	FAR_{Stoich}	%Δ
	Cruise	% Δ	Take-off	% Δ				
CU-Jet-K	662972	-	368762	-	43.1	-	0.0678	-
CU-Jet-C	676935	2.1	376706	2.13	44.1	+2.15	0.0667	-1.9
CU-Jet-M	672725	1.1	372707	1.4	43.5	+1.2	0.0668	-1.76
CU-Jet-J	683075	2.5	378105	2.8	44.3	+2.66	0.0665	-2.2

Table 5-11: Comparison for fuel related properties among the candidate fuels and reference fuel

5.4.2.2 Effect of LHV and FAR on Combustion temperature

Lower Heating value is the measure of energy obtainable from complete combustion of a given quantity of fuel. The lower heating value (expressed as MJ/kg) is influenced by the fuel's H/C ratio. Camelina SPK, Microalgae SPK and Jatropha SPK have been determined to possess 11%, 10% and 13% higher hydrogen mass content respectively, relative to Conv. jet fuel (Jet-A1).

The higher hydrogen content is expected to aid Bio-SPKs burn relative cooler resulting from low levels of dissociation and hence denser combustion gases. This phenomenon is expected to reduce fuel consumption by improving thermal efficiency and reducing SFC of CU-Jet. This phenomenon can be expressed even through Energy Specific Fuel Consumption (ESFC) of the biofuel candidates which is is more or less similar to the difference in their LHV, relative to that of Conv.Jet-A1 [Table 5-11]. According to a comparative experimental study on engine performance conducted by other studies [73], the two Bio-SPKs were able to provide an average saving in fuel flow by 0.7% and 1.2% for 25% and 50% blend of Bio-SPKs with Jet A-1 respectively.

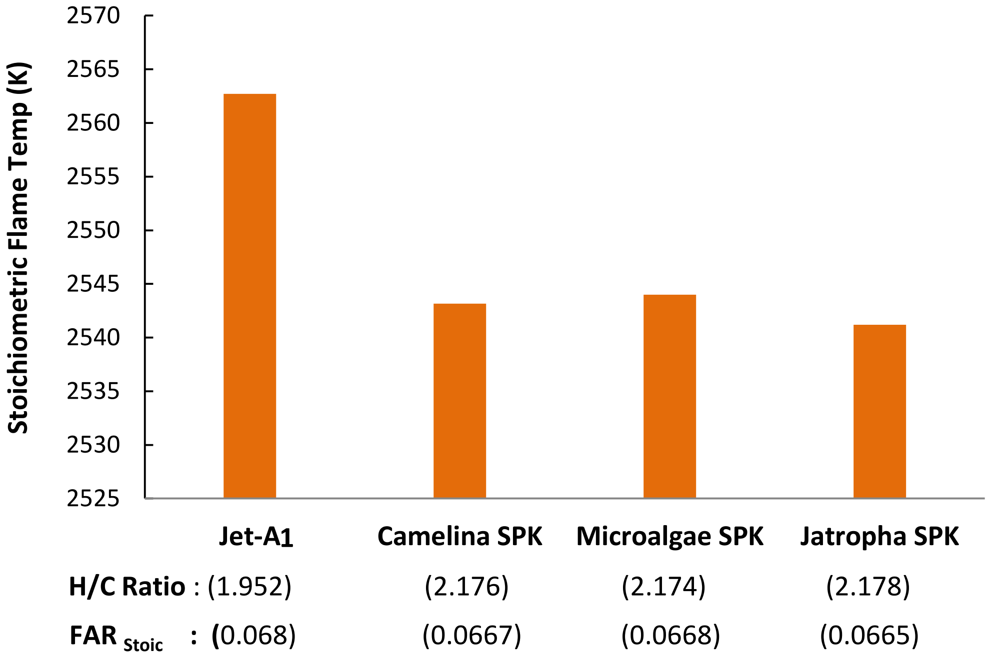


Figure 5-13: Effect of fuel H/C ratio and FAR_{stoic} on combustion temperatures of the candidate fuels

Flame temperature related to a given fuel is influenced not just by the LHV but also the fuel-air ratio (FAR). The influence of higher H/C ratio in terms of lower combustion temperatures has been observed in this analysis [Figure 5-13], a phenomenon which has significantly observed in studies of reference [21], [73] & [142]. Stoichiometric flame temperature has been chosen as a reference and it is observed that the higher hydrogen content of the Bio-SPKs lowers the corresponding flame temperature. The improved thermodynamic parameters of the post combustion gases e.g. increased enthalpy release, increased fluid density and isobaric specific heat (Cp) markedly improve the energy to work transfer and boost thermal efficiency of the overall engine. Fuel –air ratio is also a crucial determinant of adiabatic flame temperature as expressed by Borman and Ragland (1998) [22] as expressed in Eq 48

$$\boldsymbol{T_f = T_0 + \left(\frac{FAR}{1+FAR}\right)\left(\frac{LHV}{Cp}\right)} \qquad \textbf{Eq 48}$$

where, T_f = *Flame Temperature, K*

T_0 = *reference temperature (298.15 K)*

FAR = Fuel to Air Ratio

LHV = Lower Heating Value of the Fuel, kJ/kg

Cp = Isobaric Specific Heat, kJ/ kg.K

The Stoichiometric FAR of the Camelina SPK, Microalgae SPK and Jatropha SPK are 1.9%, 1.76% and 2.2% lower relative to that of the Conv.Jet-A1. Since the combustor is of fixed geometry, the primary equivalence ratio of the primary zone is assumed to be solely influenced by the fuel. Therefore, the Bio-SPKs, with their relatively lower FAR reduce the primary equivalence ratio of the primary zone leading to lower flame temperatures. Level of dissociation and associated energy loss reduces with lowered flame temperatures thereby resulting in the betterment of the core jet stream fluid properties.

5.4.3 Mission Level Performance analysis with Bio-SPKs

5.4.3.1 Aircraft Validation

The aircraft model (Lokair), comprising the model airframe equipped with two numerically modelled engine (CU-Jet), was developed with carefully assumed fuel load and aircraft weight to match the baseline specification of the aircraft model, A321-112. A comparative PLR diagram between the baseline and the modelled aircraft has been provided for the purpose of validation. The % deviation between the model and the existing baseline was restricted to <2% as presented in Figure 5-14 and Table 5-12.

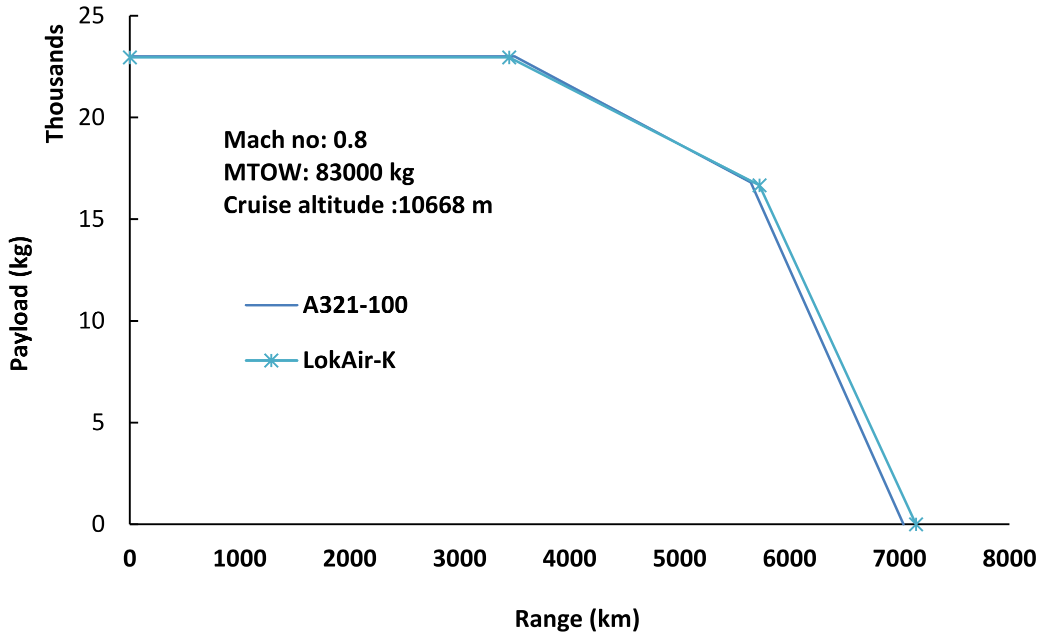


Figure 5-14: Comparative validation of LokAir-K with baseline aircraft A321-100

Specifications	A321-112		LokAir-K		% deviation
	Payload (kg)	Range (km)	Payload (kg)	Range (km)	
Max payload	23000	3500	22950	3450	1.43
Max fuel	16800	5649	16658	5728	1.4
Max ferry	0	7037	0	7150	1.6

Table 5-12: Comparison and validation of LokAir-K vs. baseline, A321-100

5.4.3.2 Mission Fuel Burn

The purpose of this analysis was to evaluate mission level performance imparted by the Bio-SPKs relative to Jet-A1. This was achieved by adopting the fuel consumption attributable to CU-Jet-K, CU-Jet-C, CU-Jet-M and CU-Jet-J from the engine performance model and zooming out to mission level analysis to measure their respective mission fuel burn. It is essential to note that mission fuel burn was measured over a fixed flight range and fuel tank capacity. This analysis concluded the % difference in fuel burned by LokAir-C, LokAir-J to be ≈-3.5% and LokAir-M to be ≈-2.8% relative to that of LokAir-K. The differences in fuel burn have been schematically represented in Figure 5-15 and numerically tabulated in Table 5-13.

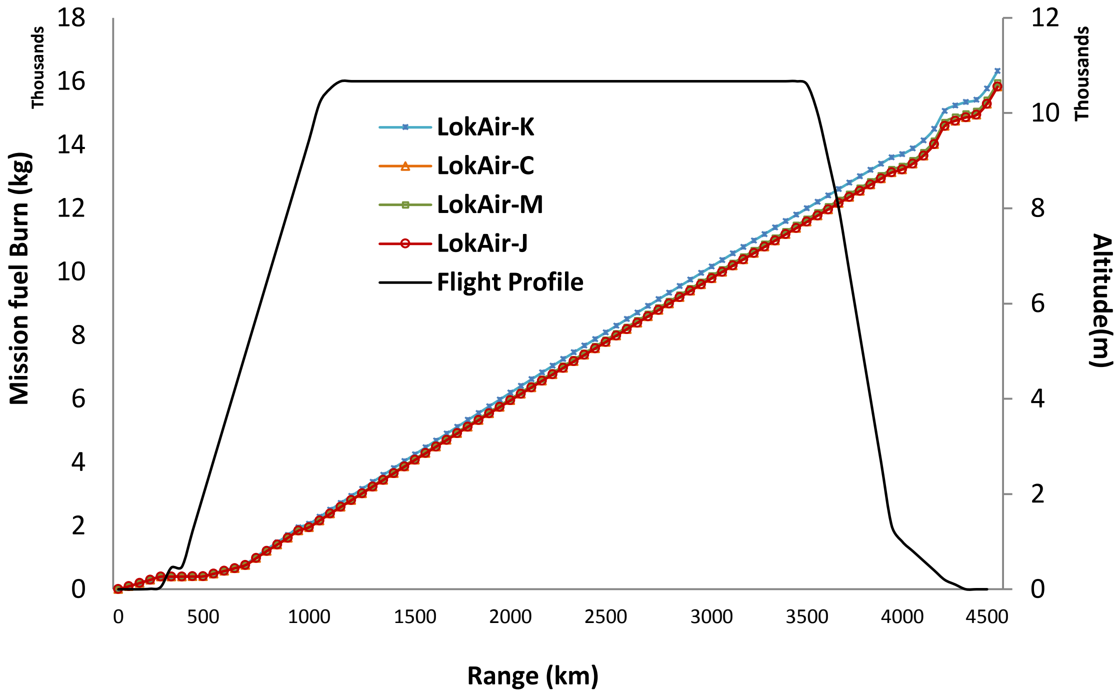


Figure 5-15: Medium-range fuel burn by LokAir with the candidate fuels

Aircraft	Mission Fuel Burn (kg)
LokAir-K	16324.3
LokAir-C	15720
LokAir-M	15817
LokAir-J	15703

Table 5-13: Mission Level fuel burn of Aircraft operated with the candidate fuels

The relatively higher LHV of Camelina SPK, Microalgae SPK and Jatropha SPK boosts the gravimetric energy content of the fuel tanks in LokAir-C, LokAir-M and LokAir-J respectively. This phenomenon delivers an average of 3.35% mission-level fuel savings, relative to that of LokAir-K. However, it is essential to note that the drop in volumetric energy content of a fixed volume tank can have a negative impact on the range deliverable by the Bio-SPKs as presented in Figure 5-16. The lower density of the fuel may be beneficial in terms of providing additional payload capacity to the airline operators. From industrial perspective, however, a relatively denser fuel is desired. It is essential to know that in practice, however, an aircraft carries fuel sufficient for the set destination and an additional 5% for contingency purposes. Therefore, the need for additional range benefit is seldom required. However, the aim is to briefly overview the significance of fuel-based physical properties on an existing civil engine/airframe configuration, for reader's reference.

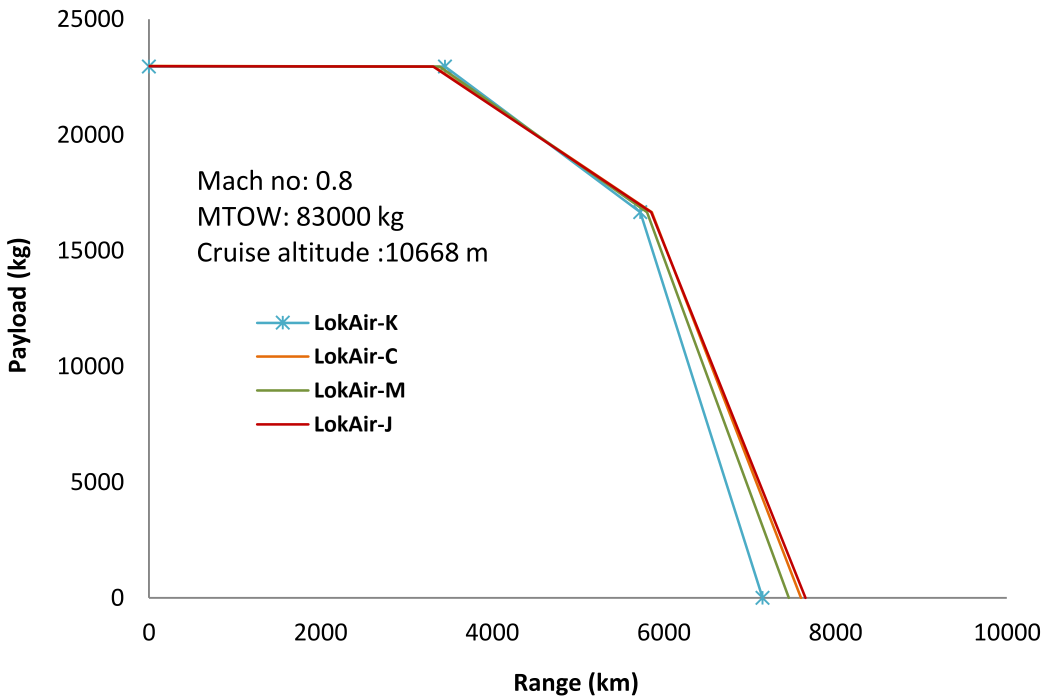


Figure 5-16: Payload-range characteristics of the LokAir operated with the candidate fuels

5.4.4 Fuel Combustion and Emissions

5.4.4.1 Validation of Emissions Model- NOx for LTO cycle

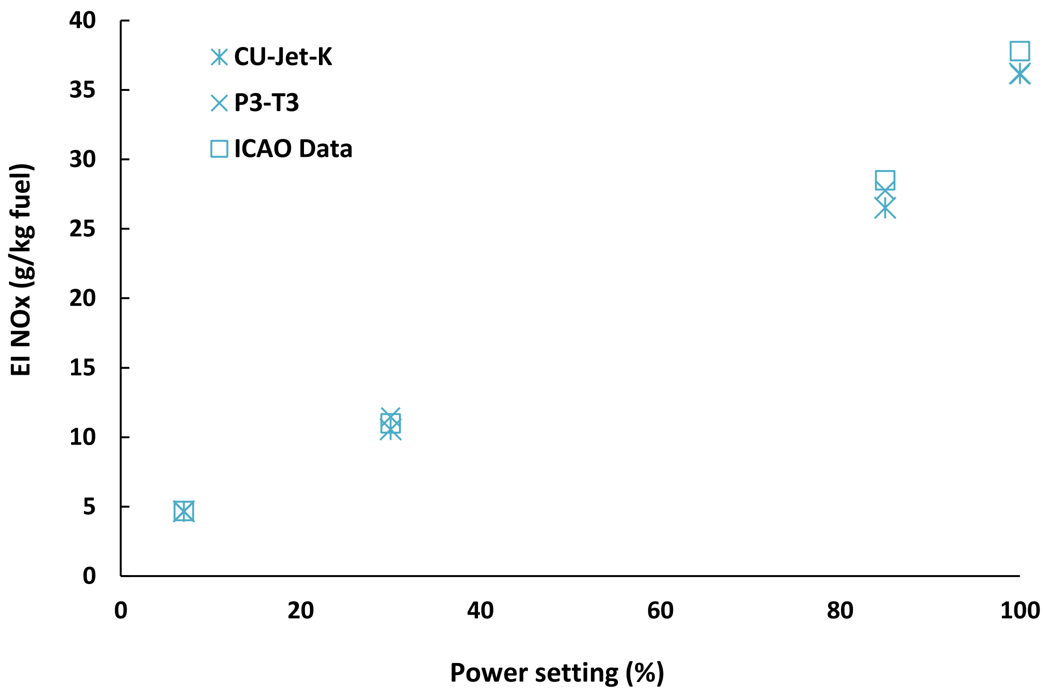


Figure 5-17: Comparison of LTO NOx emissions of model combustor with that of the baseline engine (CFM56-5B/2)

The combustor, numerically modelled on HEPHAESTUS, must be matched and validated with baseline combustor, CFM56-5B/2. The modelled combustor that was operated with the reference fuel (Jet-A1) was matched with that of the baseline (CFM56-5B/2) based on their ICAO-LTO cycle based EI-NOx emissions. The percentage deviation between the modelled combustor and the baseline have been restricted to <2%. The closeness of the match (-1.3%) between the model and the baseline is evident from Figure 5-17. The developed CU-Jet engine combustor has also been validated against the P_3-T_3 based EINOx emissions and the percentage difference was determined to be an average of 0.9% over the LTO cycle.

5.4.4.2 Estimation of NOx emissions

The need to mitigate NOx emissions have heightened in recent years due to its inevitability in a combustion process and apprehended atmospheric deterioration both at ground level and tropospheric level emissions.

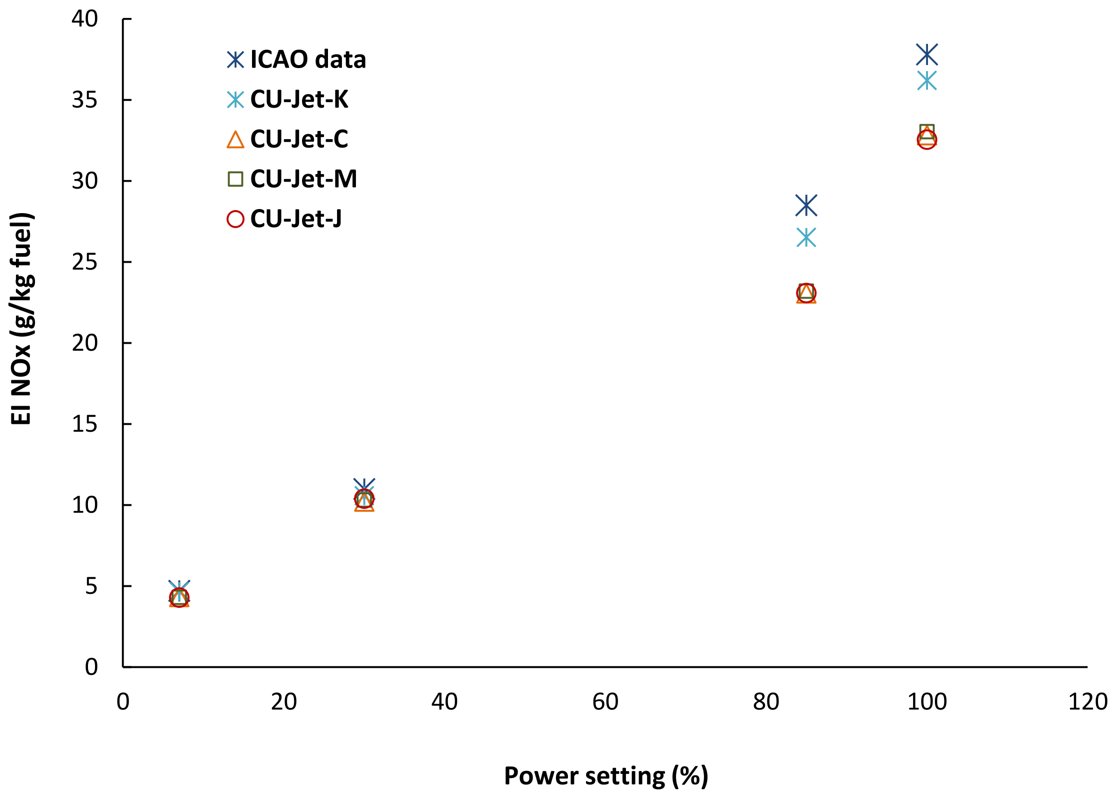


Figure 5-18: Comparison of NOx emissions attributable to candidate fuels

Fuel bound NOx is omitted due to its negligible content in the fuel (<0.4 ppm). EI NOx predicted for the modelled engine operated with 100% Bio-SPKs has been plotted against that of ICAO EI for CFM56-5B/2 and CU-Jet-K [Figure 5-18]. A clear tabulation of EI NOx emissions (g/kg of fuel) predicted for each of the LTO power settings when operated with the candidate fuels has been presented in Table 5-14.

Numerical modelling and simulation of the combustion through stirred reactor approach when the engine is operated with the Bio-SPKs lead to prediction of lower NOx emissions at higher throttle settings (take-off and climb out). However, these emissions were close to that of the reference fuel at lower power settings (approach and idle conditions). The overall difference in the LTO-NOx emissions between Camelina SPK, Microalgae SPK and Jatropha SPK (under ICAO-suggested LTO specifications) were determined to be -8.1%, -7.7% & -8.3% respectively, relative to Conv.jet fuel.

LTO Power setting (%)	Fuel Type	Fuel Flow (kg/sec)	EI Nox (g/kg fuel)
100	Jet-A1	1.389	36.2
	Camelina SPK	1.316	32.8
	Microalgae SPK	1.318	33.0
	Jatropha SPK	1.3155	32.5
85	Jet-A1	1.1137	26.5
	Camelina SPK	0.994	23.1
	Microalgae SPK	0.996	23.2
	Jatropha SPK	0.994	23.1
30	Jet-A1	0.3503	10.6
	Camelina SPK	0.3407	10.2
	Microalgae SPK	0.342	10.3
	Jatropha SPK	0.3406	10.2
7	Jet-A1	0.124	4.7
	Camelina SPK	0.1196	4.3
	Microalgae SPK	0.1204	4.3
	Jatropha SPK	0.1196	4.3

Table 5-14: Comparison of Fuel flow and EI NOx emission among Bio-SPKs at LTO power settings

NOx emissions that stem from greater adiabatic flame temperature is influenced by the equivalence ratio of the primary zone in the combustor. Primary Equivalence Ratio is defined as the ratio of Fuel-Air ratio (FAR) to stoichiometric fuel-air ratio (FAR_{Stoic}). Stoichiometric fuel air ratio (FAR_{Stoic}) corresponds to the ratio of fuel to air where all the oxygen in the oxidant (air) is utilised only to completely oxidise the fuel, leaving no excess moles air or fuel component. For the purpose of this analysis, FAR_{stoic} has been chosen to explain the outcome of low NOx emissions from Bio-SPKs. The Stoichiometric FAR of the Camelina SPK, Microalgae SPK and Jatropha SPK is 1.9%, 1.76% and 2.2% lower, relative to that of the Conv.Jet-A1. Since the combustor is of fixed geometry, the primary equivalence ratio of the primary zone is assumed to be solely influenced by the fuel. Therefore, the Bio-SPKs, with their relatively lower FAR reduce the primary equivalence ratio of the primary zone leading to lower flame temperatures. Improved fuel burn calls for a reduction in the amount of fuel required to deliver the desirable performance which again has an effect on NOx emission reduction.

The minor variations in EINOx among the candidate biofuels were a function of their fuel-caloric properties e.g. LHV and FAR as discussed in section 5.4.2.2. It is essential to note that this outcome was in line with the experimentally predicted ~1-5% reduction in NOx emissions observed from analysing 25% and 50% Jet-A1 blended Bio-SPKs [28] & [29]. Validation of EINOx for Bio-SPKs could only be compared with reference data mentioned above due to lack of further literature which in turn stems from the novel nature of the fuel studied.

An attempt to locate the engine operating with the candidate fuels on the CAEP-LTO/NOx charts was also made as presented in Figure 5-19. The inclination of OEMs towards development of engines with high OPRs stems from the benefit of lowering fuel consumption and subsequently reduced CO_2 emissions. However, higher OPRs contribute to increased flame temperature leading to an increase in NOx emissions which is well acknowledged (further illustrated in section 5.4.4.2.1). To mitigate LTO/NOx CAEP-NOx regulation was conceived in 1986 by CAEP, a subcommittee of ICAO. These standards are renewed every 4 years and any new aircraft that aims to enter commercial service will have to qualify this certification process.

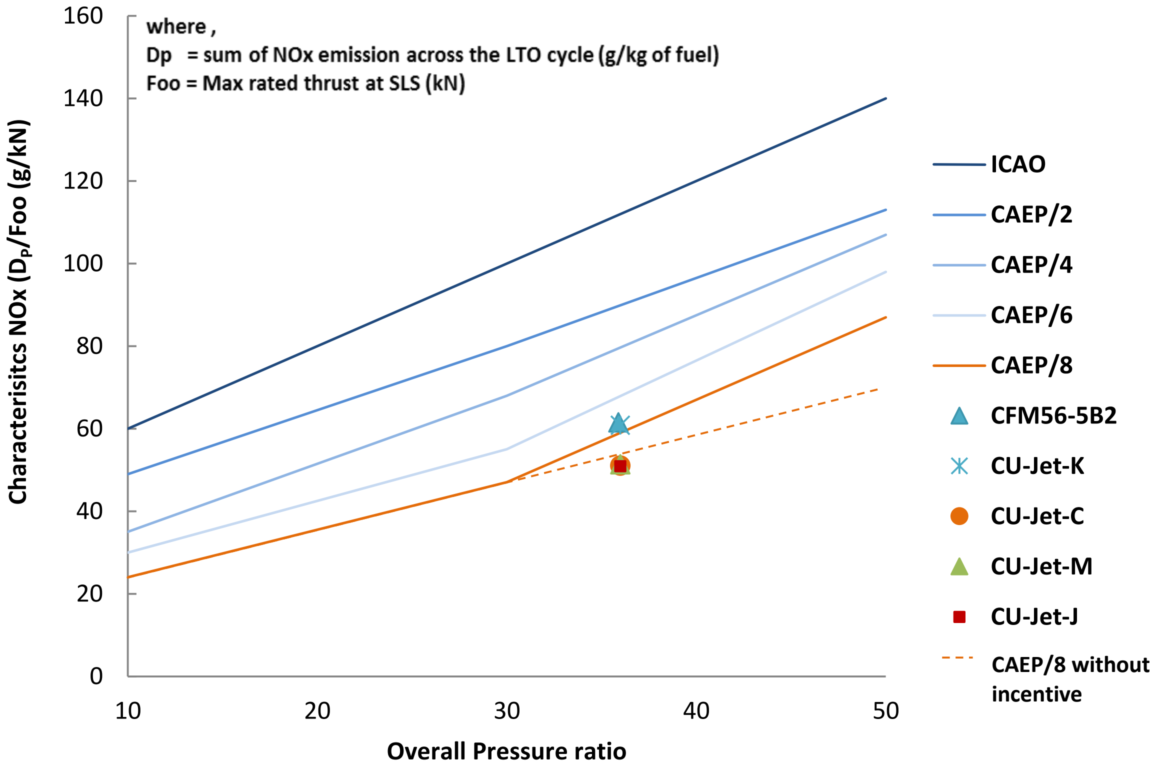


Figure 5-19: Location of candidate engines on the CAEP-LTO NOx chart

The conception of such a standard has aided the reduction of LTO-NOx emissions by an average of 55%, relative to aircraft that were operational 40 years ago. One may notice a kink on CAEP/4 regulation which permits a slight flexibility to engines operating at OPRs higher than 30. This kink is an incentive for engines that deliver better fuel economy from increased OPRs. The parameters considered for identification of engines on the CAEP/LTO-NOx chart are the Overall Pressure Ratio (OPR) and Characteristic NOx (D_p/F_{oo}). Characteristic NOx is defined as the ratio of the sum of NOx emissions produced across the LTO cycle (g/kg of fuel) and maximum rated thrust (kN) at sea level static conditions (Take-off mode). This study includes CAEP/8 regulation which came into force in January 2014 and has capped the CAEP/6 standards by an additional 11-14%.

The Bio-SPKs were able to demonstrate improved fuel burn and lowered characteristic NOx (Dp/Foo) emissions with no compromise on the overall pressure. It is essential to note that the characteristic NOx emission determined for the candidate fuels is applicable only to engine's design OPR at ISA-SLS condition.

It is also evident from Figure 5-19 is that the engine operating with the Bio-SPKs would still qualify the LTO-NOx certification even without the incentive for fuel economy (kink on the CAEP/8). This ability of the Bio-SPKs is a valuable motivation to establish more stringent CAEP limits in the future thus encouraging the development of biofuel compatible aircraft and eventually the use of alternative fuels.

5.4.4.2.1 **Effect of Fuel Caloric Properties**

HEPHAESTUS calculates adiabatic flame temperature based primarily on fuel based properties (Lower Heating Value (LHV) and Fuel Air Ratio (FAR)) and combustor inlet conditions [31]. The CAEP-LTO NOx chart presented in Figure 5-19 clearly indicates that the Bio-SPKs deliver lower LTO-NOx with no compromise on the OPR of the engine. This infers that the CU-Jet engine operating with the biofuel candidates and the reference fuel are operating at the similar inlet conditions (T&P) and the combustor inlet temperature and pressure are constant in both the cases. The constant OPR between the engines operated with Bio-SPKs and Jet-A1 (due to fixing of net thrust) results from the better fluid characteristics (relatively higher gas density and viscosity that helps the engine not compromise on its power output).

Adiabatic flame temperature is mainly influenced by the combustor inlet temperature and pressure. At higher engine OPRs, the temperature and pressure ratios across the compressor will be relatively higher than the same engine operating with lower OPR. Increased combustor inlet temperature may boost the combustion efficiency, but also contributes to formation of NOx through Thermal NOx mechanism. Similarly at high pressure conditions, their formation of NOx emissions appears to have a square root dependence on pressure.

The Bio-SPK-operated engine, in this virtual scenario, has a combustor inlet temperature and pressure similar to that operated with conv.jet fuel. However, the relatively lower FAR_{stoic} of the biofuel candidates creates a low equivalence ratio atmosphere across the length of the combustor thus resulting in lower adiabatic flame temperatures and subsequently lowered NOx emissions.

5.4.4.3 Estimation and Significance of Cruise NOx

As universally accepted, a given aero-engine is expected to operate at cruise mode for the longest period of its mission profile. Cruise mode is therefore as prominent as the LTO cycle with medium and long range flights. This significance stems from the amount of fuel consumed and resulting emissions. Currently there are no metrics available for the engine specific estimation of cruise NOx, unlike that of LTO segments, owing to the difficulty involved in measurement or modelling of this phenomenon at higher altitude and its dependency on “difficult to predict” local ambient conditions or weather patterns. The technical module, however, has made a preliminary attempt to estimate cruise NOx and determine its significance from user-defined medium-range mission.

The medium-range mission NOx attributable to LokAir-K, LokAir-C, LokAir-M and LokAir-J have been graphically presented in Figure 5-20. The scenario considered for the preliminary estimation of cruise NOx was obtained from medium-range mission fuel burn estimates for CU-Jet-K, CU-Jet-C, CU-Jet-M and CU-Jet-J.

From this assessment, fuel burn at cruise mode was estimated to be ≈12,000kg which accounts to 58% of total fuel carried by the LokAir. It is evident from Figure 5-20 that cruise NOx become significant in terms of levels of production and the environmental impact (i.e. depletion of stratospheric ozone) at higher altitudes. The Bio-SPKs were able to deliver savings in mission level NOx emissions in the range of 15-19% relative to that of Jet-A1. This phenomenon is once again a twin effect of lowered adiabatic flame temperature and reduced fuel requirements to cover the desired mission range.

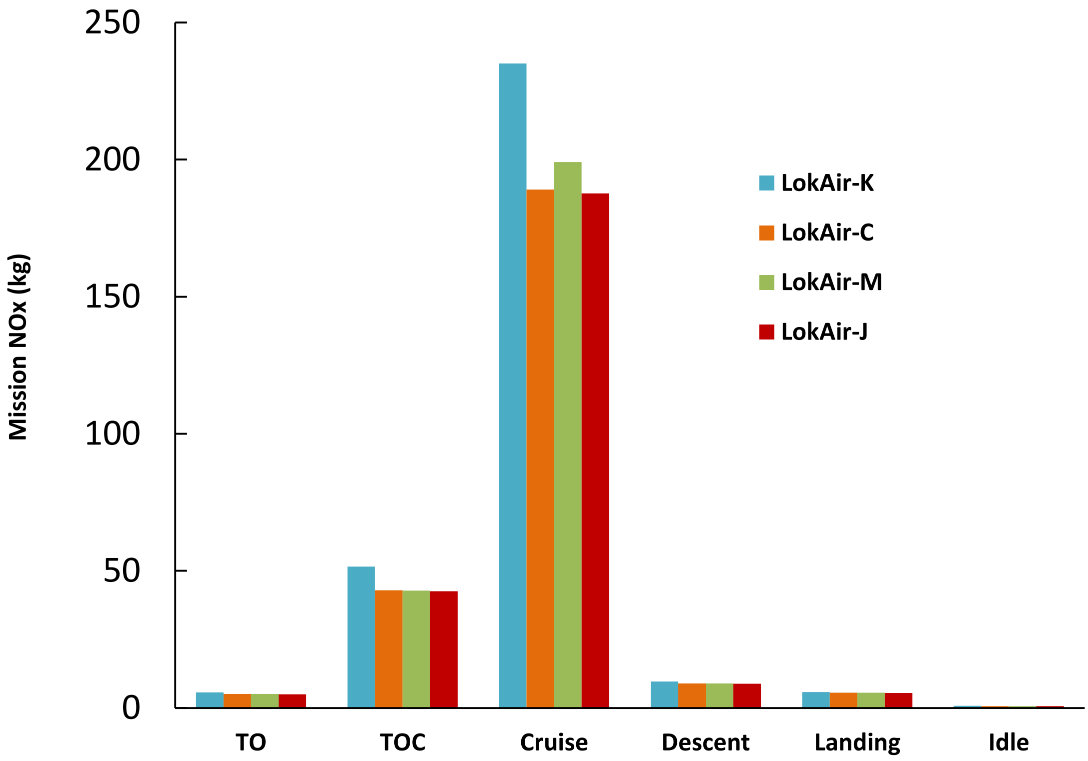


Figure 5-20: Comparison of Mission level NOx between LokAir operated with Bio-SPKs and Jet-A1

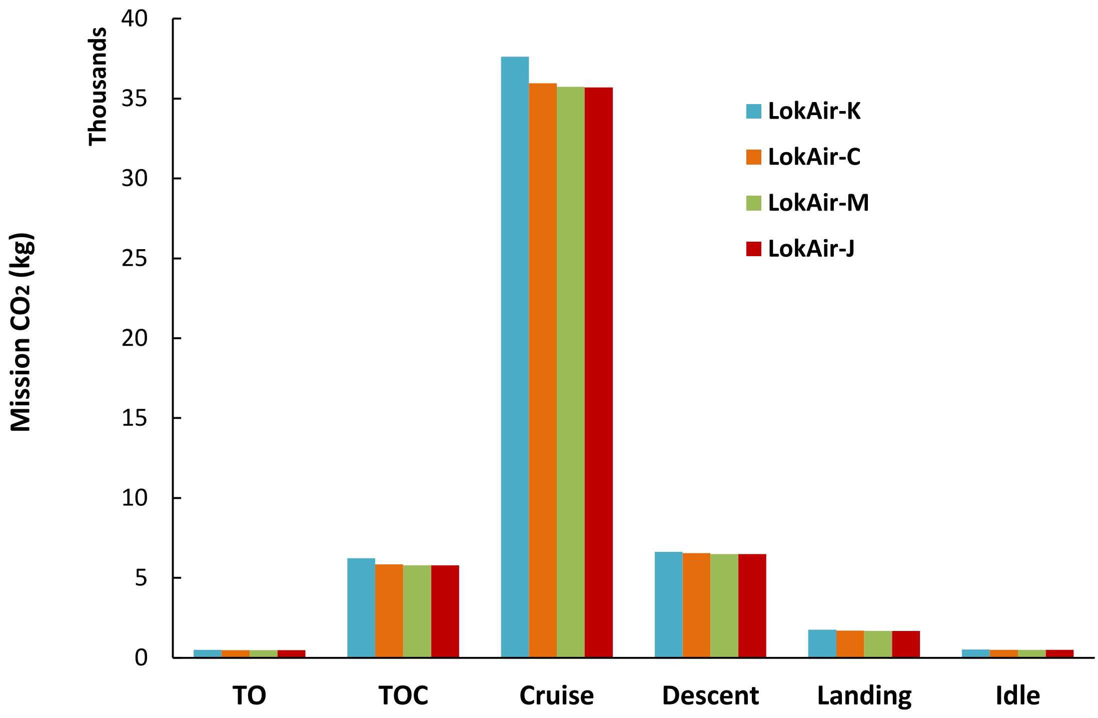


Figure 5-21: Comparison of Mission level CO_2 between LokAir operated with Bio-SPKs and Jet-A1

5.4.4.4 Estimation of CO_2 emissions

The degree of CO_2 emissions is assumed to be directly proportional to the fuel flow in a given engine. CO_2 emission resulting from LTO and cruise mode of CU-Jet engine coupled with their % difference in relation to Jet-A1 has been presented in Appendix I. The outcome has also been addressed in the corresponding LCA unit of gCO_2/MJ of fuel. This is the most common functional unit used in life cycle emission studies to estimate the environmental impact of a given fuel. Carbon savings delivered with the use of Camelina SPK, Microalgae SPK and Jatropha SPK have been presented in Table 5-15.

It is essential to note that these CO_2 emissions were estimated as average figure over the entire flight profile. This data was essential to systematically ascertain the empirically predicted combustion based CO_2 emission from ALCEmB model. The combustion emissions were certainly observed to be less than 0.5% deviated from that predicted through ALCEmB. The % difference in CO_2 emission that were calculated between the ALCEmB based empirical method and that of HEPHAESTUS were >0.3%

Fuel Type	% Diff in H/C ratio	% Diff in fuel burn	CO_2 emission (Cruise mode*)		ALCEmB based CO_2	% Diff between HEPHAESTUS and ALCEmB
			g CO_2/kg of fuel	gCO_2/MJ of fuel	gCO_2/MJ of fuel	
Jet-A1	-	-	3150.0	73.2	73.0	+0.28
Camelina SPK	+11.3	-3.7	3131.1	71	71.0	0.0
Microalgae SPK	+9.6	-3.1	3137.0	72.1	72.0	+0.1
Jatropha SPK	+13.0	-3.8	3127.6	70.8	70.6	+0.28

Note:

*An aircraft engine operates the longest at cruise mode and thus was chosen as the reference point for determination of CO_2 emissions

Table 5-15: Comparison of CO_2 emissions from LokAir operated with the candidate fuels

CO_2 emissions released over the medium-range profile of LokAir when operated with the different fuel candidates has been presented in Figure 5-22. Mission level emission estimation has indicated that LokAir-C, Lokair-M and LokAir-J deliver an overall mission level carbon saving of 6.2%, 5.8% and 6.3% relative to LokAir-K. CO_2 emission attributable to each mode of aircraft mission profile has been tabulated in Appendix I. The drop in CO_2 emissions is a twin effect from lower carbon content of the fuel coupled with improved fuel burn thus leading to fuel savings.

5.4.4.5 Estimation of H_2O emissions

Water vapour released by jet engines at cruise altitudes has captured as much attention as NOx emissions owing to its potential to heat up earth's surface though its effects are short lived. Water vapour released at upper troposphere causes an increase in earth surface temperatures through formation of contrails (condensation trails). Contrails are anthropogenic cloud formations resulting from quick freezing of water vapour around a condensation nuclei (soot particles). Contrails have the capacity to trap long wave radiations emanating from earth surface than reflecting such radiations back into space which is termed positive radiative forcing. It is essential to understand that these effects are persistent as the contrails are intact. Paoli et al, (2004), [100], Formation of Contrails and subsequent cirrus clouds is influenced by local atmospheric conditions and the fuel type used [145]. Bio-SPKs, chosen for this study, are subjected to a brief qualitative analysis on their contrail forming potential.

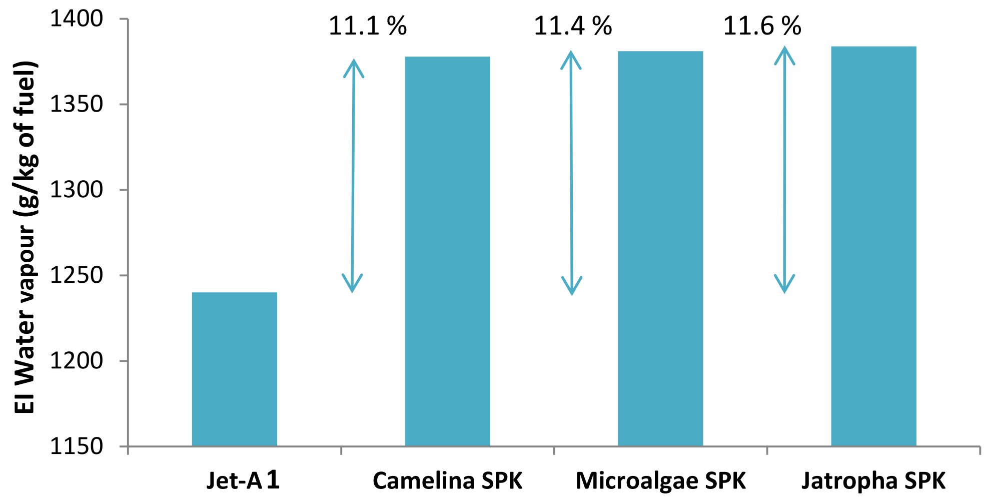


Figure 5-23: Estimated H_2O emissions for Bio-SPKs and % difference relative to Conv.Jet

Water vapour emissions from Bio-SPKs were determined to be significantly higher by an average of 11.4% relative to the reference fuel. With the consideration of direct conversion of a fuels hydrogen content to water vapour, an increase in water vapour emission was observed with the Bio-SPKs due to the 9% higher hydrogen content of the Bio-SPK, relative to that of Conv.jet fuel.

5.4.4.6 Environmental Impact of Contrails and its cirrus clouds

Efforts to understand the microphysics of contrail formation and to determine ways to mitigate the same have been carried out by the scientific community for decades [53], [91] & [100]. The environmental impact of water vapour at lower altitudes (LTO cycle) is minimal owing to comparatively warmer temperatures at sea level static conditions. However at cruise conditions (upper troposphere) a power setting at which the engine operate the longest and where the static temperatures fall below -50°C, sudden cooling of this by-product results in the formation of super cooled water particles called as condensation trails. These trails form cirrus clouds the ability of which to remain intact is influenced by the local weather conditions. Contrails dissipate with ease in dry weather conditions or will be retained in saturated conditions [48].

In general, any fuel with higher hydrogen content is expected to produce higher water vapour emissions thereby increasing the prevalence of contrail formation. However, Noppel, F.G, (2007), has delivered a simple equation to predict the contrail forming potential of fuels based on fuel based properties as mentioned below

$$\textit{Contrail forming potential} = \frac{EI_{H2O}}{LHV} \quad \text{Eq 49}$$

Where, EI_{H2O} = *water vapour emission index (g/kg fuel)*

LHV = Lower heating value of the fuel (MJ/kg)

Lower CFP implies to lesser contrail forming potential. Bio-SPKs were predicted to contain slightly higher potential at contrail formation compared to our reference fuel with an average value of 31.1 g/MJ as opposed to 28.9g/MJ of given fuel. It is however, essential to note that the environmental impact of contrails stems from aerosols and soot emission index which induce the initial formation of condensation nuclei. Since we are considering neat Bio-SPKs, the lack of sulphur content leading to reduction of aerosols in the exhaust has to lead to lower incidence of contrail formation.

5.4.4.7 Estimation of Total Mission Emissions

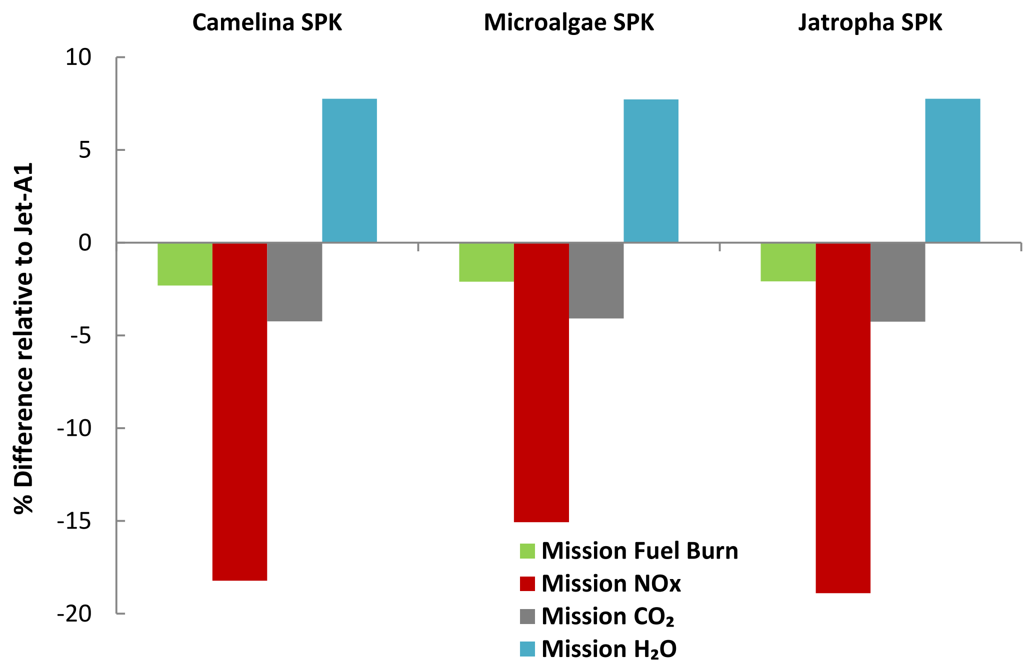


Figure 5-24: Difference in selected mission level emissions among the three Bio-SPKs relative to Jet-A1

Mission level emissions attributable to each of the Bio-SPKS were predicted from medium-range mission performance analysis with the virtually modelled aircraft, LokAir. The detailed tabulation of emissions estimated for ICAO specified power settings were used to calculate the overall mission related emissions [provided in Appendix H]. It is essential to note that the quantities, fuel burn and emission attributable to the mission level performance have been measured in kilograms. A graphical representation of the missions based quantities have been presented in Figure 5-24 and tabulated in Table 5-16.

Fuel Type	Mission Fuel burn (kg)	% Dif	Mission NOx (kg)	% Dif	Mission CO_2 (kg)	% Dif	Mission H_2O (kg)	% Dif
LokAir-K	16324	-	309	-	53263	-	20611	-
LokAir-C	15720	-3.7	252	-18.2	49960	-6.2	22474	7.8
LokAir-M	15817	-3.1	262	-15.1	50173	-5.8	22205	7.7
LokAir-J	15703	-3.8	250	-18.9	49907	-6.3	22211	7.8

Table 5-17: Total emissions from LokAir operated with the candidate fuels

5.5 CONCLUSION

The engine performance evaluation of CU-Jet, numerically modelled two-shaft turbofan engine, operated with the fuel candidates Camelina SPK, Microalgae SPK and Jatropha SPK against that of conv.jet fuel, was undertaken. The outcome of this analysis was measured as specific fuel consumption at fixed thrust rating. It was observed that the thermodynamic influence, imparted by the Bio-SPKs, on the performance of CU-Jet manifested as savings in fuel flow and consequentially as a reduction in engine SFC. Camelina SPK, Microalgae SPK and Jatropha SPK delivered a reduction in SFC by 1.78%, 1.75% and 1.8%, which was influenced by an average drop in fuel flow by 1.6%. Influence of fuel specific characteristics, primarily the lower heating value (LHV) and the Fuel-Air ratio (FAR) were determined to have significant impact on fuel consumption characteristics of the engine. The engine level assessment was zoomed out to mission level evaluation through user-definition of a fixed flight profile to determine the mission fuel burn specific to each of the fuel candidates.

The mission fuel burn delivered by LokAir, when operated with Camelina SPK, Microalgae SPK and Jatropha SPK was determined to deliver 3.7%, 3.1% and 3.8% reduction relative to that of Jet-A1.

These observations infer that the Bio-SPKs are capable of delivering fuel savings in the range of 3.0-3.8% relative to conv. jet fuel. However, a study to assess the degree of fuel economy achieved with a short and long range mission must be undertaken to fully comprehend their ability at fuel savings.

“Cradle-Grave” GHG emission analysis of Bio-SPKs, [Chapter 3] showed an avg. 60-70% reduction in life cycle emissions relative to that of, Conv.Jet fuel. However, for the purpose of ascertaining their systemic combustion emissions [highest LCE contributor, ≈70%], technical assessment entailing engine/ aircraft performance with the candidate fuels was undertaken. This outcome paved way to analyse Bio-SPKs from the context of systems level emission assessment through a representative virtual experiment.

Combustion emissions were predicted and quantified with additional importance to CO_2 and NOx emissions. It was determined that Bio-SPKs lowered LTO-NOx emissions by 7.1-8.3% without a compromise on engine performance. Consequently, at medium-range mission based emissions analysis, Camelina SPK, Microalgae SPK and Jatropha SPK were able to reduce their NOx emission by 18.2%, 15.1% and 18.9% respectively, relative to Jet-A1. The reported reduction in CO_2 emission was 6.2%, 5.8% and 6.3%, respective fuel candidates. However, there was an increase in water vapour emissions resulting from combustion of Bio-SPKs increasing their contrail forming potential. On an overall basis, the level of pollutant (except water vapour) formation was the lowest with Jatropha SPK among the fuel candidates. Aviation CO_2 emissions released from fuel combustion were almost similar (<0.28% difference) to the figures empirically predicted through ALCEmB.

6 SIGNIFICANCE OF FUEL PROPERTIES OF BIO-SPKS – A Qualitative Discussion

The "Drop-in" nature of the Bio-SPK implies that it can be incorporated in its pure composition into existing aero-engines without the need for mechanical modifications. On the other hand, any discrepancies observable in their performance properties may not be acceptable for aero-engines, unlike land-based gas turbines for energy generation and propulsion. Fuel compatibility with the existing engine scheme is a crucial techno-economic determinant to both the engineers and stakeholders. Fuel-engine incompatibility will only prove to be cumbersome demanding redesign, optimisation of the entire engine scheme, increased maintenance costs, consequentially affecting reliability and passenger safety.

There are inter-continental regulatory bodies which lay down standards and specifications for aviation fuel upon extensive visual, laboratory and site based evaluation. Some key examples of these authorities are ASTM (American Standard for Testing and Materials) and DEF-STAN (UK Defence Standards). Novel alternative fuels that are aimed for aviation purposes have to pass through a set of standard assessment through these regulatory bodies to be qualified for their commercial use. Among a range of performance and thermal properties tested, there are certain essential bench test properties which are prioritised as first-line specifications. They can be broadly classified into handling and combustion properties. Handling properties corresponds to the physico-chemical characteristics of a given fuel which are of significance to processes involving transportation, pipeline transfer and storage up to the point of fuel injection in an aero-engine. Some of the main handling properties discussed in this chapter are as follows

- Aromatic content
- Fuel Density
- Fuel Viscosity
- Freeze point
- Fuel Lubricity

- Vapour Pressure
- Flash Point

Combustion properties, as suggested, correspond to the caloric properties of the fuel which are significance to its oxidation. Key combustion properties which are qualitatively assessed here include

- Fuel Calorific Value
- Spontaneous Ignition Temperature

Bio-SPKs (also called as Hydrotreated Renewable Jet (HRJ), are synthesised through Hydrotreatment, a process where the plant lipids are pressurised with excess hydrogen in the presence of a multifunctional catalyst at varying temperature and pressure conditions. This process consequentially improves the hydrogen content of the final jet fuel fraction, thus boosting its lower heating value. It is essential to note that any variation in the performance and thermal properties of the Bio-SPKs, discussed in the upcoming section, are in relation to their fossil-derived counterpart, Jet-A1. An increase in the hydrogen content of the fuel is likely to reduce fuel density and leading to variations in their thermodynamic behaviour. In-depth evaluation of Bio-SPKs performance properties can be comprehended only through bench-test and experimental analysis. However, a qualitative attempt to appreciate the effect of fuel composition on their performance properties has been made.

6.6.1 Aromatics Content

Prior to approval for commercial deployment, Bio-SPKs have been rigorously scrutinised from laboratory scale bench test through to rig and flight tests. Bio-SPKs have been determined to clear most specifications except that of aromatic and fuel density. A fuel's aromatic content causes the rubber seals used in the high pressure fuel system to swell thus preventing fuel leaks during operation at various altitudes. Therefore, ASTM D1319 specifies that aviation fuels must contain a minimum of 8% by volume of aromatics for qualification into commercial use.

Bio-SPKs contain insignificant or no aromatic content in their pure composition. There are three kinds of seal materials currently in use: fluorosilicone, fluorocarbon-O rings and Nitrile compounds. According to an experimental reference quoted by Lefebvre and Ballal, (2010),

[83], 50% Bio-SPKs (blended with JP-8 to increase aromatic content by 7% by vol.) showed no effect on the Fluorosilicone and Fluorocarbon-O rings, but created satisfactory volume swell with nitrile rubber. Lack of aromatic content in Bio-SPKs is therefore a major limitation towards consideration of higher blend percentages. This limitations could cause fuel leaks and coke depositions due to kinetic heating and eventually higher maintenance costs. The newer fleet of aircraft may adopt state-of-the-art elastomers which may be biofuel compatible. Since, the regional aviation fuel standards are generalised for the global fleet of carriers, these specifications must be met by any alternative fuels aiming for approval. It is also essential to note that these fundamental/ historic specifications for the aviation fuel approval is currently under review and will be revived towards the newer fleet of aircraft to pave way for deserving sustainable fuel candidates. In view of the shortcoming at compatibility with hardware specifications and to ensure the operability of the fuel systems of aircrafts, Bio-SPKs have been currently approved for commercial use to a maximum of 50% blend with conventional aviation fuel.

In terms of advantages from handling perspective, lack of aromatics in the Bio-SPKs provides them ideal storage and handling specifications in addition to lowered emissions of volatile organic compounds from fuel combustion. Tin Conv. fossil derived fuels, double-rings in the aromatics become unstable upon prolonged exposure to varying temperatures degrades and results in the formation of “gums” which settles in the fuel tanks and fuel line obstructing fuel flow [106]. This issue if eliminated from renewable jet owing to their lack of aromatics.

6.6.1 Fuel Density

Fuel Density defined as the mass per unit volume of the fuel (kg/L of liquid fuel and kg/m^3 for gaseous fuel). This is a key bench test property that is defined by the fuel composition. Different fuels (Hydrocarbons) possess different H/C (Hydrogen/Carbon) ratios and simply, a fuel with higher H/C ratio is likely to be less dense. This behaviour is dictated by the hydrogen component which is less dense than carbon.

Fuel Density is a key handling parameter which is significant from the pipeline transfer to the storage facilities of a fuel’s life cycle process. Fuel pump pressure, storage, aircraft fuelling procedures and more importantly, capacity to contribute to chosen range of destination in addition to sufficiently being accommodated in a fixed fuel tank are crucial factors dictated by fuel density. Fuel density plays a significant role in fuel line/pumps right onto pre-combustion phase such as the formation of fuel droplets. Combustion efficiency which is defined by the fuel evaporation, mixing and reaction rate as presented in eq 50 is dependent on many factors and mainly fuel density.

$$\boldsymbol{\eta_{Comb}} = \boldsymbol{f(airflow\ rate)^{-1}}\left(\frac{1}{evaporation\ rate}+\frac{1}{mixing\ rate}+\frac{1}{reaction\ rate}\right)^{-1} \quad \textbf{Eq 50}$$

Fuel density also influences a number of other fuel factors including LHV, viscosity, H/C ratio, surface tension and is influential on combustion efficiency in terms of fuel atomization and consequently mixing/ evaporation rates. This property is of vital significance to fuel spray characteristics (spray penetration, droplet size and eventually mass-flow rate of evaporated fuel) which is crucial to the concentration of fuel vapour in the vicinity of the flame-front and primary zone. Improved fuel atomisation improves evaporation and mixing rate thus having a positive impact through ignition enhancement.

It is evident from specifications indicated in Table 6-1 that Bio-SPKs are less dense compared to the reference fuel, Jet-A1 (8% less dense ±1%). Bio-SPK is capable of increasing the gravimetric energy content of a fixed fuel tank. However, it is essential to know that the fixed capacity of fuel tank filled with less dense fuel leads to lower volumetric energy content of the same. This leads to a loss in obtainable range, as demonstrated in section 5.4.3.2. In order to meet the specification for fuel density in accordance to ASTM D4052 and DEF-STAN IP 365, Bio-SPK had to be blended with Conv.Jet fuel in 50/50 ratio. The lower density of the Bio-SPKs is again a major limitation in their consideration for higher % blend. In order to accommodate the less dense 100% Bio-SPKs, the upcoming fleet of aircraft will have to be biofuel compatible and require certain modifications which include fuel tank re-design. This modification can have technical implications such as increase in aircraft weight and eventually drag which in turn can take a toll on fuel burn. An evaluation of this nature was not conducted in this study since it lies outside the scope of this study, however, would be a valuable addition to existing literature, if undertaken.

6.6.2 Fuel Viscosity

Fuel viscosity defines the flow characteristics of a given fuel. Fuel viscosity is an important handling property which plays a crucial role in fuel transfer through pump lines during fuel transportation, storage and aircraft fuelling. On the other hand, fuel viscosity dictates pump pressure required to facilitate fuel transfer through fuel lines (desirably without creating air-locks) and mainly on the fuel injection system. Fuel viscosity at pre-combustion phase determines the fuel spray characteristics, rate of evaporation and mixing, creating sufficient fuel-air mixture for ignition which in turn defines the combustion efficiency. Simply put, highly viscous fuel degrades combustion efficiency only to result in relatively larger fuel droplets thus increasing incidence of incomplete combustion products such as CO, soot and particulates.

Viscosity of a given fuel is highly dependent on fuel temperatures, which is crucial to aero-engines operating at very low ambient temperatures. As universally acknowledged, fuel viscosity is inversely dependant on temperature and therefore, the cold characteristics of a given fuel must be well assessed. According to an experimental examination conducted by Boeing [107], the viscosity of blended and 100% Bio-SPKs (measured at -20°C) was determined to be in the range of 3.33-3.6 mm^2/s. This viscosity of the Bio-SPKs were well below the jet fuel specifications listed for Jet-A1 and blending Bio-SPK with Conv.Jet fuel (50/50) only seemed to reduce the viscosity of the mixture. This property is advantageous in terms of assuring the acceptable levels of fluidity at low ambient temperature conditions (during cruise).

6.6.3 Freeze Point

Among the four cold bench tests, Freeze point analysis is the most realistic determinant of fuel solidification point. Freeze point can be defined as the temperature at which a stirred fuel sample begins to precipitate a cloud of wax crystals on cooling which immediately disappears on warming [54]. This test is to identify the threshold of fuel liquidity at low temperature conditions (as in flight mode) and this is a crucial flight safety parameter as well. Some fuels which are relatively viscous than jet fuels may tend to solidify at relatively higher temperatures than jet fuel variants. Such fuels are capable of clogging fuel injectors leading to coke deposits (clogged pipelines) or affect the atomisation process itself, degrading the overall combustion efficiency.

With respect to the Bio-SPKs the lower density and relatively lighter composition of the fuel (higher hydrogen content) advantageously renders the alternative fuel tolerant to relatively lower low-temperature threshold compared to jet fuel.

6.6.4 Fuel Lubricity

Fuel Lubricity defines the ability of a given fuel surface boundary to interact with surface material (mostly hardened steel) without causing wear and tear over a period of time. Any new fuels are assessed against the reference fuel Jet-A1. Finished product, Jet-A1, contains sufficient amount of sulphur (derived from the refining process) to aid its lubricity within the engine fuel systems. However, lack/negligible amount of sulphur in Bio-SPKs (<0.0003% by mass) does not deter the Bio-SPKs from exhibiting its sufficiently lubricious characteristics. Further to the above observations and despite lower fuel viscosity, the benchmark fuel pump pressure (Jet-A1) required to circulate the fuel through the line was observed to remain unaffected [127].

6.6.5 Vapour Pressure

Vapour pressure of a given fuel is a measure of the degree of fuel volatility and this property plays a vital role in transportation of a fuel to storage facilities, refuelling an aircraft through to the fuel injection. Vapour pressure is defined as the absolute pressure exerted by a given fuel at standards temperature (37°C). Vapour pressure is mainly a handling property governed by the fuel density. In terms of denser fuels, the heavier molecules of the hydrocarbon construct tend to be less volatile thus exerting less pressure relative to less dense fuels. Vapour pressure is also fuel temperature dependent whereby the fuel volatility increases with temperature.

Fuel temperature in a standing system (fuel tank) is influenced by the mission characteristics such as mission altitude, climb rate and subsequently the aerodynamic heating of the engine system which without proper measures could lead to fuel reaching boiling temperatures. This is generally mitigated through use of a fuel pressure venting system or pressurising the fuel tanks to absolute pressure (in excess of vapour pressure) to prevent fuel wastage from venting losses. Formation of potential vapour locks in the fuel lines and injection system could affect pump pressure and eventually blow-out which makes vapour pressure an important qualification criteria in terms of passenger safety consideration.

Bio-SPKs are less dense resulting from relatively lower Initial Boiling Point (IBP) alternative fuel variants. Bio-SPKs are expected to exhibit higher vapour pressure relative to the reference fuel, Jet-A1 [Figure 6-1]. In addition to this observation, laboratory based vapour pressure measurements by Kinder and Rahmes (2009) reported similar observations [107]. Use of low vapour pressure fuels (Bio-SPKs) in engine systems that were built around reference fuel specifications can prove to be technically challenging. For instance, the vapour vent requirements for Bio-SPK's vapour lock formations may lead to fuel evaporation losses and eventually aircraft safety issues respectively.

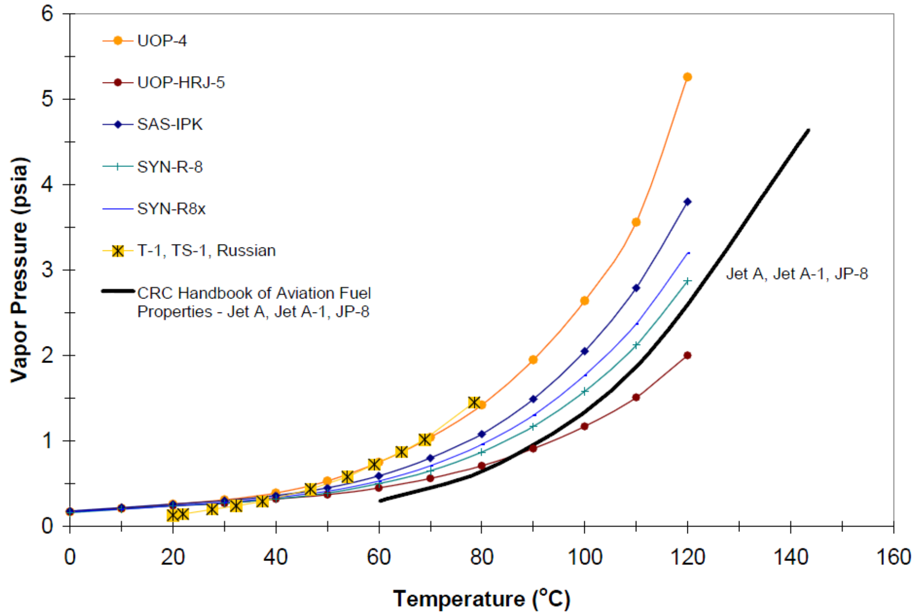


Figure 6-1: Vapour pressure of 100% Bio-SPKs and FT-SPKs against reference fuel (Jet-A1) [107]

From combustion perspective, high volatile fuels can evaporate faster upon atomisation boosting combustion efficiency. This accounts for the lower FAR of the Bio-SPKs (FAR_{stoic} range 0.0675-0.0677) relative to that of conventional jet fuel (0.068). The lean burn benefit of Bio-SPKs is advantageous in terms of fuel savings over an established flight trajectory. However, modifications to the fuel metering system (altitude and acceleration sensory units [57]) may be required in order to maintain the optimum flammable mixture limits for the Bio-SPKs in order to prevent blowouts or eventually successful altitude relights.

6.6.1 Thermal Stability

Thermal stability tests are predominantly conducted to determine the maximum temperature at which the fuel begins to degrade and develop carbonaceous deposits. Thermal stability is a key handling property for a given fuel which is of significance to bulk storage in the fuel tanks and flow through the fuel lines (coking from kinetic heating due to flight's forward speed). Blockages in the fuel lines could affect the fuel flow into the injection system; result in formation of coke deposits thus increasing the requirements for checks and shop-maintenance. Thermal stability is a function of the fuel density where denser fuels (due to lower levels of volatility) tend to degrade and form coke deposits. Bio-SPKs, with their relatively lower densities form coke deposits at higher temperatures compared to the reference fuel Jet-A1.

6.6.2 Flash Point

Flash point is an important fuel handling (fire safety) characteristic with significance to fuel transportation and refuelling procedures. Flash point of a fuel is defined as the temperature at which the vapour above the liquid fuel forms sufficiently lean mixture to become flammable. This temperature can also be interpreted as the lean mixture of flammability which is generally quantified as fuel-air mixture of 1% [54]. This property which is fuel volatility dependant is a function of fuel density similar to that of vapour pressure. According to this principle, less dense fuels, in comparison to Jet-A1, are expected to have higher flash points which are concluded to be safer in terms of handling specifications.

6.6.6 Calorific value

Calorific value of a fuel is defined as the amount of energy (heat) released per unit mass of the combustion of a given fuel (MJ/kg). The calorific value of a given fuel is dictated by the fuel composition where fuels with higher H/C ratio increase the calorific value of a fuel. Use of highly calorific fuels in existing aero-engine (built around jet fuel specification), at constant TET, is likely to improve their thermal efficiency thus improving the thrust output. In economic and environmental sense, higher calorific value of the fuel can be interpreted to fuel and carbon saving respectively.

Bio-SPKs, as mentioned earlier, have higher hydrogen content which has subsequently shown a boost in their calorific value relative to that of jet fuel. The dynamic performance characteristics influenced by the fuel types on an operating aero-engine have been studied in detail and reported in section 5.4.

6.6.3 Spontaneous Ignition Temperature (SIT)

Spontaneous ignition temperature defines the high temperature threshold of a given fuel sample where the fuel ignites spontaneously when subjected to extreme heat. It is an important handling property which defines safety and fire hazards both during gate to refuelling phase of the life cycle process and within an operational aircraft. In terms of compositional influence, denser fuels (lower H/C ratio) fuels are likely to spontaneously ignite at higher temperatures. This behaviour is due to the ability of denser molecules to dissociate bonds with each other and re-associate with oxygen in air improving their chances for ignition. In terms of Bio-SPKs, which are less dense than the conventional jet fuel, the spontaneous ignition temperatures are relatively higher. The purpose of this section is to provide the reader a qualitative idea on the effect of fuel composition and thermal-physical properties on the handling, combustion and system operability capabilities of the alternative fuels under discussion against the baseline fuel (Jet-A1). Fuel properties of significance to application in aero-engine have been tabulated in Table 6-1.

Thermo-Physical Properties	ASTM Tests	Jet A/ Jet-A1	Camelina SPK	Microalgae SPK	Jatropha SPK	Units
Aromatics	D1319	25	0.3	0.0	0.0	%
Flash Point	D 3828	38	42.0	39	46.5	°C
LHV	D4529	42.8	44.1	43.2	44.3	MJ/kg
Viscosity @-20°C	D445	8.0	3.336	3.91	3.663	mm^2/s
Lubricity	D5001	0.85	0.76	-	0.76	mm
Hydrogen	D3345	13.96	15.1	15.2	15.5	% mass
Density @15°C	D4052	831	753	755.2	749	kg/m^3
Initial Boiling Pt	D86/D2887	165	162	130.9	164.5	°C
Final Boiling Pt	D86/D2887	265	251.2	296.7	254.9	°C
Freeze point	D2386	-43.5	<-63.5	<-48.6	<-54.5	°C
Sulphur	D1266	0.03	<0.0001	<0.0001	0.0001	% mass
H/C ratio *		1.952	2.176	2.174	2.178	
Empirical Form*		$C_{12.5}H_{24.4}$	$C_{11.2}H_{24.4}$	$C_{11.5}H_{25}$	$C_{11.2}H_{24.5}$	

Note:

***** Estimated from carbon distribution data (refer to [107] for further data)

Table 6-1: Thermo-chemical properties of candidate fuels of analysis

7 ASSESSMENT OF LIFE CYCLE COST OF BIO-SPKS Part I -Biofuel Pricing (ALCCoB-BP)

(Economic module)

7.1 INTRODUCTION

The performance and progress of civil aviation, or any other transportation sector, have been influenced by the efficiency of petroleum infrastructure for more than 6 decades. However, this capriciously complex business is currently facing challenges in terms of uncertainties in feedstock availability (from fast depleting crude oil deposits).

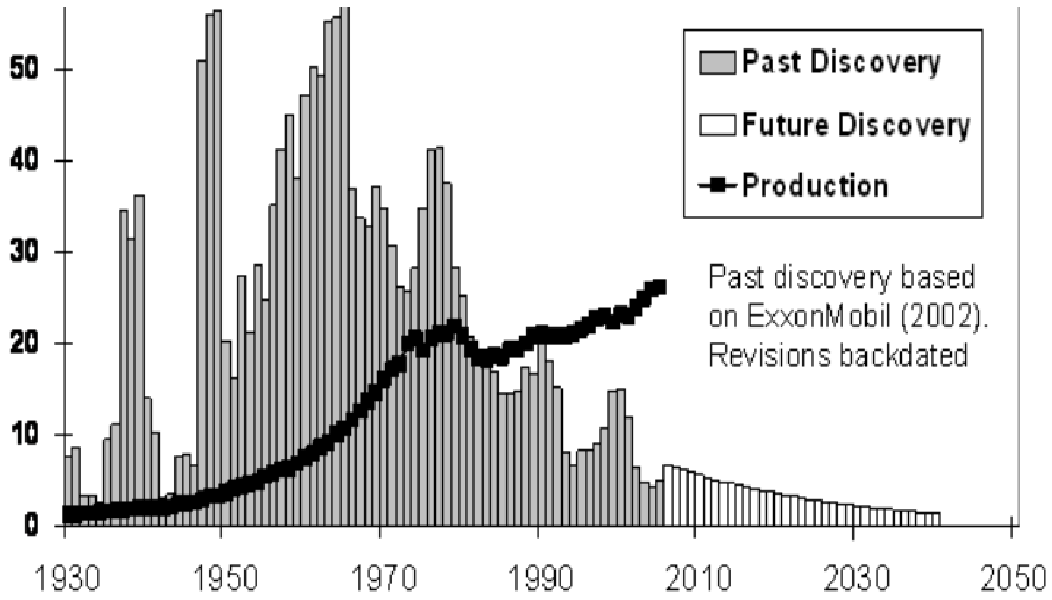


Figure 7-1: Global Oil Deposits as predicted by ExxonMobil (2002) [39]

Substitution of a well-established liquid fuel infrastructure with sustainable alternative fuels can be quite a challenging task. In-spite of their ability to reduce the "Cradle-grave" carbon intensity by 60-80%, their struggle to balance supply-demand equilibrium (stemming from its technological infancy), appears to make alternative fuels economically unsound.

7.2 LITERATURE REVIEW

The financial impact of deploying Bio-SPKs into the existing aviation infrastructure is a topic of immense interest with least number of studies. The reason for the rarity in such studies is the uncommercial nature of the biofuels in question and the high levels of associable uncertainties. These uncertainties include

- Price volatility of fossil derived energy
- Fluctuations in biofuel feedstock costs (influenced by differences in demand and supply)
- Variation in “feedstock to fuel” conversion efficiency

Among the uncertainties indicated above, price volatility of the fossil fuel is the most dreaded parameters for a financial analyst in the energy business. Two methods for hypothetical fuel price prediction were realised from consulting earlier literature. The first and common method of biofuel price prediction is quantification of material, energy and associated costs ([55], [72], [108] and [125]) and the second method is solely based on the energy intensity of the base commodities (feedstock) of the fuel product [30]. Studies following the first method largely focussed on the life cycle costs analysis assessing the risks and gains associated with investing into operation and maintenance of the biofuel plant and were based on an elaborate process-level techno-economic analysis. Other more simplistic empirical methods of price prediction is the Petroleum Intensity (PI) method [30] proposed by Cazzola et al, (2014) [30]. This method is based around the most important variable, the energy feedstock cost and is expressed as follows.

$$\boldsymbol{Input\ Cost}_{\boldsymbol{i}} = \boldsymbol{Base\ Cost}_{\boldsymbol{i}} + (\boldsymbol{PI}_{\boldsymbol{i}} \times \boldsymbol{PC} \times \Delta \boldsymbol{Pp}) \qquad \textbf{Eq 51}$$

where, *I = any feedstock ($/GJ of feedstock)*

PI = Petroleum Intensity of the feedstock (MJ/GJ of feedstock)

PC = Cost of Petroleum ($/MJ)

ΔPp = Change in Petroleum price from benchmark price ($60/bbl)

According to the PI method, the market price of the finished product is solely influenced by its petroleum intensity (feedstock production and transportation). Use of this method overcomes the uncertainties associated with price volatility. However, it is essential to note that among the three biofuel feedstock, two are assumed to be located in a developing country. With the PI method, regional rates of inflation and subsequent fluctuations in energy prices cannot be captured with the PI method. Adoption of the first method would improve the robustness of cost prediction in the current time period but will be time intensive and deviate from the scope of this analysis.

The aim of this economic module is to identify the financial competence of advanced biofuels when introduced into commercial use over at medium (2020), long-term (2050) and very long term (2075) periods, at varying environmental taxation and fuel price scenarios. ALCCoB (Assessment of Life Cycle Assessment of Biofuels) is a cost analysis model that has been developed to fiscally evaluate the advanced biofuels from two perspectives.

ALCCoB- BP (Biofuel Pricing) - To calculate the hypothetical market price of advanced biojet fuels.

ALCCoB-DOC (Direct Operating Cost) - To analyse and interpret the consumer level financial competency of the advanced biojet fuels.

The First part of the economic model ALCCoB-BP addresses the limitations commonly encountered in fuel pricing through the following approaches

- The cost of energy and material specifications are user-defined and therefore, these costs can be instantly factored into ALCCoB-BP
- “Feedstock-fuel” conversion efficiency corresponds to the plant production capacity. As in the earlier case, the plant capacity is calculated from the user-defined specifications.

The market price of conventional jet fuel can be fractioned and classified as follows: Cost of Crude Oil (52%); Refining Expenses (19%); Taxes (20%); Distribution and Marketing (9%). However, this study will not account the taxes attributable to fuel candidates since it would increase uncertainties into the cost predicted. In general, life cycle cost analysis is a method of quantifying the commercial feasibility of a given project. This work uses a similar approach, however, only to predict only the market cost. Therefore, this study will omit cash flow and present value analysis since it would deviate from the scope of the overall research.

Consultation of earlier literature concluded unavailability of any previous work on consumer-level economic feasibility studies of 100% Bio-SPKs. Therefore, this study has adopted a number of assumptions in addition to the contemporary method of aircraft's DOC estimation [20], [30] and [72]. In order to handle the uncertainties associated with these assumptions, rational sensitivity studies accompany the main analysis. Further reading into this section will assist the reader identify and rank advanced biofuels based on the fiscal saving they offer in a commercial backdrop of fuel costs and environmental taxations, relative to that of Conv.Jet fuel. This study contributes to the existing literature by developing a method of predicting hypothetical market prices of novel biofuels and their impact on the aircraft operating cost over a medium-range mission on medium (2020), long (2050) and very-long time (2075) periods. This is a novel element in this analysis since consultation of earlier available literature establishes that an elaborate analysis of such nature has never been conducted.

7.3 METHODOLOGY

Biofuel pricing is conducted through a Life Cycle Cost (Cradle-gate) model termed ALCCoB (Assessment of Life Cycle Cost of Biofuels). This model paves way for future studies where process based input specifications can be defined by the user for prospective biofuels to predict their cradle-gate costs (CGC) and eventually their market price. The costs of the inputs, equipment and its maintenance have been identified from market based information. As universally acknowledged, any life cycle cost assessment encounters uncertainties from fluctuations in the global commodity costs and therefore, costs attributable to the each of the feedstock have been fixed at Feb 2014, for this study. Though this study does not address all the uncertainties, fossil energy price volatility has been studied through sensitivity analysis which will be detailed in section 7.4.1. The upcoming sections will elaborate on the material, energy, machinery and process based costs for each of the Bio-SPK on a stage-stage basis.

7.3.1 Input Data- Commodity and Cost specifications

The Material and energy inputs specific to each of the three Bio-SPKS have to be fed into the ALCCoB-BP model. The components of the input specifications are mainly unit costs of commodities from the point of raw material generation (cradle) to the point of distribution and storage of the final product at its intended destination (grave). The list and cost of commodities were sourced from global trading websites, recently published government documents and regional energy trading websites [appropriate references listed in Table 7-1]. The cost of each of the commodities was converted to UK sterling pounds (£) accounting the conversion rate of $1= £0.603 (12th Feb 2014).

Commodities	Camelina SPK	Microalgae SPK	Jatropha SPK	Units	References
Marginal land	135.816	75.68	75.68	£/ha	[56], [72], [133]
Arable Land	694.29	326.7	326.7	£/ha	[56], [72], [133]
Tillage costs	36	0	24	£/ha	[56], [72], [133]
Seed costs	3.24	5.87	4.23	£/kg seeds	[52], [72], [95]
Fertilizers					[40], [47]
K2O	0.162	0.162	0.162	£/kg fert	
P2O5	0.2	1.2	2.2	£/kg fert	
Urea	0.078	0.078	0.078	£/kg fert	
Hexane	27.732	27.732	27.732	£/L	[147]
Diesel	0.87	1.87	1.87	£/L	[128] [132]
Electricity	0.03	0.08	0.08	£/kWh	[63], [128] [135]
Water	0.0012	0.0012	0.0012	£/kg	[99]
CO_2 supply	0.021	0.021	0.021	£/kg	
Hydrogen (Pathway)					
Natural gas	0.68	0.68	0.68	£/kg	[128]
Coal	1.836	1.836	1.836	£/kg	

Table 7-1: Regional commodity cost of Material, Energy and process inputs

7.3.1.1 Assumptions

It is essential to realise that ALCCoB-BP is used to predict just the gate cost (cradle-gate) of each of the Bio-SPK and not the feasibility of the operation and maintenance of the Cradle-Gate biofuel infrastructure. In support of this objective, this study incorporated the following assumptions

- Use of matured biofuel plantations and agricultural facilities (start-up costs have been excluded)
- The predicted market price of the Bio-SPKs is assumed to be not influenced by its supply-demand equilibrium. The productivity of the biofuel infrastructure is assumed to be constantly improving with technology maturity and expanding acreage of plantations. It is essential to note that the biofuel feedstock chosen for this assessment can be cultivated on non-arable

land. With the availability of ample acreage of non-arable land the assumption on expanding acreage [244 and 251], is considered valid.

- Overhead costs such as tax, maintenance fees, insurance and utilities have been evaluated but excluded from estimation of buying price since it hold its significance only towards evaluating project feasibility
- The market price of commodities listed in the input section are region-specific unit prices

7.3.2 Biomass Cultivation

The economic model ALCCoB-BP works in conjunction with the environmental model ALCEmB to access the life cycle inventory of each of the Bio-SPKs. The cost of material and energy inputs is calculated by accounting the temporal commodity prices specified by the user in commodity cost section. Distribution of the biomass cultivation Costs (BC) across the by-products of the Bio-SPKs is crucial to the objective of this analysis. BC_{Cost} (£/kg of Bio-SPK) is the sum of feedstock costs (starter seeds/culture, CO_2 costs), Energy Costs (Fuel and electricity costs), Labour cost and water supply cost and is represented as in Eq 52.

$$(\boldsymbol{BC_{cost}}) = \left[\frac{\boldsymbol{FC+EC+LC+WsC}}{\boldsymbol{BY} \times \left[\left(\frac{\boldsymbol{BcY}}{\boldsymbol{100}}\right)\times\left(\frac{\boldsymbol{Bio-SPK\ Conv.Eff}}{\boldsymbol{100}}\right)\right]}\right] \quad \textbf{Eq 52}$$

Where, BC = Biomass Cultivation cost (£/kg)
FC = Feedstock Cost (£/kg)
EC = Energy Cost (£/MJ)
LC= Labour Cost (£/year)
WsC = Water supply Cost (£/litre)
BY = Biomass Yield (kg)
BcY = Bio-crude yield (kg)
Bio-SPK Conv. Eff = Feedstock to fuel conversion efficiency (%)

Feedstock costs is the sum of costs involving purchase of starter seed/ culture costs, fertilizer/ pesticide, CO_2 supply costs (Microalgae) and land preparation (tillage) required for an area of 1 hectare. Energy cost is contributed by the use of diesel in equipment for land preparation, and electricity costs towards operation of facilities over an area of 1 hectare. The value for labour cost was cross-predicted with information indicated by [56] and [72]. Agricultural water supply costs are solely dependent upon the energy intensity of the pumping up the water from underground sources. It is essential to note that all the cost factors accounted in this study are region-specific since this study assumed Camelina to be cultivated in the Montana, IL, USA and Microalga and Jatropha to be cultivated in Tamil Nadu, India.

7.3.3 Biomass Harvest

The Biofuel plantation has to mature to produce oil-bearing seeds ready for the annual harvest. Similar to the approach used in ALCEmB, the cost incurred during the harvest process is influenced by its corresponding energy intensity. This includes the cost of fuel and electricity mix used for operating the harvesting equipment and storage in the case of Camelina. To harvest a hectare worth of stock of microalgae, two units of Disc centrifuge each of which consumes 1.04 kWh/kg of biomass were assumed to have been used. The equipment's energy consumption was obtained through personal conversation with online equipment sellers [115] and available online literature [71]. The manually harvested Jatropha fruits are sun-dried and the oil-bearing seeds are mechanically extracted. BH_{cost} is calculated as (£/kg Bio-SPK) presented in Eq 53. Biomass harvest costs are calculated as follows

$$(\boldsymbol{BH_{cost}}) = \left[\frac{\boldsymbol{HeC}}{\boldsymbol{BY} \times \left[\left(\frac{\boldsymbol{BcY}}{\mathbf{100}}\right) \times \left(\frac{\boldsymbol{Bio-SPK\ Conv.Eff}}{\mathbf{100}}\right)\right]}\right] \qquad \textbf{Eq 53}$$

where, BH Cost = Biomass Harvest Cost (£/kg)

HeC = Harvest Energy cost (£/MJ)

7.3.4 Biomass transportation

The Biomass harvested earlier is transported to the site of oil extraction and refining. The transportation costs incurred here is primarily from fuel (Low Sulphur Diesel) consumption. As assumed in the environmental module, the feedstock is assumed to be transported over a distance of 150km using medium-duty truck with a payload capacity of 5000 kg and an average vehicle mileage of 6km/L.

$$\boldsymbol{BT_{cost}} = \frac{\boldsymbol{Ds} \times \boldsymbol{Dc}}{\boldsymbol{BY} \times \left[\left(\frac{\boldsymbol{BcY}}{\mathbf{100}}\right) \times \left(\frac{\boldsymbol{Bio-SPK\ Conv.Eff}}{\mathbf{100}}\right)\right]} \qquad \textbf{Eq 54}$$

where, Ds = Diesel Supply (L)

Dc = Diesel Cost (£/L)

7.3.5 Oil Extraction

The Bio-Crude (plant oils extracted from the oil-bearing seeds) is extracted following the methods indicated in the environmental module. The oil bearing Camelina seeds are mechanically dehusked and the corresponding energy use were identified to be 0.215kWh/kg bio crude. On the other hand, Jatropha bio-crude is assumed to be extracted through the conventional screw press method which demands manual labour thus requiring no energy needs. Microalgae bio-crude is extracted through mechanical means. Initially, a sludge belt drier is used to dry the wet algal biomass which uses power generated using natural gas. The quantity of hexane fed into the extraction process is also accounted [72] and [119]. Oil Extraction costs are calculated as follows

$$\boldsymbol{OE_{cost}} = \left[\frac{(\boldsymbol{EC+SC+LC})}{\boldsymbol{BcY} \times \left(\frac{\boldsymbol{Bio{-}SPK\ Conv.Eff}}{\boldsymbol{100}}\right)}\right] \qquad \textbf{Eq 55}$$

where, OE_{cost}= Oil Extraction Cost (£/kg)

SC = Solvent Cost (£/L)

7.3.6 Hydrotreatment

The extracted Bio-crude is assumed to be directed towards Hydrotreatment. The essential feedstock of this process is the bio-crude and abundant supply of hydrogen. The fossil derived energy and hydrogen requirement demanded by the Hydrotreatment process are listed below and were sourced from works of reference [94], [123] [124] and [143].

Energy costs associated with the Hydroprocessing of bio-crude were calculated using the region-specific energy prices and the above mentioned information on process specifications. ALCCoB paves way for the user to define the unit cost of the final product (Bio-SPKs) as £/kg, £/L or £/gal of Bio-SPK.

Commodities	Quantity	Units
Electricity	1.2	kWh/kg bio-crude
Natural gas	6.5	MJ/kg bio-crude
Hydrogen	1.4	kg/kg bio-crude

Table 7-2: Energy Inputs for Hydroprocessing of Bio-crude

Hydrotreatement costs are calculated as follows

$$HT_{cost} = \frac{(ElC+NgC+HC+LC)\times\left(\frac{Conv.eff_{Hydrotreatment}}{100}\right)}{SPK_{yield}} \quad \textbf{Eq 56}$$

where, ElC = Electricity Cost (£/kWh)

NgC= Natural Gas Cost (£/MJ)

HC = Hydrogen Cost (£/MJ)

SPK_{yield} = Bio-SPK Yield (kg)

7.3.7 Fuel Transportation

The energy intensity of the Bio-SPKs transported from refining facility to the storage facility (located 150km away) follows a similar approach of assumption from the biomass transportation phase. In this case, the Bio-SPKs are transported using large tank trucks with a payload capacity of 4000 gallons and a mileage capacity of 6km/litre. Fuel Transportation costs are calculated as follows

$$FT_{Cost} = \frac{Ds \times Dc}{SPK_{yield}} \quad \textbf{Eq 57}$$

7.3.8 Market Price Estimation

The outcome of ALCCoB-BP, the market price of Bio-SPKs is calculated by summing all the costs incurred by the life processes. It can be represented as follows

$$Estimated\ Market\ Price\ of\ Bio-SPKs = BC_{cost} + BH_{cost} + BT_{cost} + OE_{cost} + HT_{cost} + FT_{cost} \quad \textbf{Eq 58}$$

7.4 RESULTS AND DISCUSSION

ALCCoB-BP, a numerical model was developed to predict the market price of Camelina SPK, Microalgae SPK and Jatropha SPK from a "cradle-gate" perspective. The market price was predicted as a function of input specification that include quantified material and energy inputs plus period-specific (temporal) commodity prices. The Market price of Camelina SPK, Microalgae SPK and Jatropha SPK were determined to be £0.86/L, £1.03/L and £0.915/L respectively. This market price was predicted using energy and other commodity prices specific to the period 02/02/2014. The average price of Jet fuel at this period was determined to be £0.82/L [130]. As evident, producing Camelina SPK is more economical when compared among the three Bio-SPKs and is only roughly 4p more expensive than conventional jet fuel in terms of £/kg. The energy use pattern of the two second generation Bio-SPKs was observed to be consistent. However Microalgae SPK was determined to be relatively more resource intense in the following aspects

- the existing cultivation practices of *Microalgae sp* is more energy intensive which is due to requirement of continuous agitation in the raceway pond.
- Most importantly, the CO_2 supply costs (specific only to Microalgae sp) also contribute to its high cultivation costs.
- Microalgae Cultivation in raceway ponds requires 40 times more fresh/marine water supply than its second generation counterparts.
- Requirement for sophisticated downstream processing technologies for dewatering and concentration of biomass makes microalgae energy intensive.

The life cycle cost intensity of the Bio-SPKs have been schematically represented in Figure 7-2. On the other hand, the cost of transporting microalgal biomass is relatively lower than that of the second generation candidates. The higher volumetric energy content of Microalgae SPK on the yield basis, transported between the processing sites is relatively higher and therefore contributes to lower energy consumption ratio in terms of fuel transportation. In relation to the various stages analysed, Hydrotreatment contributed the highest to the cradle-gate cost of the Bio-SPKs most of which is attributable to the major reactant, hydrogen and electricity supply costs for heat/ steam generation. The stage in the life process of Bio-SPK which follows

Hydrotreatment is Oil Extraction. With the Oil extraction procedure, the morphological specifications and high biomass productivity of the microalgal biomass demands the use of sophisticated downstream processing technology which are energy and labour intensive. For instance, in the current analysis microalgal biomass requires 850 kWh/yield of biomass relative to 124 kWh for Camelina seeds and 46.2 kWh for Jatropha seeds. Therefore, energy consumption, in the form of electricity plays a significant role in the influencing the market price of Bio-SPKs.

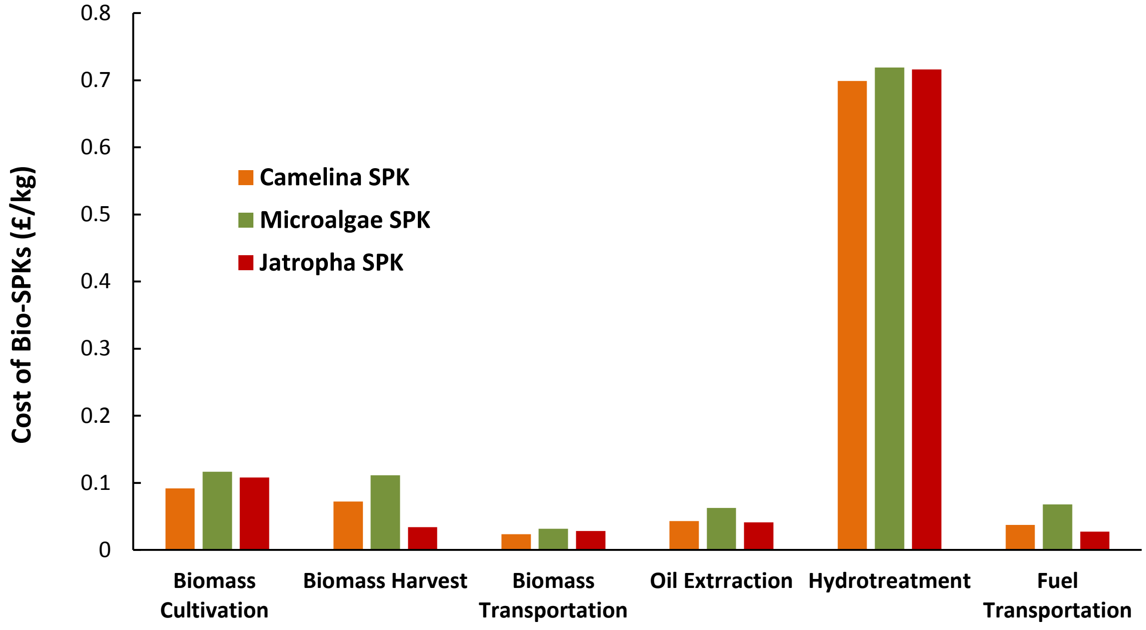


Figure 7-2: Life Cycle Cost breakdown of Bio-SPKs as calculated by ALCCoB-BP

7.4.1 Sensitivity Analysis

For this sensitivity analysis, ALCCoB adopted elements of the "Petroleum intensity method" from a study by Cazzola et al, (2014) [30] and evaluates the impact of price volatility of the energy feedstock on the final market price of the Bio-SPKs. The fossil energy sources considered in this analysis include the following mentioned below and the past price data for each of the commodity have been sourced from [128] and [135]

- Diesel (used for processes including field based operations, pumping underground water, feedstock transportation)
- Coal (for electricity generation)
- Natural Gas (choice of feedstock for hydrogen generation)

Uncertainty of future fuel prices is inevitable. This study was conducted through use of regional historic price fluctuations of the above mentioned feedstock classified as high, base and low Fossil-fuel price (FFP) scenarios. The period of fuel price reference was set between 2008 and 2013 for two reasons. Firstly, the global economy and the relying industries have seen the min/max of fuel prices within this period. Secondly, the Bio-SPKs were introduced into the commercial market from 2009 onwards. To evaluate the effect of this uncertainty on the predicted fuel prices, a sensitivity analysis was conducted in a similar approach to the PI method [30] where the biofuel prices were predicted as a function of low, baseline and high fossil fuel prices (FFPs) The candidate fuel prices predicted for the year 2014, from ALCCoB under high, baseline and low FDE price scenario, have been presented in Table 7-3.

Fuel Type	ALCCoB- Market price of Bio-SPKs (£/kg)		
	Low FFP	Baseline FFP (calculated)	High FFP
Jet-A1	0.42	0.64	1.89
Camelina SPK	1.06	1.28	1.51
Microalgae SPK	1.28	1.37	1.72
Jatropha SPK	1.12	1.32	1.45

Table 7-3: Variation in Market price of Bio-SPKs as a function of petroleum price volatility

7.4.2 Limitations

Market growth, an important factor which influences the pricing of fuels, has been assumed to increase consistently with the analysis years. This assumption has a significant effect on the quality of the predicted biofuel prices. The author wishes to indicate that this economic analysis relies on the nature and quality of assumptions indicated in section 7.3.1.1. This analysis does not explore or explicitly predict the cost impact of future expansion of fuel infrastructure on fuel price. However, ALCCoB-BP solely devoted to preliminary prediction of biofuel prices. Cash flow evaluation, project risk and feasibility assessment fall outside the scope of this analysis but, they can be accommodated with further development of the model.

Part-II: Direct Operating Cost Model

(ALCCoB- DOC)

7.5 INTRODUCTION

Commercial air-transport is a capriciously complex business with immense competition for passenger volume. The profitability, for an airline operator, stems from any savings in the fuel costs which occupies as much as 35% of the variable operating cost of an aircraft per annum [66]. In order to ensure a stable profit margin, some airline operators "hedge" or "fix their fuel prices" a year earlier, to avoid losses from price hike. However, the fuel price is volatile to an extent that this "hedging" can either protect or penalise the operators in billions of dollars on a global scale. Any fuel that aims to be commercially deployed must therefore by analysed for economic viability from consumer's perspective.

7.6 LITERATURE REVIEW

The volatility in fuel prices is pre-dominantly influenced by the market demand. Aviation fuel costs contributed to about 30% of an aircraft's direct operating cost, as of 2014 [66]. This is a 28% increase from the average of operating cost between the baseline years (2004-2006). In context of the volatility of the fuel prices, current jet fuel price has lowered since April 2014 and remained constant at a rate of $2.87/gallon of Jet-A1 (in contrast to highest price in the last 2 decades at $3.89/gallon reported in Jul 2008 [130]. In financial terms, aviation fuel costs on the global scale amounted to $210 billion in 2013 [68]. The instability in fuel price can only be resolved through establishment of an equilibrium between global demand and supply. This equilibrium is achievable with advanced biofuels where the supply and demand are controllable factors. Studies which entail the industry-based financial impact of advanced biojet fuels have rarely been reported [125].

In view of lack of literature attributable to the biofuels, this study has opted for contemporary method of "Direct operating cost" analysis factoring the various fixed and variable costs. This study is expected to contribute to knowledge through prediction of direct operating cost of a representative model aircraft (LokAir equipped with two CU-Jet engines) operating on a user-defined medium-range trajectory using advanced biofuels accounting the following parameters

- Capital Cost
- Standing Cost
- Crew cost
- Maintenance Cost
- Mission Cost
    - *Fuel Cost*
    - *Emission Cost*

Suitable sensitivity studies with extreme environmental taxations and fuel prices over medium (2020), long (2050) and very long (2075) periods have also been undertaken. The purpose of this sensitivity study is to deliver an insight into the threshold of cost volatility associated with the Bio-SPKs relative to that of Conv.Jet-A1.

7.7 METHODOLOGY

The purpose of this Direct Operating Cost (DOC) analysis is to determine the economic feasibility of Camelina SPK, Microalgae SPK and Jatropha SPK, in the current scenario of commercial aviation. An accompanying sensitivity analysis conducted over medium (2020), long (2050) and very long (2075) term period accounts for prospective economic measures (strict environmental taxations). Direct operating costs define the yearly expenditure and thus the annual profit margin for the airline operator. Direct operating cost is the sum total of the following costs

1. Fuel Costs – First biggest operating cost contributor
2. Airframe and Engine maintenance cost – Second major cost contributor and is influenced by the size, weight and range of component application
3. Flight & Cabin crew cost- depend upon the size and the range of application
4. Landing cost
5. Ground maintenance costs
6. Depreciation Costs

7. Insurance and Interest on Total investment costs

8. Carbon Emissions and Noise Tax costs

1,2,3,5 and 8 are highly variable costs and depend upon a variety of variable factors such as market demand, fuel price fluctuations, economic climate, and unexpected maintenance requirement demanding shop visits. Other parameters are likely to remain fixed over the entire timeframe considered for this analysis, irrespective of persistent inflation and market growth.

7.7.1 Capital Costs

Capital Costs (cost of the aircraft) are dependent on the cost of assets (aircraft and range). Capital costs determination is a pre-requisite to calculate standing charges (Depreciation, insurance and interest costs) which are asset dependent costs and contribute to fixed costs in addition to crew cost and airport charges. Consultation of earlier published literature [8] and [118] and method of cost distribution over engine and aircraft components enables prediction of their component and material costs with relative ease. For instance, the airframe (Wing, Tail and Fuselage) and engine costs contribute to 41.5% and 17.1% of the total aircraft cost. Other components which contribute to the total aircraft cost include the following

- Furnishings including lighting = 14.5%
- Avionics (communication and navigation) = 12.7%
- Flight control and guidance = 5.3%
- AC power systems = 2.4%
- Hydraulics and auxiliary power systems = 2.1%
- Air-conditioning and pressurisation = 1.9%
- Landing gear; wheels, tires and brakes = 1.7%
- Miscellaneous systems and components = 0.8%

7.7.2 Standing Charges (Depreciation, Interest and Insurance Costs)

As mentioned earlier, the depreciation, interest and insurance costs are a fraction of the annual operating costs which are asset price-dependent and fixed over the life of the aircraft. These costs were calculated by the following method

$$\boldsymbol{Depreciation\ Cost\ per\ year}\ \left(\frac{\$}{yr}\right) = \boldsymbol{Aircraft\ price} + \boldsymbol{Cost\ of\ Aircraft\ spares} + \boldsymbol{Cost\ of\ engine\ spares} \quad \textbf{Eq 59}$$

$$\boldsymbol{Interest\ per\ year} = \boldsymbol{Investment\ cost}\ \times \left(\frac{\boldsymbol{Interest\ rate}\ (\%)}{\mathbf{100}}\right) \quad \textbf{Eq 60}$$

$$\boldsymbol{Insurance\ per\ year} = \boldsymbol{Investment\ Cost} \times \left(\frac{\boldsymbol{Aircraft\ cost\ based\ insurance\ rate}}{\mathbf{100}}\right) \quad \textbf{Eq 61}$$

$$\boldsymbol{Total\ Standing\ Charges\ per\ year} = \frac{\boldsymbol{Depreciation\ costs}}{\boldsymbol{year}} + \frac{\boldsymbol{Interest}}{\boldsymbol{year}} + \frac{\boldsymbol{Insurance}}{\boldsymbol{year}} \quad \textbf{Eq 62}$$

7.7.3 Crew Cost

According to a report published by EUROCONTROL programme CARE INO III, Flight and cabin (2+3) crew costs related to A321 family of aircrafts in 2008 was determined to be £240/FH [127]. The yearly rate of inflation over the 6 yr period was assumed to be 21% for which the flight and cabin Crew Cost were determined to be £545/FH in 2014 pounds. The rate of inflation from 2008 to 2014 was calculated using the online inflation calculator available at the Bank of England website [16].

7.7.4 Maintenance Cost

Maintenance cost analysis forms an underpinning element when evaluating the economic feasibility of a novel concept or an optimised process. The baseline engine/airframe configurations (two CFM56-5B2/B engines in A321-112) adopted for these analyses have been operational since 1999 and therefore, there is abundance of information available regarding their maintenance regime. The costs incurred from maintenance of the given engine/airframe configurations relating to A321-100 were assumed to remain unchanged for LokAir-K. Yearly utilisation and the associated cost data have been presented in Table 7-4 upon consultation of earlier literature [9].

The chemical compositions of Bio-SPKs (Camelina SPK, Microalgae SPK and Jatropha SPKs) have dictated a difference upon their performance properties (i.e. h, Cp, γ, viscosity, density). Having elaborately assessed these properties, it is evident that Bio-SPKs burn relatively cooler (combustion flame temperature) and deliver the same level of thermodynamic performance similar to Jet-A1. From practical point of view this phenomenon is likely to pose an impact on the life of engine components (hot and cold section) thus having a marked effect on the life of the engine/aircraft combination. Qualitatively discussing, the relatively cooler flames of the Bio-

SPKs would have a positive effect on the combustor lining and the hot-end components. On the other hand, thermodynamic effect of the biofuels boosting the thermal efficiency and thus the overall performance of the engine may also affect the mechanical integrity and eventually the engine life. Therefore, considering both scenarios, one has to entertain the possibility of change in maintenance costs with use of 100% Bio-SPKs in their annual operating cost analysis. However, maintenance characteristics attributable to biofuel operated engine/aircraft combinations can be understood only through experimental investigations.

Utilisation Parameters	Values		Units
Flight Hour	3500		-
Flight Cycle	1830		-
FH/FC	1.9		-
Maintenance Parameters	**2006 £**	**2014 £**	**Units**
Line and Ramp Checks	112.76	146.93	£/FH
A Checks	14.89	19.40	£/FH
Base Checks	68.08	88.71	£/FH
Heavy Components	63.82	83.16	£/FH
Line-replacement Unit support	95.74	124.75	£/FH
Total Airframe & component Maintenance	355.29	462.94	£/FH
Engine Maintenance	244.68	318.82	£/FH
Total Direct Maintenance costs	600	781.80	£/FH
Total maintenance Cost per year	2,100,000	2,736,300	£/year

Note:

- 2006£ have been adjusted to 2014£ accounting the annual rate of inflation [16].
- For FH of 3500 and FC of 1830
- Sourced from reference [9]

Table 7-4: Maintenance parameters assumed into ALCCoB-DOC

Additionally, personal communication with experts on experimental fuel property evaluation have indicated that even the least of temperature dependant engine/aircraft-life implications can only be observed for fuel with adiabatic flame temperature exceeding 50K relative to that of reference fuel [110]. The only available literature on maintenance implication of advanced biofuels on existing engine/ aircraft combination has been provided [127]. A 6-month trial conducted by Lufthansa on A321 operated with 50% blend biofuels between Hamburg and Frankfurt yielded successful results without any operation anomalies and technical issues. Visual investigation made on fuel tanks, lines and seals for deposits were negative with the engine tank appearing in “good condition” as claimed by the studies. However, the maintenance implications of aircraft operated with 100% biofuels is unavailable in the open domain. With careful consideration of the above mentioned this study assumes that the advanced biofuels under consideration do not impart major mechanical implications over the life of the engine-airframe configuration, and therefore, the maintenance cost of aircraft operated with the candidate fuels (including reference fuel) is assumed to remains constant.

7.7.5 Mission Costs

The mission costs were predicted from a representative engine/ aircraft performance evaluation that was conducted in the technical module [section 5.3.2]. The mission level assessment involved operation of LokAir (equipped with two CU-Jet engine) operating on a user-defined profile with a mission range of 4650 km, a typical travelling distance between London Heathrow (LHR) and Bahrain International (BAH). The two parameters which contribute to calculation of missions are fuel cost and aviation CO_2 emission cost. Further information elaborating each of the parameter can be found in section 7.7.5.1 and 7.7.5.2. ALCCoB-DOC will also adopt the outcome of the mission level assessment (fuel burn and aviation CO_2 emissions) technical assessment into the sensitivity studies to create a business case.

7.7.5.1 Fuel Cost

The aim of this economic module is to predict the financial feasibility of using Bio-SPKs in an existing engine/airframe configuration over a user-defined mission profile through operating cost analysis. The prices of each of the Bio-SPKs have been predicted through ALCCoB-BP. The hypothetical market price of Camelina SPK, Microalgae SPK and Jatropha SPK was integrated into the ALCCoB-DOC module to predict the mission fuel cost. Mission fuel burn attributable to LokAir-K, LokAir-C, LokAir-M and LokAir-J were adopted from the outcome of the technical module [section 5.4.3.2].

7.7.5.2 Emission Costs

European Union- Emissions Trading Scheme (EU-ETS) is expected to tax commercial airline operators based on the aviation CO_2 emitted above the allowance cap (95% from 2014). The price of aviation CO_2 for 2014 was determined to be £4.98/ metric ton [13] which will be levied on excess aviation CO_2 emissions produced above the carbon cap, by flights travelling through the EU airspace. Regrettably, the full-fledged global deployment of aviation emissions taxation faces protests from intercontinental aviation associations which has resulted in the EU having to "stop the clock" on carbon emission taxation. Consequentially, there are no functional, globally-deployed aviation CO_2 taxation mechanisms in existence. The EU aviation industry is, however, headstrong to become carbon neutral by 2050, carbon emissions and the efforts to introduce carbon taxation on aviation emissions are expected to take force in the near future. ALCCoB-DOC considers EU-ETS based aviation CO_2 taxation for LokAir-K, under current scenario, where 5% of its excess emissions will be charged.

A number of studies including [19], [29], [39] and [46] have acknowledged that the commercial intrusion of sustainable aviation fuels is possible only through global implementation of economic measures. These measures include ambitious environmental goals/ standards and stringent emission caps/ taxes. These taxes could be invested into techno-economic development of both the aviation and biofuel infrastructure and thus towards a greener sustainable growth. LokAir-C, LokAir-M and LokAir-J, on the other hand, are exempt from these taxes due to the 60-80% carbon offset achieved with the biofuel plantations. This data was adopted from the sustainable fuels policy conceived by the European Commission in 2012 [26].

It is essential to note that the baseline scenario is restricted to the analysis year 2014. To investigate the impact of these variables costs (fuel and mission costs) in the near and long term future, appropriate sensitivity studies have been undertaken. Further information on this sensitivity study will be provided in the upcoming section.

7.7.6 Sensitivity Analysis

It is essential to note that this study considers some of the "difficult to forecast" data which include

- fuel prices
- aviation CO_2 cap
- aviation CO_2 tax

However, the parameters which have the most impact on the annual mission cost are future fuel prices and emission cap/ taxations. In order to alleviate the associated uncertainties, an elaborate sensitivity analysis was conducted, over medium (2020), long (2050) and very long term (2075). The method and assumptions for predicting fuel prices, between the analysis periods (2014-2075) has been elaborated in sections 7.7.6.1.1 and 7.7.6.1.2.

7.7.6.1 Prospective Fuel Prices (2014-2075)

7.7.6.1.1 Conventional Jet fuel prices

Prediction of future fuel prices is a pre-requisite to the estimation of aircraft's mission cost evaluation over the mid- term (2020), long-term (2050), and very-long term (2075) periods. The purpose of this analysis is to determine the economic competence of the advanced biofuels against the backdrop of varying fuel (Bio-SPKs and Conv.Jet fuel) prices.

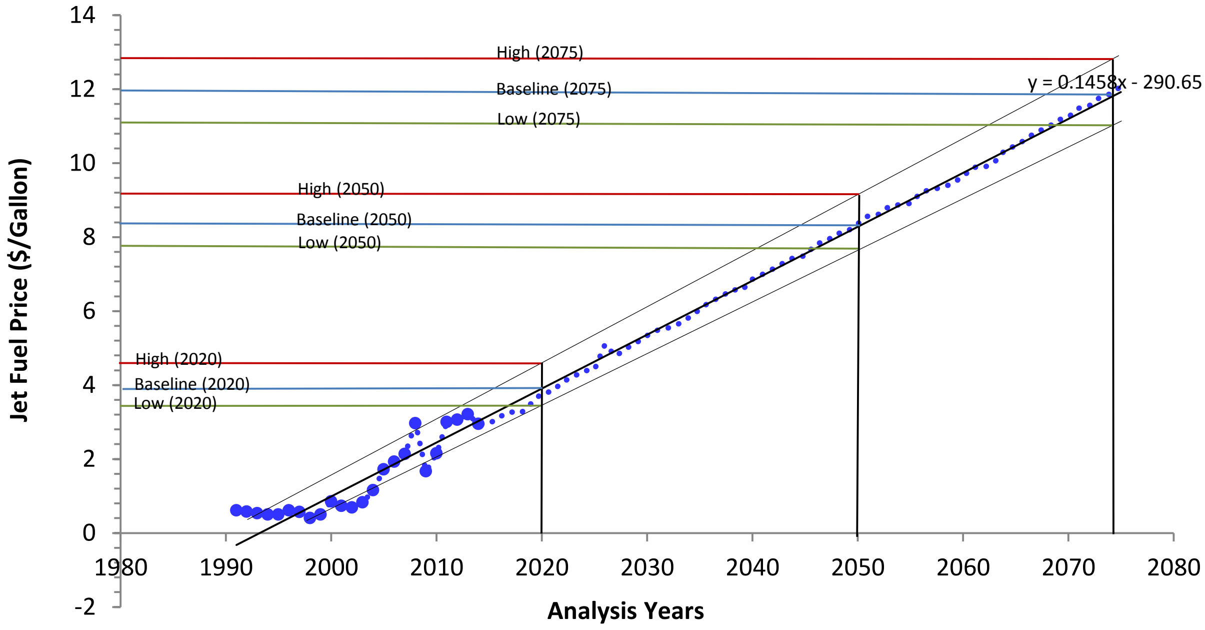


Figure 7-3: Future projections of Jet fuel price

This study was initiated with the prediction of future fuel prices for Conv.Jet fuel. Historic prices for Jet-A1 were obtained from a reliable source in the open domain, Energy Information Administration [129] and [130] for the prices between the periods Jan 1990- Jan 2014. Prospective Jet fuel prices were carefully extrapolated through regression. The volatile nature of this commodity is well acknowledged by this study and to avoid uncertainties in this analysis, a high and low fuel price scenario has been introduced. A schematic representation of the high, baseline and low jet fuel price chosen, extrapolated over till 2075 has been presented in Figure 7-3 .

7.7.6.1.2 Bio-Synthetic Paraffinic Kerosene

Future pricing of Bio-SPKs is highly speculative due to their uncommercial nature and lack of information in the open domain. However, biofuel prices for 2020, 2050 and 2075 have been consistently predicted based on the assumed expansion of biofuel production infrastructure and improvement in biofuel conversion efficiency from technology maturity. It is also essential to note that the expansion of Bio-SPK processing infrastructure could be as twice or more than jet fuel production capacity in a "business as usual" scenario owing to the current and potential land availability as indicated in literature [125]. The biofuel industry is assumed to expand and increase the overall production capacity to keep up with the global demand for jet fuel from 2020 to 2075. Existing global biofuel acreage allotted for cultivation of Camelina, Microalgae and Jatropha and the possibility of their technology maturity have been adopted from consultation with earlier literature [52] and [71]. The Bio-SPK process specifications modelled in ALCEmB will be accounted to forecast prospective Bio-SPK production capacities upto 2075. The production capacities were measured and compared in metric-tonnes of jet fuel produced per year. This method (Eq 63) of future biofuel price prediction simply follows the principle involved with pricing conv.jet fuel i.e. the supply-demand equilibrium and has been presented in Eq 63.

$$\boldsymbol{Conv.Jet\ fuel\ to\ Biofuel\ production\ ratio}\ \left(\frac{PC_{Jet\ K}}{PC_{Bio-SPK}}\right)_x = \frac{\boldsymbol{Production\ capacity}_{Jet-A}}{\boldsymbol{Production\ capacity}_{Bio-SPK}}$$

Eq 63

where, x= analysis year

$$\boldsymbol{Biofuel\ Price}_x = \boldsymbol{Predicted\ Biofuel\ Price}_{2014} \times \left(\frac{PC_{Jet\ K}}{PC_{Bio-SPK}}\right)_x \qquad \textbf{Eq 64}$$

The price of the Bio-SPKs progressing into the future was also assumed to be influenced by technology maturity. Further information on the impact of technology maturity on fuel prices has been provided in section 7.7.6.3. The market price of Camelina SPK, Microalgae SPK and Jatropha SPK predicted through above mentioned method have been predicted for the analysis years 2020, 2050 and 2075 [Table 7-5].

[**NOTE**: It is also essential to note that this study does not explicitly address or account the market growth, realistic increase in air-traffic, techno-economic improvement to the existing and future fleet of aircraft over the analysis years. This would only increase the degree of uncertainties with the price prediction]

7.7.6.2 Prediction of Future aviation CO_2 Tax

In the wake of stringent environmental goals and policies, emissions taxes can be considered variable parameters like fuel prices. The aviation industry in EU aims to become carbon neutral by 2050. The "four pillar" strategy clearly demonstrates that the gap in achieving carbon neutral growth, even after implementation of technological, infrastructure and operational improvements, can be bridged only with economic measures [Figure 1-1]. Therefore, incorporation of aviation CO_2 taxations is crucial to this assessment.

The CO_2 price for analysis years 2020, 2050 (goal year of carbon neutral growth) and 2075 have been assumed to be £50, £100 and £1000/ metric ton. These figures were adopted from an industrially, reputable Massachusetts Institute of Technology (MIT) based techno-economic-emission mitigation model for climate change solutions called MERGE (Model for Evaluating Regional and Global Effects of GHG Reduction Policies) and MiniCAM (MINI-Climate Assessment Model). MERGE and MiniCAM are techno-economic aviation emission mitigation models which have predicted these prices based on the carbon intensity of the aviation industry [88]. They are recursive (looking-forward) dynamic models which are capable of estimating future carbon price by accounting prospective investments made into emission mitigation efforts. These efforts range from retrofits and techno-economically improved maintenance programs, use of advanced biofuels, ATM improvement to incorporation of cutting edge-technology (e.g. open rotors and distributed propulsion systems) ([41]. Further information on these models can be obtained from literature of references [41] and [88].

The fuel and aviation CO_2 prices attributable to the operation of LokAir with the candidate fuels over medium (2020), long (2050) and very-long term (2075) periods have been tabulated below.

Fuel Types and parameters		**2014**	**2020**	**2050**	**2075**
Fuel Price (£/kg)	Conventional Jet fuel	0.6	0.9	1.8	2.5
	Camelina SPK	1.3	1.1	1.0	0.34
	Microalgae SPK	1.4	1.3	1.2	0.35
	Jatropha SPK	1.3	1.1	1.0	0.35
Aviation Carbon Price (£/MT)		5	50	100	1000

Table 7-5: Specifications for long term economic viability evaluation of Bio-SPKS

These the above mentioned figures assumed for this assessment have been adopted based on the following assumptions.

7.7.6.3 Assumptions

It is essential to note that this sensitivity analysis has been conducted only for baseline scenario with the assumptions listed below.

Emission Taxation

- It is imperative to realise that the aviation CO_2 taxation proposed by EU-ETS apply only emissions from burning Conv.Jet fuel and that produced above the carbon cap of 95%. Any aviation CO_2 emissions resulting from their combustion are exempt from emission taxation. However, this study assumed that the roughly 35-40% carbon emissions resulting from systemic combustion of Bio-SPKs (balance from life cycle emissions) being taxed from 2050 onwards since the civil aviation industry aims to achieve “carbon neutral growth” from then on.
- In addition to the baseline emission taxes from MERGE and MiniCAM, two other scenarios defining the “high” and “no tax” threshold over the analysis period have also been included. The price of CO_2 emissions in this scenario will be +/-100% tax on the predicted medium, long and very long term CO_2 prices. This supplementary scenario was additionally factored in to evaluate the mission costs of biofuel operated flights against a backdrop of extreme environmental taxation scenario

Future Fuel Price

- The fuel management infrastructure (factory gate to airports) is assumed to remain unchanged for handling Bio-SPKs and therefore, airport charges are constant.
- Prediction of future Conv.Jet fuel price comes with the following assumptions
    - Crude oil supply is assumed to remain unaffected over the analysis period by external factors (use of shale gas and oil as jet fuel feedstock, fluctuations in the global economy or political conflicts) to ensure that the jet fuel supply-demand equilibrium and thus the jet fuel price follows the trend presented in Figure 7-3.

- The medium (2020), long terms (2050) and very long term (2050) prices of the Bio-SPKs were predicted as a function of two factors.
    - **Increase in technology maturity and thus production capacity-** Conversion efficiency of crude oil to jet fuel is currently 98.97% and this was achieved over 50 years [75]. According to a study conducted by Cazzola et al, (2014), [30] most unconventional jet fuel infrastructure is assumed to achieve technology maturity of almost 50% in 50 years. This figure was arrived at accounting the rate of technology maturity achieved by the Conv.jet fuel infrastructure. The rate of technology maturity achieved by the advanced biofuel infrastructure may be required to be quantified precisely. However, this study assumes that any growth in this industry improves the production efficiency, and reduced the cost of production by 20% in 2020, by 50% in 2050 and 75% in 2075.

Fuel Demand

- At a global level, older fleet of aircraft are still functional. From the quantitative and qualitative discussions conducted in chapter 5 and 6, it is evident that the Bio-SPKs are not absolutely compatible with their systems and configurations. Therefore, the demand for conv. jet fuel is assumed to persist.

7.8 RESULTS AND DISCUSSION

The Direct operating cost of an existing aircraft operated with 100% Bio-SPKs was observed to be a gap in literature and also a valuable contribution to knowledge. In view of this shortcoming, the second part of the economic module, ALCCoB-DOC was developed. The various cost parameters which contribute to the prediction of DOC of LokAir-C, LokAir-M and LokAir-J have been provided in the upcoming sections.

7.8.1 Fixed cost parameters – Capital Cost

The costs which have been fixed between the aircraft operated with the candidate fuels have been tabulated in Table 7-6. This study clearly comprehends that this cost analysis is solely fuel centred and not asset/ operation-based, as in, technological improvement, operational efficiency or an optimisation study. For the purpose of uniformity, flight cycles and flight hours have been assumed constant and this assumption is also validated by the outcome of the mission based aircraft performance assessments from the technical module [section 5.4.3.2]. This study concluded that LokAir-C, LokAir-M and LokAir-J performed just as efficiently as the baseline LokAir-K with no major discrepancies.

Standing charges are dependent on airport regulations and in this study, they were predicted from the aircraft cost. For the purpose of simplicity, airport costs were also fixed between the chosen destinations assuming that the fuel management infrastructure for the Bio-SPKs will be similar to that of Jet-A1. This is highly unlikely in reality since Bio-SPKs may require different fuel management and infrastructure [for storage, transfer and refuelling procedures] which is dictated by their fuel property.

Parameters			Values	Units
	Aircraft Life		20	Yrs
		Airframe Cost	30147466	£
		Engine Cost	7143771	£
		Aircraft Spares cost	3014746	£
		Engine Spares cost	2143131	£
		Total Investment Costs	**42449116**	**£**
	Aircraft utilisation	Annual Flight Hours	2800	FH/year
		Annual Flight Cycles	1830	FC/year
Aircraft utilisation		Flight Hr /Flight Cycle	1.530054645	FH/FC
	Aircraft Max take-off weight		83000	kg
	Aircraft cost		42449116	$
		Depreciation	10	%
		Interest rate	4	%
		Insurance	0.5	%
		Depreciation cost	38204204	£/year
		Interest costs	2573435.2	£/year
		Insurance costs	1697964	£/year
		Total Standing Charges	**40114415.2**	**£/year**
	Crew Cost (Flight and Cabin crew)		3000	£/FH
		Total Crew cost	**831354**	**£/year**
	Airport Charges	Ground handling charges	200	£/FC
		Navigational fees	100	£/FC
		Landing charges	0.01	£/FC
		Total Ground handling charges	386381	£/year
		Total Navigational fees	181116	£/year
		Total landing charges	1453157	£/year
		Total Airport charges	**2020655**	**£/year**
	Total Fixed Operating Cost		42966423.6	£/Year
			15345	£/FH
			23478.92	£/FC

Table 7-6: Cost parameters fixed over the flight operations with the candidate fuels

7.1.1 Maintenance Cost

The maintenance cost associated with the operation of Bio-SPKs was assumed to be similar to that of Conv.Jet fuel and the maintenance cost related for the operation of LokAir on an annual basis has been tabulated in Table 7-7. The rational for this assumption of similar maintenance cost has been elaborated in section 7.7.4.

Parameters	Values	Units
Engine Maintenance Labour rate	46	£/MH
Aircraft Maintenance Labour rate	48	£/MH
Default Engine maintenance hours	2441	MH/year
Default Airframe maintenance hours	3035	MH/year
Engine Material Cost	66000	£/year
Aircraft material cost	114740	£/year
Engine Maintenance costs	75000	£/year
Airframe Maintenance costs	221562	£/year
Total Engine maintenance cost	1688440	£
Total Aircraft maintenance cost	5210675	£

Note:
Maintenance rates and data for the baseline aircraft [A321-112], [9], were adopted for LokAir

Table 7-7: Maintenance cost incurred by LokAir per annum

7.1.2 Mission Cost

Mission costs (fuel and emission costs) is the key financial parameters, in this study of interest since the maintenance costs attributable to LokAir-C, LokAir-M, LokAir-J and LokAir-K have been standardised for this fuel centred feasibility study. The market price of the Camelina SPK, Microalgae SPK and Jatropha SPK predicted from ALCCoB were factored into the DOC model with respective quantity of fuel consumed by LokAir-C, LokAir-M and LokAir-J.

[Note: It is essential to note that this includes a sensitivity assessment conducted at three different scenarios: Low, baseline and high FFP. The cost of the Bio-SPKs for year 2014 has been predicted at three different scenarios as a function of fossil fuel prices. These prices were tabulated in Table 7-3 through the economic model ALCCoB-BP]

Baseline mission costs (for analysis year 2014) have been presented as m£ (million pounds). Mission costs attributable to each of the Bio-SPKs were higher than that of the reference fuel for low and baseline FFP scenario. The main contributor to this outcome was the fuel price of each of the Bio-SPKs which is roughly twice as high as the reference fuel. In terms of emission costs, it is essential to know that the Bio-SPKs are exempt from carbon taxation owing to their environmental competence at a “Cradle-Grave” life cycle level. However, this analysis determined that the benefits from emission tax exemptions was overshadowed by their relatively high market prices.

- The % increase in mission cost encountered LokAir-C, LokAir-M and LokAir-J were determined to be 103%, 125% and 155% higher relative to that of LokAir-K under low fossil fuel price (FFP) scenario.
- This percentage difference appears to reduce to 92%, 100% and 95% respectively during the baseline scenario.
- A shift occurs during the high FFP scenario where the cost of the conventional jet fuel overtakes the Bio-SPKs and creates a favourable fiscal scenario towards biofuel commercialisation.

This analysis infers that volatility of jet fuel prices are able to create an advantage for the Bio-SPKs during the high FFP scenario, airline operators using 100% Bio-SPKs would be able to fix their costs or make significant financial savings unlike reference fuel dependant operators.

Parameters	LokAir-K	LokAir-C	LokAir-M	LokAir-J	Units
Mission Costs (high)					
Mission Fuel Costs	93	71	84.5	69	m£/year
Mission CO_2 Costs	1.4	0	0	0	m£/year
Total Emissions Costs	2.9	0	0	0	m£/year
Total Mission Costs (no NOx costs)	94.3	71	84.5	69	m£/year
Mission Costs (baseline)					
Mission Fuel Costs	31.69	61	66	63	m£/year
Mission CO_2 Costs	0.10	0	0	0	m£/year
Total Emissions Costs	1.45	0	0	0	m£/year
Total Mission Costs (no NOx costs)	48.2	61	66	63	m£/year
Mission Costs (low)					
Mission Fuel Costs	25	51	61	53	m£/year
Mission CO_2 Costs	0.15	0	0	0	m£/year
Total Emissions Costs	1.39	0	0	0	m£/year
Total Mission Costs (no NOx costs)	25	51	61	53.12	m£/year

Table 7-8: Mission Cost Calculated at High, Baseline and Low fossil fuel price scenarios

7.1.3 Future Biofuel prices

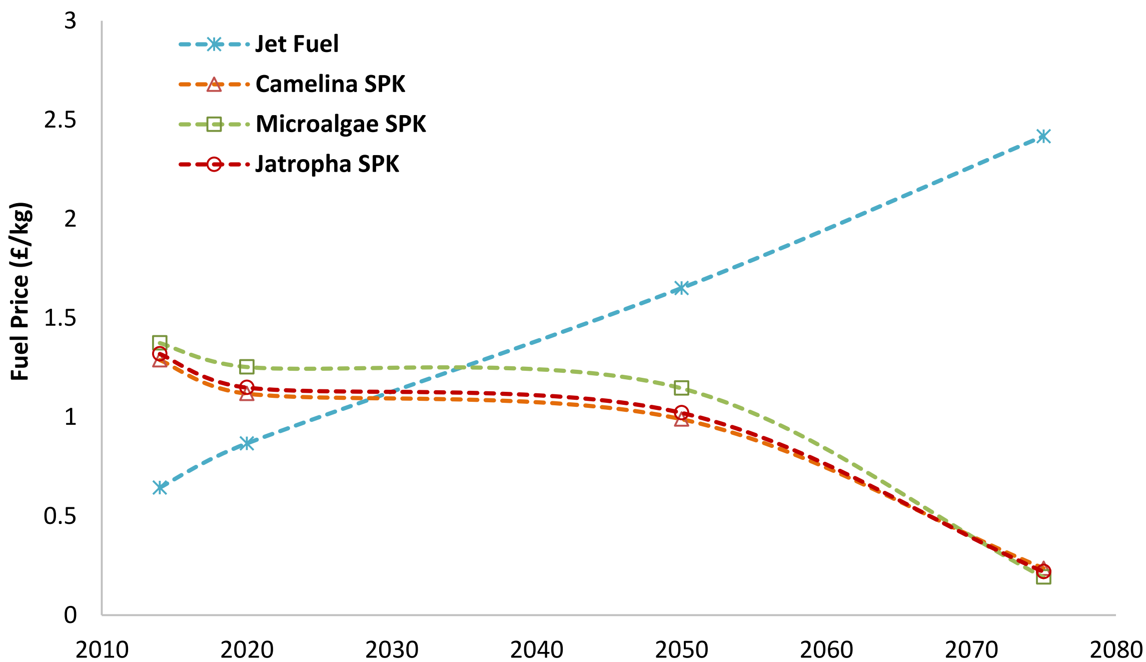


Figure 7-4: Estimated price of fuel candidates between analysis years 2014-2075

The future fuel prices were required to be estimated as a part of the sensitivity analysis which involves prediction of mission cost of LokAir-K, LokAir-C, LokAir-M and LokAir-J as a function of varying fuel prices and emissions taxation scenarios. As presented in the methodology [section 7.7.6.1.2], the hypothetical market prices of each of the Camelina SPK, Microalgae SPK and Jatropha SPK has been predicted as a function of increasing plant production capacity production (plant expansion and technological maturity) over the analysis period (2014-2075).

Unlike Conv.Jet fuel, the supply-demand equilibrium of the biofuels is a controllable factor and therefore, are less likely to undergo market based fluctuations in terms of market price. The level of certainty attained with the biofuel prices (under user-defined boundary) is likely to be an advantageous factor to the profitability of airline operators.

This analysis is extended to 2075 since the aviation industry will be keen to become carbon negative through with full-fledged deployment of emission mitigation efforts and existing “futuristic” technology. With the intrusion of stringent emission caps, high levels of aviation CO_2 taxes and incessant increase in Conv.Jet fuel prices, a clear demand for Bio-SPKs is expected to be created. Bio-SPK become an economically feasible choice of fuel from 2030 onwards.

Continuous demand for the Bio-SPKs creates an opportunity for the expansion of Bio-SPK processing infrastructure and boosting the production capacity over the upcoming years. With the supply-demand equilibrium clearly established for the Bio-SPKs, the cost of Bio-SPKs stabilise upon commercial deployment between 2020 and 2050. The desire to become “carbon neutral” from 2050 will motivate the civil aviation sector to seek more futuristic “zero carbon” alternatives such as electric hybrids and hydrogen thus leading to a drop in the Bio-SPK prices.

7.1.4 Sensitivity Analysis

A sensitivity study was conducted to examine the economic viability of the Bio-SPKs (through mission cost analysis) over medium (2020), long (2050) and very long (2075) term periods as a function of varying fuel price and emission taxation scenario.

It is essential to note that the aviation carbon tax prices chosen for this assessment were used for its closeness to the future universal carbon price predicted by renowned MERGE (Model for Evaluating Regional and Global Effects of GHG Reduction Policies) and MINICam (MINI-Climate Assessment Model) models.

From mission cost analysis, sensitivity study, undertaken for the year 2014, concluded that the flight mission operated with each of the Bio-SPKs costs higher than the baseline fuel despite their emission exempted from taxation. The benefit of fuel savings and emission tax exemptions obtainable with Bio-SPK use is overshadowed by its relatively high market price. The fuel costs seem to account for 97% of the total mission cost and 65% of the overall direct operating cost calculated. A clear challenge from the well-established Conv.Jet fuel infrastructure on the assumedly expanding biofuel production capacity is evident up to 2020 (medium term). However, the benefit of stabilising biofuel price (from its predictable supply-demand equilibrium) establishes a case for economic feasibility from 2020 and improves against the backdrop of constantly increasing conv. jet fuel price and aviation emissions taxation.

"No emission Tax" scenario (-100% from baseline) is an unrealistic long (2050) and very long (2075) terms since there are ambitious environmental goals to be achieved. However, this setting has been chosen to depict an "existing situation" as opposed to +100% increase (from baseline) in emission taxes, "the high tax" scenario, which is also included in this assessment to set up a threshold for extremes in environmental taxation.

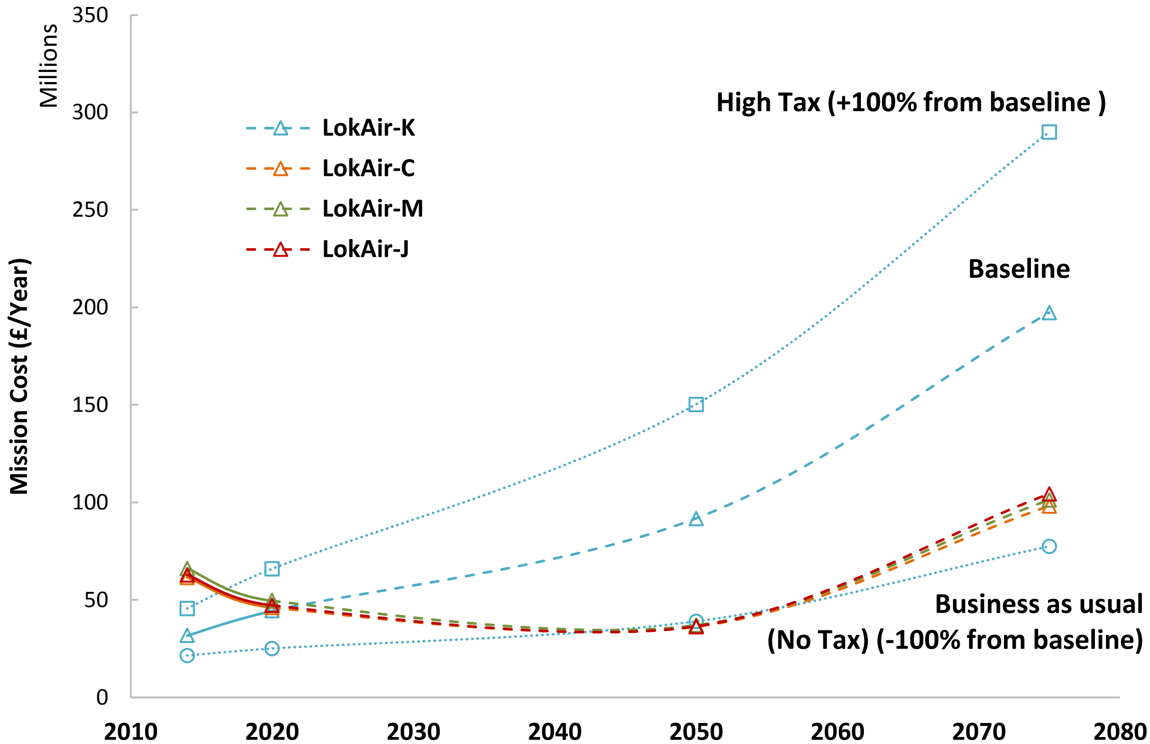


Figure 7-5: Effect of annually increasing fuel prices and emission taxation scenario on Mission Cost per annum

When comparing the mission cost trends for Camelina SPK, Microalgae SPK and Jatropha SPK, it was observed that the Bio-SPKs appeared to fall close to but still higher than the "no emission tax" scenario of Conv.Jet fuel. This particular observation infers that Bio-SPKs or any sustainable and radical energy technologies will be economically unfeasible and will be viable only with global deployment of stringent emission taxations (market based measure). From roughly 2023 onwards, Bio-SPKs demonstrate phenomenal viability over conventional jet fuel, dictated by the both the competent fuel price and exemption from the very high cost aviation CO_2 taxation (£50/ton). This outcome was observed to be in favour of the Bio-SPK beyond 2020.

The mission costs for LokAir operated with the Bio-SPKs increases gradually from 2050. As mentioned earlier, this scenario is supported by the civil aviation's inclination to become "carbon neutral" by 2050 and therefore, an interest to infuse more radical energy technology (such as hydrogen fuel) will be pursued. The aviation CO_2 tax attributable to the Bio-SPKs will be based on their ability to reduce their overall life cycle emissions (adopted from ALCEmB). Upon accounting Bio-SPK emission taxes, their mission cost was observed to be increasing in line with that of Conv. Jet fuel as observed in Figure 7-5. Nevertheless, Bio-SPKs are likely to be economically viable option from 2023 onwards.

7.2 CONCLUSION

The ultimate purpose of ALCCoB was to determine the economic competence of advanced biofuels against its fossil-derived counterpart, Jet-A1, when commercially deployed into the existing civil aviation infrastructure. This study entailed a two-part analysis consisting fuel price prediction and its incorporation into mission cost prediction.

This study concluded that for the current period, the cost of producing Bio-SPKs is relatively higher than that of conventional Jet fuel. It is essential to acknowledge that Convectional Jet fuel had a 50 year early start and its methods where techno-economically optimised improving their process efficiency by over 50% over 5 decades. Technological advancements in biofuel process engineering and their deployment can be expected to take effect by 2020 as quoted by a study [30]. In any case, ALCCoB projects that the Bio-SPKs, from fuel price perspective, become economically feasible from 2035 onwards. The cost competence of these alternative fuels have to be assessed through an elaborate aircraft direct operating cost analysis where the actual effects of fuel price on mission cost can be quantified. Direct operating cost evaluation indicates that the expensive (roughly 100% higher) biofuel price makes these alternative fuels appear economically unsound between 2014 and 2020. However, a number of factors including

- Constantly increasing jet fuel prices

- Constantly increasing emission cap and aviation CO_2 taxations
- Stability in supply-demand equilibrium achieved with the Bio-SPKs

The above mentioned factors make Bio-SPKs economically feasible from 2035 onwards creating a "cross-over" with conventional jet fuel price. From mission cost analysis, the Bio-SPK appears an economically feasible option only with ambitious and globally deployed emission taxation mechanisms as opposed to "no emission tax" which is the current state of aviation emission mitigation strategy.

7.3 LIMITATIONS

Assessment of Life Cycle Costs of Biofuels (ALCCoB) is an economic model developed to predict the cost of yet uncommercial alternative fuels. In order to predict the cost of these fuels, a number of assumptions had to be adopted. Among the assumption, the highly uncertain entity, fossil fuel prices had to be included to account the energy-cost intensity of each of the biofuel feedstock. A crude attempt has been made to account for fossil fuel price volatility in the sensitivity analysis, however, the uncertainties associated are extremely high.

ALCCoB-DOC developed to predict the direct operating cost of the aircraft operated with Camelina SPK, Microalgae SPK and Jatropha SPK were based on the list of fixed and variable direct operating parameters. Consideration of constant maintenance cost for LokAir operated with the candidate fuels is a limitation. Though this study has adopted this assumption upon careful consideration, the analysis would be complete only with the inclusion of quantitative analysis and technical evidence on any similarities/ discrepancies in the maintenance schedule (Time between Overhaul [TBO]) identified with Bio-SPK operated "LokAir".

8 QUALITATIVE DISCUSSION

8.1 Conventional Alternative – Shale Oil

Shale gas and oil are currently believed to be more reliable substitutes to conventional crude, beside the biofuels and natural gas. Shale oil, being literally a precursor to conventional crude, appears a promising solution in two ways.

- Conversion from Shale oil to conv. jet fuel is an established, functional process
- No major modifications to the existing "liquid fuel refining" infrastructure is demanded by the feedstock (shale oil).
- No major modifications will be demanded of the aircraft and the airport infrastructure to accommodate shale derived jet fuel. This particular benefit cuts short the major techno-economic commitments that would be encountered with radical alternative technologies like hydrogen and natural gas.
- Shale deposits have been determined to be abundantly available securing future energy demands for over 450 years. Currently the Alberta shale deposits in Canada are extracted at 1.32 million barrels per day (59% through surface mining and 41% through in-situ extraction). However, more reserves are discovered at a global scale which ensures global level energy security.

To briefly introduce shale oil, it is a non-refined form of Crude oil (does not undergoes decomposition through naturally occurring heat and pressure over a period of time to form conventional crude oil deposits). However, the method of their conversion to jet fuel has been established and this particular section briefly reviews and discusses the life cycle processes and emissions attributable to these alternative conventional fuel sources. The process of Jet fuel synthesis from Oil shale can be determined to be of the following stage

Method of Jet fuel Synthesis

Extraction of Shale oil involves complex, expensive and energy intensive processes. The intensity of the processes varies with the depth of oil shale location. There are two types of extraction process which are **Ex-situ** in which the oil shale is extracted and transported to the refining facility Ex-situ technique is carried out for surface mining procedures. The shale oil extracted upgraded to lighter synthetic crude oil through hydrogenation cracking. The Shale deposits extracted through surface mining is crushed and subjected to pyrolysis in an anoxic environment at 480-550C. The solidified high molecular weight Kerogen which composes Oil shale is decomposed to gas, condensed oil phase and solid residue the fraction of which forms 84%, 6% and 10% respectively. This process is called retorting.

In-situ process is employed for deeper oil shale deposits which are steamed with pipes drilled into the ground to reduce the viscosity of shale oil. The melted shale oil is pumped to the surface and this technique has been determined to be 86% more efficient than surface mining technique (Wong, HM, 2008). A more recent process patented and successfully operated at a sub-commercial level by SHELL involves the following process. Shell claims to have devised this method to reduce the environmental risks involved in the extraction of shale oil through in-situ method thereby promising an increase in oil productivity per cell. The In-situ process involves a series of processes which are as follows [17] & [24].

1. **Identification of Shale deposits and preliminary operations** (Layout of production cells)
2. **Construction of Freeze wall** around the production cell: In-situ process is retorting of the shale deposits within the ground. In order to avoid the risk of oil seepage and contamination of water resources and soil, a freeze wall 3 meters thick is constructed around the production cell. The freeze3 wall is constructed at -40C and is maintained at the same temperature of the period of shale oil extraction.
3. **Removal of water** from production pits is to ensure that the oil shale deposits are extracted with utmost efficiency and avoid extraction based difficulties.

4. **Drilling and insertion of Rods** to facilitate heating of the shale deposits. The deposit is heated with closely spaced rods to cut down on energy spent for heating. However, more holes have to be drilled to cover the area of production cell. The Shale deposits are heated through electrical resistance method to a temperature of 480-550C. The temperature of the productivity cells are increased at a rate of 3C per day at a pressure of 0.2-2MPa. It is also essential to understand that addition of excess pore pressure may result in the fracturing of the shale formation which could lead to a geologic fracturing. Heated kerogen is decomposed to natural gas, Shale oil and residual coke similar to product of the surface mined produce.
5. **Extraction of Shale oil** from the production wells. The oil, in its vapour phase reaches the production well. However, it has been reported that oil tends to move towards to the perimeter as a result of this heating process through capillary mechanisms underground and remain trapped. The nature, quantity and composition of shale oil extraction may vary with the location of extraction site. However, from the process point of view, it was observed that low temperatures and high pressure reduce extraction efficiency to a reasonable extent. Shale oil (composed of very long chain hydrocarbons) is recovered from the well through conventional pumping method at a reduced temperature of 200C.
6. **Remediation of Production cells** is essential owing to the deleterious effects of shale hydrocarbons. The production well is saturated with 20 pore volumes of water and is thoroughly flushed in order to prevent seepage of trapped oil contaminants into surrounding soil or water sources. The flushed water is thoroughly treated to reduce its toxicity levels to legal limit before being released into the environment.
7. **Upgrading and refining** extracted shale oil to consumable jet kerosene.

   The process involved in upgrading the extracted Shale crude is as follows.

- The crude is distilled at atmospheric pressure to obtain an atmospheric distillate and a heavy residual fraction
- Vacuum distillation of the atmospheric distillate to obtain intermediate vacuum distillate and a vacuum residue similar to the earlier case

- The distillates obtained earlier are subjected to a solvent de-asphalting process which is installed with the vacuum distillation unit. It is essential for the crude to be de-asphalted to improve downstream process efficiency and not affect the catalyst life. This is also reflected on the stability properties of the final fuel product.
- The atmospheric distillate is mixed with the de-asphalted crude which form the feedstock for hydrocracking.
- Hydrocracking of the feedstock enables cracking long chain hydrocarbons into smaller chains in the presence of excess hydrogen and a hydrocracking catalyst at elevated temperatures and pressures of 360C. This process is called as single step hydrocracking. Formation of lower boiling point (<360C) hydrocarbon concludes the upgrading face of Shale crude.

8. **Refining** process of shale oil to consumable jet fuel is expected to follow the conventional petroleum refinery process in this study

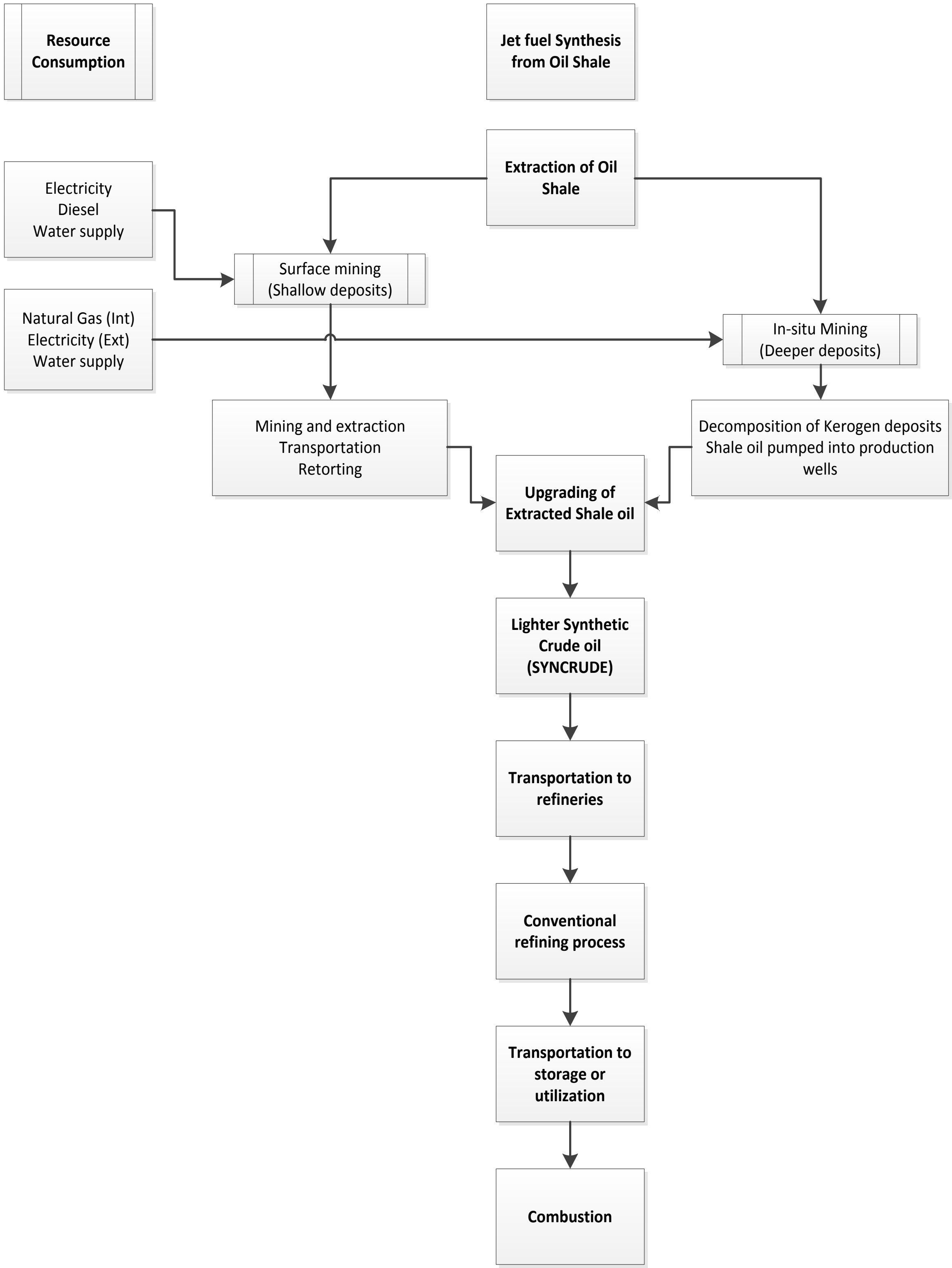


Figure 8-1: Life cycle process of Jet fuel derived from Shale oil

Results of life cycle emissions

A Brief Life cycle assessment of Shale generated jet fuel is expected to provide an insight into its environmental impact. This life cycle has adopted the methodology of Shale oil generation and conversion to consumable jet fuel developed and patented by Shell Corporation. The methods and subsequent impact will be discussed below. However, the environmental impact reported to the European Parliament by the Economic and Scientific Poly department, European Union Commission have been discussed below. According to the report, major health and safety hazards arise from the air pollution through accidental leaks of methane and leakage of melted kerogen or shale oil into the underground aquifers due to fracturing of the deposit and the freeze wall during drilling and unidentified anomalies in the surface topography. Shale mining activities in the US have been reported to face 1-2% of such environmental violations resulting from leaking and improper handling of equipment [81].

Stages of Jet fuel production	Emissions (gCO_2e/MJ)	
	SJF (24)	Bio-SPKs (107)
Construction of Freeze wall **Maintenance of Freeze wall** **Drilling of holes into deposits** **In-situ heating** **Plantation/ Feedstock harvest and affiliated equivalent activities**	41.2	30.3
Upgrading and refining	13.5	10.3
Combustion	73.2	71.2
Biomass Credit	0.0	-71
Total Emissions	128	40.8

Table 8-1: Life Cycle Emissions of Shale Derived Jet fuel

It is essential to consider the Land use change arising from shale oil extraction.

- The original ecosystem and biodiversity may be lost due to the requirement of extensive area of land from oil extraction process (Located on nation forest reserves).
- Conversion of landscape for paving routes for transportation of extracted oil or drilling machinery.

- Extraction of melted kerogen from shale deposits and use of drilling components may leads to possibilities of earthquakes and in extraction site or the surrounding land scape
- Heating up the deposits and its surrounding soil may render the site unsuitable for remediation.
- Toxicity levels in the surrounding soil may increase owing to the trapped shale oil extracts discussed in the earlier section.

Report of environmental hazard

The proper disposal of waste water seems to be a major issue in North America. The core problem is the huge quantity of waste water and the improper configuration of sewage plants. Though recycling might be possible, this would increase project costs. Many problems associated with the improper disposal are reported. For instance:

- In August 2010 'Talisman Energy' was fined in Pennsylvania for a spill in 2009 that sent over 4200 gallons (~16 m^3) of hydraulic fracturing flow-back fluid into a wetland and a tributary of Webier Creek, which drains into the Tioga River, a cold-water fishery. [81]
- In January 2010 'Atlas Resources' was fined for violating environmental laws at 13 well sites in south-western Pennsylvania, USA. Atlas Resources failed to implement proper erosion and sedimentation control measures, which led to turbid discharges. Furthermore, Atlas Resources discharged diesel fuel and hydraulic fracturing fluids into the ground. Atlas Resources holds more than 250 permits for Marcellus wells.
- 'Range Resources' was fined for an October 6, 2009 spill of 250 barrels (~40 m^3) of diluted hydraulic fracturing fluid. The reason for the spill was a broken joint in a transmission line. The fluid leaked into a tributary of Brush Run, in Hopewell Township in Pennsylvania [102].
- A comparative view on the fuel based properties of SJF against CJK indicates that shale derived jet fuel has been synthesized to possess better fuel performance e.g. lower carbon and higher hydrogen content thereby leading to a higher specific energy. However certain discrepancies such as lack of aromatic content, higher pour point can be detrimental on hardware specifications for certification. It is essential to note that these superficial observations can be verified only through experimental operations on a given jet.

8.2 Societal Impacts and Ethical Concerns

Advanced “Drop-in” biofuels were brought under lime light only since the last 5 years and one of the key hurdles to their commercialisation is the acknowledgement of their inability to cope with global jet fuel demand. Even if the meticulous task of establishing supply-demand equilibrium is achieved with the biofuels, their supply must be ensured to be sustainable and environmental friendly. This section briefly touches upon the ethical benefits and concerns associated with Bio-SPKs. The Biofuel will required to be produced sustainably in terms of the following aspects

Land Acquisition and Use- Land Use is an essential criterion that must be included into biofuel policies to address their sustainability and ethical concerns. It is essential for international biofuel companies to not target forested (rich soil) landscapes as it will have a negative impact on the landscape biodiversity and the thinly- populated local indigenous communities leading to human-ethical violations. Land acquired for biofuel plantations must be free of legal entitlements.

The three biofuel feedstock chosen for this assessment are called second generation since they are “non-food” crops and thus eliminating the “fuel vs food” conflict. They do not compete with arable land designated for food production. However, some earlier studies have identified plant species like Jatropha and Camelina to perform better in fertile land relative to average/poor soil, by convention. The volatility of the fossil fuel market and its impact on the biofuel prices were observed from the economic module. Therefore, any volatility in the fossil fuel prices (like the baseline fuel) and the increased plant productivity (derived from fertile soil) could tempt farmers to transform their choice of crop cultivation from food based to fuel based. This could be identified as a major societal risk which can be affect the food-fuel balance. However, microalgae cultivation is independent of soil quality requirement and this makes it an ideal option which eliminates its land-use issues.

Water Consumption- Fresh water resources have been globally acknowledged as non-renewable. Fresh water intensity of the feedstock (crude oil) of the baseline fuel is observed to be less than that required for irrigational purposes with biofuel plantations [141]. The performance of Camelina and Jatropha, in terms of productivity improves with increase in water supply which becomes a mandatory requirement for microalgae cultivation [1], [158] and [149]. However, the yield-water supply ratio of the biofuels has been determined to be equivalent to that of conventional jet fuel by the studies mentioned above. In any case, water consumption is one among the essential sustainability feature to be taken into account.

Trade and Labour- Establishment of a biofuel infrastructure on a commercial scale is likely to have a positive impact on national socio-economic growth through creation of employment and international trade opportunities. This aspect plays a crucial role in developing nations where commercial scale biofuel production infrastructure ensures the improvement local rural economic and agronomic developments. However, it is essential to note that these developments occur in an ethical fashion in terms of uniform work hours, pay scales and not having a negative impact on the livelihood of the local population. The trade policies between the international biofuel production network and the local governments/ communities must be just and fairly communicated/ optimised to balance the culture shock.

9 RESEARCH CONCLUSIONS

Techno-Economic Environmental Risk Analysis (TERA) of advanced biofuels for Civil Engines was undertaken to holistically evaluate and quantify the prospects of advanced biofuels in civil aviation. This TERA study contributes to knowledge through conception plus application of quantitative/ qualitative approaches to assess the technical viability, financial feasibility and environmental competence of advanced biofuels from their application into the existing civil aviation infrastructure, relative to conventional jet fuel. The above mentioned objectives were achieved with the following quantitative/ qualitative approaches

- Development of a comprehensive "Cradle-grave" GHG emission prediction tool titled ALCEmB (Assessment of Life Cycle Emissions of Biofuels) to report the life cycle carbon intensity of existing and prospective aviation biofuels.
- Development and integration of a thermodynamic model for the jet performance simulation code, TURBOMATCH towards prediction of Bio-SPK directed engine/ aircraft performance prediction as a function of their systemic thermodynamic behaviour
- Assessment of Engine/ aircraft level performance and emissions imparted by the use of the advanced biofuels over user-defined engine cycle and mission profile specifications.
- Development of a two-part life cycle economic model titled ALCCoB (Assessment of Life Cycle Costs of Bio-SPKs) comprising ALCCoB-BP (Biofuel pricing) and ALCCoB-DOC (Direct operating cost) to predict the hypothetical cost of the Bio-SPKs towards prediction of aircraft operating cost over a user defined mission for a selected analysis period.

The assessments were undertaken and the key finding of this TERA study have been summarised as follows

9.1 Environmental competence

ALCEmB is a "Cradle-Grave" GHG emission prediction model devoted to advanced biofuels. Life cycle carbon savings delivered by 100% blends of Camelina SPK, Microalgae SPK and Jatropha SPK with respect to Jet-A1, were determined to be 70%, 58% and 64% respectively. The GHG emissions of each of the Bio-SPKs were calculated through ALCEmB by accounting region-specific feedstock-carbon intensity (e.g. fertiliser, water, fossil fuels) as opposed to standardised figures used in earlier literature [15], [18], [21], [58] [60] & [143]. The Bio-SPKs were able to clearly demonstrate their environmental competence at process level and system level against the reference fuel, Conv.Jet fuel. Among the Bio-SPKs, Camelina SPK was determined to possess the lowest carbon intensity among the biofuel candidates. Camelina feedstock may appear to be more environmentally viable option. However, the natural carbon sequestration and waste land reclamation capabilities of Microalgae and Jatropha can have an equally significant positive impact coupled with improvement of social-economic conditions and energy independence of developing nations. Further reductions in life cycle emissions may be achievable through

- Use of organic fertilizers and pesticides derived from Bio-crude production process
- Improvements in Plant/ strain yield characteristics.
- Further developments in management of biofuel plantations and Bio-crude extraction processes.
- Use of potential fuel type by-products of Bio-SPK production process.

However, upon grading the Bio-SPKs based on their "Cradle-grave" emissions, ALCEmB reports Camelina SPK has a relatively lower carbon intensity relative to the other two biofuel candidates.

Secondly, the rate of carbon sequestration is proportional to the carbon content of Bio-crude and subsequently Bio-SPKs, provided the mass and energy balance across the hydrotreatment process (for all the three types of bio-crudes) is maintained constant. The higher the capacity of biomass to fix CO_2, the higher will be the carbon content of Bio-SPK. Recent strain development efforts which include higher CO_2 fixation rate is expected to have a marked effect on the chemical composition of resultant biojet fuel [148]. However, there is a probability for UOP's Renewable jet process to find a solution to this issue through techno-economic improvements to the existing hydrocracking process; resulting in Bio-SPKs of standard compositions. Bio-SPKs, on an overall scale of study, have been determined to be a valuable asset in terms of following benefits associated with it besides sustainable method of energy generation. They include

- Afforestation,
- Waste land reclamation,
- Community uplift in developing countries

These benefits are likely to outweigh the drawbacks associated with life cycle emissions. However, this can be demonstrated only through long term life cycle assessment. The combustion emissions reported in this study, through theoretical calculations, will be required to be verified through simulation techniques to get a clearer portrait of Bio-SPKs combustion emissions within in aircraft engine. This study, however contributes to knowledge through a holistic environmental analysis of the carbon emissions allied with processes of each of the Bio-SPKs synthesis and the potential of these “Drop-in” biofuels in the aviation industry.

In terms of system level-emissions, Bio-SPKs were able to deliver CO_2 saving by 5.8- 6.3% on a complete mission level assessment. The higher hydrogen content improved their combustion characteristics in terms of comparatively cooler adiabatic flame temperature which was reflected as significant reduction in LTO NOx by 7-8% and mission NOx by 15-19% relative to Jet-A1.

9.2 Technical Viability

The engine performance of a numerically modelled (and validated) two-shaft CU-Jet, operated with the fuel candidates Conv.Jet fuel, Camelina SPK, Microalgae SPK and Jatropha SPK was predicted. The outcome of this performance was measured as specific fuel consumption (SFC-g.kN.sec) at fixed thrust rating. It was observed that the thermodynamic influence, imparted by the Bio-SPKs, on the performance of CU-Jet manifested as fuel savings and consequentially resulted in a reduction in engine SFC. Camelina SPK, Microalgae SPK and Jatropha SPK delivered a reduction in SFC by 1.78%, 1.75% and 1.8%, which was influenced by an average drop in fuel flow by 1.6%. Influence of fuel specific characteristics, primarily the lower heating value (LHV) was determined to have significant impact on fuel consumption characteristics of the engine. Increase in the LHV attributable to the Bio-SPKs (roughly +2.5%) boosts the enthalpy release from fuel combustion coupled with reduction in dissociation losses. The reason for this behaviour exhibited by the Bio-SPKs is their naturally higher hydrogen content (9-10% mass content) [Note: the enthalpy release of hydrogen is 4 times higher than that of carbon].

The engine level assessment was zoomed out to mission level evaluation, through user-definition of a fixed flight profile spanning over 4650km, to determine the mission fuel burn specific to each of the Bio-SPKs relative to the Conv.Jet fuel. Missions level performance was measured as kg of fuel burnt. LokAir operated with Camelina SPK, Microalgae SPK and Jatropha SPK delivered 3.7%, 3.1% and 3.8% fuel savings, relative to that of Jet-A1. Among the three Bio-SPKs, Jatropha SPK was determined to deliver the highest of fuel savings due to its relatively higher LHV (3.5%). However, a study to assess the degree of fuel economy achieved with a short and long range mission must be undertaken to fully comprehend their ability at fuel savings.

“Cradle-Grave” GHG emission analysis of Bio-SPKs, [Chapter 3] showed an avg. 60-70% reduction in life cycle emissions relative to that of, Conv.Jet fuel. However, for the purpose of ascertaining their systemic combustion emissions [highest LCE contributor, ≈70%], technical assessment entailing engine/ aircraft performance with the candidate fuels was undertaken. This outcome paved way to analyse Bio-SPKs from the context of systems level emission assessment through a representative virtual experiment.

Combustion emissions were predicted and quantified with importance to CO_2 and NOx emissions. It was determined that Bio-SPKs lowered LTO-NOx emissions by 7.1-8.3% without a compromise on engine performance. Consequently, at medium-range mission based emissions analysis, Camelina SPK, Microalgae SPK and Jatropha SPK were able to reduce their NOx emission by 18.2%, 15.1% and 18.9% respectively, relative to Jet-A1. The reason for the reduction in NOx emissions were determined to be due to the FAR ratio attributable to the Bio-SPKs (roughly 1.9-2% reduction) which in turn lowered the primary equivalence ratio within the modelled combustor. This created a drop in the adiabatic flame temperature which reflected as a reduction in NOx emissions. The reported reduction in mission CO_2 emission attributable to LokAir-C, LokAir-M and LokAir-J, relative to Conv.Jet fuel were quantified to be 6.2%, 5.8% and 6.3% respectively. This reduction in mission level CO_2 emissions were twin effect of innately lower C/H ratio of the Bio-SPKs and the fuel savings (from improved fuel burn).

9.3 Economic Feasibility

The market price of each of the Bio-SPKs was predicted through development of an elaborate life cycle cost prediction model (ALCCoB-BP) based their process resource and energy intensity. It is essential to note that the process technology currently devised for the Bio-SPKs are required to be perfected overtime and therefore this study has been conducted over medium (2020), long (2050) and very long (2075) term periods.

The second segment of the economic module developed to predict the DOC of the aircraft was termed "ALCCoB-DOC. The predicted market prices (cradle-gate cost) of each of the Bio-SPKs were adopted towards the DOC estimation of biofuel operated aircraft. The purpose of this analysis was to determine the financial competence of the advanced biofuels through a representative business case against a backdrop of varying emission taxation and fuel price scenarios. The market prices of each of the Bio-SPKs at baseline scenario have been determined to be £1.28, £1.37 and £1.32 /kg of Camelina SPK, Microalgae SPK and Jatropha SPK respectively, relative to £0.64/kg of Conv. jet fuel. The high biofuel prices result from the technology infancy attributable to the biofuel processing infrastructure. A sensitivity analysis was conducted to evaluate the effect of changing fossil-derived energy costs (regional unit costs of Natural gas, diesel and electricity) on biofuel prices under three scenarios: high baseline and low fossil fuel price (FFP) scenarios. Direct operating Cost of an aircraft operated with the Bio-SPKs produced in high, baseline and low FFP scenarios. This assessment was conducted from mission cost perspective since the cost parameters specific to the fuel (fuel cost and emissions cost). It is essential to note that the Conv.Jet fuel price was assumed to increase persistently without being affected by the global economic climate, supply-demand equilibrium or the political strategies. The missions cost evaluation resulted in Bio-SPKs exhibiting economic competence only at high FFP scenario in the current time period (2014).

A sensitivity analysis was conducted was conducted with varying fuel prices and aviation CO_2 emission taxation scenario. The price of conv. jet fuel was assumed to increase persistently without being affected by the supply demand equilibrium, global economic climate or political strategies over the period of analysis (2020-2075). On the other hand, the price of the Bio-SPKs were assumed to drop owing to technology maturity over the analysis period. From emissions cost perspective, the Conv.Jet fuel based CO_2 aviation was assumed to be taxed, unlike that of Bio-SPKs which are exempt from taxation as declared by EU biofuel policy. Bio-SPKs exhibit financial viability [measured in terms of mission cost (£/year)] from 2024 onwards by stabilising their fuel price through technology maturity and eventual improvement to the annual biofuel production capacity. However, the outstanding life cycle emissions of the Bio-SPKs begin to be taxed from 2050 onwards causes their mission cost to gradually rise. The reason for such taxation is due to the civil aviation's goal to move towards carbon neutral growth that will cause the industry to wean away from liquid fuels and look for "non-CO_2 emitting" technologies such as hybrid engines and aviation H_2. The rise in Bio-SPK specific mission cost (from 2050 onwards) was still observed to fall below that of the baseline fuel mission costs, providing an advantageous edge to the biofuel candidates. This study clearly acknowledges and informs the reader that the biofuels can prove to be economically viable only with market based measures as proposed in the "four pillars" strategy.

10 RECOMMENDATIONS FOR FUTURE WORK

Techno-economic Environmental Risk Assessment of Advanced Biofuels for Civil Aviation is a broad spectrum topic of interest and its ever expanding scope for analysis is a major advantage. A huge range of plant species are available as valuable biofuel feedstock. The environmental competence, economic feasibility and technical viability may vary depending on a number of factors including geographical locations, method of synthesis and resulting fuel properties. This is particular study was conducted with specifically chosen biofuel feedstock for their capacity to alleviate need for arable land use and claimed “drop-in” capability with the existing aero-engines. TERA of biojet fuels motivated the development and use of a models and tools of a variety of specialism indicated below to gather and bridge the limitations of earlier study.

- Life cycle studies
- Fuel chemistry
- Thermodynamic analysis
- Engine/ mission level performance modelling and simulation
- Environmental and
- Economic assessments

This study was instrumental in the development of the life cycle model called ALCEB – Assessment of Life CyclE of Biofuel which is composed of two main modules: the environmental module (ALCEmB) which evaluates and reports the “cradle-grave” life cycle emissions of any biofuels and the economic module which evaluated and reported the “cradle-gate” life cycle cost of any biofuels. The aim of these models was to deliver a method of exhaustively assessing alternative fuels (biofuels in specific) to achieve the TERA objective.

This study investigates the technical viability, economic feasibility and environmental competence of 100% Bio-SPKs, unlike any earlier studies. Due to lack of available literature, a number of educated assumptions had to be made to handle uncertainties encountered. An uncertainly analysis to evaluate the effect of the varying the different parameters assumed in this analyses on the outcomes would be a valuable addition to knowledge. For instance, the impact of increased fertiliser use on biomass yield and eventually the overall life cycle emission is crucial to environmental evaluation. From technical perspective, an uncertainty evaluation on the effect of fuel "performance properties (fuel LHV and density) on mission level fuel burn and range characteristics and eventually the associable emissions would expand the certainty of this assessment. From economic perspective, an elaborate evaluation on the effect of the uncertainties in Conv.Jet fuel price and the energy feedstock of the alternative fuels assessed could be a valuable addition to the certainty of this study.

10.1 Environmental Module

The aim of ALCEmB and ALCCoB were developed to aid prospective users to incorporate, evaluate and quantify the carbon intensity and the cost of any type of biofuel they may wish to investigate. Owing to the proprietary nature of the biojet fuels, this work involved exhaustive data extraction from available literature and use of industrially acceptable assumptions with the technical, economic and environmental modules.

A relatively higher quantities of water vapour released from combustion of Camelina SPK (+7.8%), Microalgae SPK (+7.7%) and Jatropha SPK (+7.8% relative to Conv.Jet-A1) is evident from the section 5.4.4.5 of Chapter 5. Though this study briefly touches upon the contrail forming potential of the Bio-SPKs, an assessment of its attributable global warming potential has not been reported due to high level of uncertainties associated with the assumptions. Besides water vapour emissions, many studies have indicated that the low carbon content of the fuel results in reduced soot emissions (a primer of condensation nuclei which leads to the formation of contrails). An elaborate contrails model which analyses and reports the environmental impact of Bio-SPKs accounting the lower soot production from Bio-SPKs combustion and the global warming potential at existing and optimised mission trajectories could be a valuable addition to existing literature. Similarly, this study was unable to account the aviation NOx emissions into overall life cycle emissions. The reason for this limitation is the lack of a definitive, standardised figure for GWP attributable to aviation NOx.

10.2 Technical Module

For the technical analysis, the system level functionality and mission level assessments were undertaken through numerical modelling and simulations at medium range. The true mission level behavioural and economic implications of these sustainable fuel candidates would have been more promising and absolutely exhaustive if conducted from short-long range mission assessments in addition to medium range.

This study was unable to arrive at conclusive evidence with other pollutant of the emission index (CO, UHC and soot) owing to uncertainties associated with their prediction. These uncertainties corresponds to estimated emissions varying with technologies used for the purpose, unavailability of specific data on fuel injection characteristics, fuel atomization and burning velocity. The above-mentioned were observed as the limitation of this techno-environmental study. With fuel specific thermo-physical properties available for Camelina SPK, Microalgae SPK and Jatropha SPK, a more precise prediction of combustion efficiency (energy release) attainable can also be determined. This would require the definition of fuel-specific parameters with include density, Reynolds number, mass transfer number and residence time to calculate the reaction and evaporation rates.

10.3 Economic Module

The outcome of the technical module: thermodynamic and system level functionality; questioned the proclaimed “drop-in nature” of the assessed biofuel candidates. One can be conclusive of its “drop-in” nature only upon undertaking experimental studies with the appropriate apparatus. In addition to these suggestions, the mechanical implications imparted by long term use of biofuels on engine/ aircraft life must also be accounted in future studies. Any wear/ tear imparted by the post combustion fluids from Bio-SPKs, on the hot end components of the engine and its subsequent feedback to the compressor can impact the overall engine life which can lead to variations in maintenance cost. However, the relatively cooler flames from biofuel combustion can have a positive impact on the combustor liner wall and eventually on the hot section which again is an issue that calls for an exhaustive virtual experiment. It is essential to carefully estimate TBO attributable to engines operated with the Bio-SPKs and the degree of this impact will be reflected as maintenance cost of the DOC of a given aircraft. The maintenance cost consideration hold significance not only to hardware reconfigurations and optimisation procedures but also on alternative fuel impact on the mechanical life of a given engine/aircraft operation.

An elaborate NPV (Net Present Value) evaluation of an aircraft operated with the candidate fuels is a valuable addition to this TERA study. An NPV evaluation is expected to educate the readers the commercial viability of biofuel application in an existing civil aviation infrastructure and open up scope for a range of techno-economical optimisation procedures appropriate for long, medium and short-haul routes.

A Techno-economic evaluation of the Bio-SPK processing infrastructure to identify the potential of this industry ability to keep up with the continuous demand for jet fuel over medium (2020), long (2050) and very long (2075) term period would be a valuable addition to this analysis. However, this has been omitted from this study since the current and future development in downstream processing technology is difficult to predict. Moreover, such an extensive evaluation falls outside the scope of this analysis but the outcome of such an assessment could improve the fidelity of future biofuel price prediction.

Comparison with Carbon Neutral Alternatives - Hydrogen

Commercial aviation aims to achieve carbon neutrality by 2050 at a global level. In order to achieve this goal, the aviation infrastructure will be required to adopt radical environmental solutions and wean-off liquid aviation fuels (due to the inevitable CO_2 emissions from their combustion). Among a range of solutions under consideration which include hybrid engines using electrical energy, H_2 is a popular contender. The choice of H_2 will demand major techno-economic commitments to the infrastructure and operation of global civil aviation infrastructure which includes conception of advanced engine and airframe designs, innovative fuel storage and management measures, optimised flight routes and trajectories (to reduce the incidence of contrail formation) on a global scale. The major advantage drawn form use of hydrogen as aviation fuel would be alleviation of CO_2 emissions. Beside the combustion based emissions, the technical, environmental, economic, societal and sustainability-based implications of aviation H_2 will have to be thoroughly analysed. H_2 has not been accounted for, in this study since TERA of advanced biofuels is devoted to evaluation of “liquid, renewable drop-in” fuels alone. Nevertheless, a holistic assessment of aviation H_2 could be valuable additions for comparative evaluation of alternative fuels.

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APPENDICES

Appendix A : Prediction of Bio-SPK composition

A.1 Estimation of Molecular formula of Camelina SPK

Carbon Type	Species Mass fraction (c)	C atoms / C-type (a)	H atoms/ C- type (b)	C atoms/ Component (d)	H atoms/ component (e)
iso 9	0.157	9	20	1.413	3.14
n9	0.025	9	20	0.22	0.5
iso 10	0.194	10	22	1.94	4.2
n 10	0.025	10	22	0.25	0.5
iso 11	0.175	11	24	1.92	4.2
n 11	0.021	11	24	0.23	0.5
iso 12	0.143	12	26	1.71	3.7
n 12	0.016	12	26	0.19	0.4
iso 13	0.109	13	28	1.41	3.0
n 13	0.013	13	28	0.16	0.3
iso 14	0.066	14	30	0.92	1.9
n 14	0.008	14	30	0.11	0.2
iso 15	0.039	15	32	0.58	1.2
n 15	0.005	15	32	0.07	0.16
iso 16	0.004	16	34	0.06	0.1
Total	1			**11.2 (x)**	**24.4 (y)**

A.2 Estimation of Molecular formula of Microalgae SPK

Carbon Type	**Species Mass fraction (c)**	**C atoms / C-type (a)**	**H atoms/ C- type (b)**	**C atoms/ Component (d)**	**H atoms/ component (e)**
iso 9	0.107	9	20	0.963	2.14
n9	0.048	9	20	0.432	0.96
iso 10	0.22	10	22	2.2	4.84
n 10	0.125	10	22	1.25	2.75
iso 11	0.05	11	24	0.55	1.2
n 11	0.058	11	24	0.638	1.392
iso 12	0.038	12	26	0.456	0.988
n 12	0.056	12	26	0.672	1.456
iso 13	0.041	13	28	0.533	1.148
n 13	0.011	13	28	0.143	0.308
iso 14	0.033	14	30	0.462	0.99
n 14	0.045	14	30	0.63	1.35
iso 15	0.046	15	32	0.69	1.472
n 15	0.042	15	32	0.63	1.344
iso 16	0.08	16	34	1.28	2.72
Total	1			**11.5**	**25.1**

A.3 Estimation of Molecular formula of Jatropha SPK

Carbon Type	Species Mass fraction (c)	C atoms / C-type (a)	H atoms/ C- type (b)	C atoms/ Component (d)	H atoms/ component (e)
iso 9	0.125	9	20	1.125	2.5
n9	0.026	9	20	0.234	0.52
iso 10	0.2	10	22	2	4.4
n 10	0.025	10	22	0.25	0.55
iso 11	0.191	11	24	2.101	4.584
n 11	0.018	11	24	0.198	0.432
iso 12	0.159	12	26	1.908	4.134
n 12	0.018	12	26	0.216	0.468
iso 13	0.123	13	28	1.599	3.444
n 13	0.01	13	28	0.13	0.28
iso 14	0.074	14	30	1.036	2.22
n 14	0.005	14	30	0.07	0.15
iso 15	0.024	15	32	0.36	0.768
n 15	0.002	15	32	0.03	0.064
iso 16	0	16	34	0	0
Total	1			**11.3 (x)**	**24.5 (y)**

A.4 Estimation of Molecular mass for Camelina SPK

Carbon Type	Species Mass fraction (c)	C atoms / C-type	H atoms/ C- type	C-type molar mass (f)	Component molar mass (cxf)
iso 9	0.16	9	20	128	20.4
n9	0.025	9	20	128	3.2
iso 10	0.194	10	22	142	27.5
n 10	0.025	10	22	142	3.55
iso 11	0.176	11	24	156	27.4
n 11	0.02	11	24	156	3.12
iso 12	0.145	12	26	170	24.6
n 12	0.016	12	26	170	2.72
iso 13	0.108	13	28	184	19.8
n 13	0.013	13	28	184	2.392
iso 14	0.066	14	30	198	13
n 14	0.008	14	30	198	1.5
iso 15	0.039	15	32	212	8.2
n 15	0.002	15	32	212	0.4
iso 16	0.003	16	34	226	0.6
Total	1				**159**

A.5 Estimation of Molecular mass for Microalgae SPK

Carbon Type	Species Mass fraction ©	C atoms/ C- type	H atoms/ C- type	C-type molar mass (f)	Component molar mass (cxf)
iso 9	0.107	9	20	128	13.696
n9	0.048	9	20	128	6.144
iso 10	0.22	10	22	142	31.24
n 10	0.125	10	22	142	17.75
iso 11	0.05	11	24	156	7.8
n 11	0.058	11	24	156	9.048
iso 12	0.038	12	26	170	6.46
n 12	0.056	12	26	170	9.52
iso 13	0.041	13	28	184	7.544
n 13	0.011	13	28	184	2.024
iso 14	0.033	14	30	198	6.534
n 14	0.045	14	30	198	8.91
iso 15	0.046	15	32	212	9.752
n 15	0.042	15	32	212	8.904
iso 16	0.08	16	34	226	18.08
Total	1				**163.4**

A.6 Estimation of Molecular mass for Jatropha SPK

Carbon Type	Species Mass fraction (c)	C atoms/ C- type	H atoms/ C- type	C-type molar mass (f)	Component molar mass (cxf)
iso 9	0.125	9	20	128	16
n9	0.026	9	20	128	3.328
iso 10	0.2	10	22	142	28.4
n 10	0.025	10	22	142	3.55
iso 11	0.191	11	24	156	29.796
n 11	0.018	11	24	156	2.808
iso 12	0.159	12	26	170	27.03
n 12	0.018	12	26	170	3.06
iso 13	0.123	13	28	184	22.632
n 13	0.01	13	28	184	1.84
iso 14	0.074	14	30	198	14.652
n 14	0.005	14	30	198	0.99
iso 15	0.024	15	32	212	5.088
n 15	0.002	15	32	212	0.424
iso 16	0	16	34	226	0
Total	1				**159.8**

Appendix B Hydrotreatment process (UOP-Honeywell)

The various stages of the hydrogenation process has been elaborated below

Hydrogenation: Hydrogenation of bio-crude takes place in the presence of a catalyst at a temperature of 320°C and elevated pressures of 1380 kPa. Hydrogenation brings about saturation of olefin compounds (replacement of double bonds with hydrogen atoms in the Hydrocarbon backbone. McCall et al, 2009, have indicated of reaction and material specification in the patent for hydrotreating bio-crude to Bio-SPKs which were also adopted into this study. The aim of Green jet fuel process is to produce higher fraction of Bio-SPKs over other lighter fuel fractions. The reaction specifications of temperature and pressure for hydrogenation have been presented in [94].

Hydro De-Oxygenation: Deoxygenation is a composite process of Decarboxylation, Decarbonylation and or Hydro-Deoxygenation. As the name of the process suggests, Decarboxylation aids the removal of carboxyl group from triglycerides. Decarbonylation is a means of removal of carbon monoxide from the treated oil. These processes are followed by deoxygenating the hydrogenated crude removing any oxygen atoms bound to the former. The oxygen atoms naturally bound to the bio-crude are removed in order to improve the specific energy of Bio-SPKs. This process also involves the conversion of olefins to straight chain paraffin in order to improve the thermal and oxidative stability of the resulting biojet fuel. The different pathways of hydrogenating the carboxyl groups have been presented in Eq 65-67.

Pathways of Decarboxylation of Hydrotreatment

$$H_2 + C_n\,COOH \xrightarrow{Catalyst} C_n + CO_2 \qquad \textbf{Eq 65}$$

$$H_2 + C_n\,COOH \xrightarrow{Catalyst} C_n + CO + H_2O \qquad \textbf{Eq 66}$$

$$H_2 + CO + H_2O \xrightarrow{Catalyst} CO_2 + H_2 \qquad \textbf{Eq 67}$$

Carbon emissions associated with this process and other by-products include CO, CO_2, H_2O, H_2S and propane. The existing paraffinic chains are to be subjected to further chemical conversion in order to make the resultant fuel meet the specification of an aviation fuels with a 14-18 carbon chain length.

Isomerization and Selective Hydrocracking: Hydrocracking is a process by which long paraffinic chain is hydrocracked to smaller carbon numbers. Hydrocracking takes place at higher temperatures of 390°C and elevated pressures of 7500 kPa in the presence of excess hydrogen supply. The cracked carbon chains will be isomerized in the isomerization reaction at temperatures of 255°C and comparatively reduced pressures of 3275 kPa. The isomerization reaction produces carbon chains of varying length, fractionated according to their density ranges in a relatively cooled separator (Equation 68-69).

Pathway of Selective Cracking and Isomerisation

$$\boldsymbol{nC_{n+1} + nC_n \xrightarrow{Catalyst} iC_{n+1} + iC_n} \quad \textbf{Eq 68}$$

$$\boldsymbol{iC_n \xrightarrow{Catalyst} iC_{n-y} + iC_y} \quad \textbf{Eq 69}$$

Appendix C Life cycle emissions of Conventional Jet-A1

Conventional Jet Kerosene

Jet Kerosene has remained the unbeatable fuel of choice, owing to its desirable handling and combustion properties. As a consequence, CJK has been adopted as the reference fuel to determine the environmental impact of the biojet fuels. The Assumptions that have been adopted for the LCA of Jet Kerosene are listed below.

- Crude oil is sourced from the North Sea
- The CO_2 emissions calculated at every step correspond to the combustion of fossil derived energy at an efficiency of 99.4% [75], [114].
- Emissions adapted from earlier literature have been corrected by adding a 7% credit to account for technological advances.

Crude Extraction

The location of the crude oil extraction site is crucial to this study owing to the emissions released from transport and acquisition of the raw material. Identification of the oil well is followed by drilling a hole into the earth. The crude oil is pumped out with the natural pressure that is built up within the oil well. The recovery % at this phase is 5-15% [85]. The excess natural gas released at this stage is released in the form of flares which in turn is legally restricted [122].

A steel casing bored into the well is expected to maintain the structural integrity of the well and the petroleum is manually pumped out. The recovery % at this stage is determined to be 45-55%. This stage is followed by tertiary oil extraction process which, at the point of completion leads to the % recovery of 98%. Crude extraction is a fossil-derived energy intensive process.

Crude Oil transportation (marine)

The extracted crude oil is transported to the petroleum refinery to be processed to consumable distillates. Location of the crude oil extraction site influences its LCE as mentioned earlier. The crude oil is assumed to be transported through sea with the aid of oil tankers using heavy fuel oil. The emissions figures for this process were adapted from two studies [75] & [85].

Refining

Crude refining is a multistage process with varying reaction conditions and thus uncertain levels of energy consumption. Lewis C.A., (1997), stated that a comprehensive emissions analysis of the refining process requires certain considerations which are feedstock parameters, frame work of refinery, demand for products and product specifications [85]. A standard refinery is adopted for the life cycle study thereby creating a baseline scenario for Jet Kerosene emissions assessment.

Desalter

The crude oil is directed to a desalter unit where it is scrubbed of its salt content (Calcium, Sodium and Magnesium chloride). This is carried out in order to prevent water hydrolysis at reaction temperature downstream of the refining process [75]. This may be quoted as the first stage of purification and the products include desalted crude, salt and water.

Distillation

The desalted crude is distilled at atmospheric conditions and varying temperatures. A range of distillates (light to heavy) are extracted through distillation of crude oil. Light fractions (Naphtha & Gasoline) are acquired between 30 to 180°C and middle fraction (Gas oil) between 180 to 360°C.The heavier fraction pass through vacuum distillation operating at >360°C to produce by-products including Heavy fuel oil. Some heavy fractions are made to pass through to catalytic reformation to produce hydrogen. The products of catalytic reformation are subjected to alkylation and isomerization to form higher octane-numbered hydrocarbons.

Merox Treatment

Merox (MERcaptan OXidation) treatment is a process by which the mercaptans present in the kerosene fraction are oxidized in the presence of a catalyst thereby sweetening the Jet fuel fraction [75].

Jet Kerosene transportation

Refined sweetened kerosene will be transported to storage facilities and airports. The distance between the refinery and storage facility is assumed to be an average of 150 kilometres. Individual GHG emissions for Jet kerosene transportation were validated with studies [18].

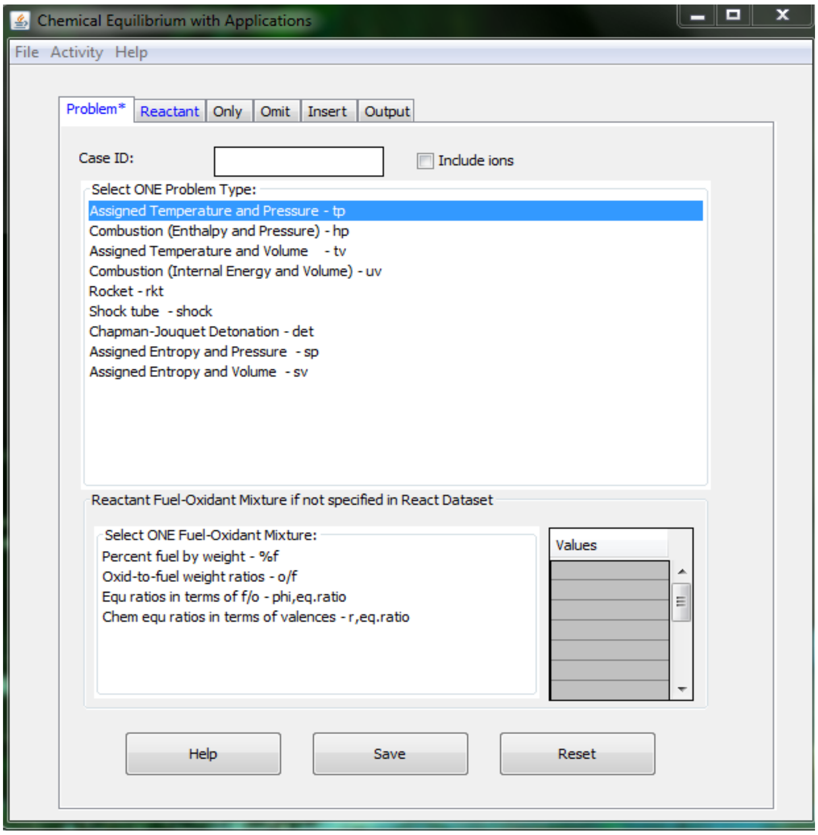
Jet Kerosene Consumption

Jet Kerosene is assumed to undergo non-dissociated combustion within an aero-engine upon operation. This assumption has been included solely for the purpose of deriving a numerical figure to complete the Well – wake life cycle emissions of the reference fuel

Life Cycle stage	GHGs and their emissions (gCO_2e/MJ)		Emissions (gCO_2e/MJ of fuel)
Crude Oil Extraction	CO_2	4.2	10.5
	NO_x	2.9	
	CH_4	1.4	
Crude Transportation (marine)	CO_2	0.6	8.5
	NO_x	4.8	
Refining process	CO_2	3.9	13.5
	NO_x	9.5	
	CH_4	0.007	
Jet Kerosene Transportation	CO_2	0.11	0.6
	NO_x	0.52	
Jet Kerosene Consumption	CO_2	72.5	72.5
Total Emissions			105.9

Appendix D : Introduction to NASA Chemical Equilibrium with Application

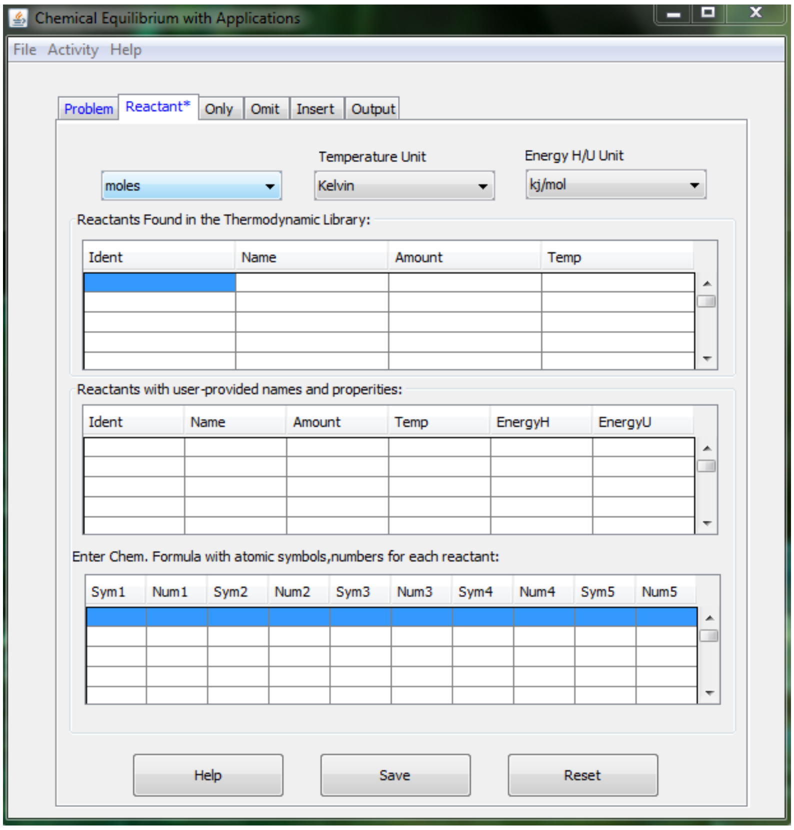
A new version of NASA CEA can be downloaded from NASA webpage resulting in a graphic user interface called as *CEAgui-win* file which is a graphic user interface- a simpler mode of getting familiar NASA CEA. The



Figure_Apx 1: A Screenshot of NASA CEA (Problem tab)

The CEA code has a series of Datasets where the user-defines the conditions for combustion and output of analysis. These datasets include the following

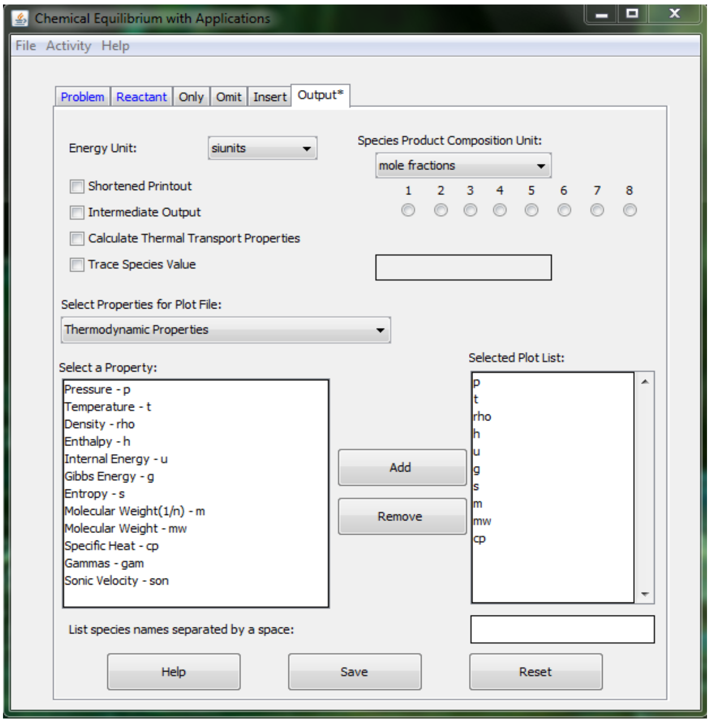
1. ***Problem* tab** - "tp" was chosen towards this gas model development. The range of temperatures (200-3000K) can be entered in the temperature section with the suitable units chosen. The range of pressures chosen for this analysis (0.5- 50 atm) is entered under the pressure section in a similar fashion.



2. ***Reactants* tab –** The reactants can be chosen from a wide range of species available from the thermodynamic library. e.g. the reference fuel, Jet A, was readily available from the library window. However, users may be required to specify the composition of the unknown reactants. For instance. The compositions of the Bio-SPKs were specified with their atomic symbols and numbers. The Oxidant in all the cases was chosen as Air. It is essential to note that Jet-A11 fuel present in the Reactant tab only has its Carbon and hydrogen make up. The aromatics content was additionally fed into the program when generating tables for the reference fuel. The amount of aromatics added was in line with the current aromatics specification of 8% by volume of Jet A-1.
3. ***Only* tab**- This tab is useful in the case of evaluation of non-dissociation combustions where the user can define a specific set of combustion products required for his/her analysis.
4. ***Omit* tab**- certain species such as H_2O (cr), H_2O (l) were omitted from this analysis to avoid problems of convergence and discrepancies in plotting the caloric properties of the combustion products.

5. ***Insert* tab** – Insert tab is used to specify the set of condensed products to be added to the set of gaseous products in the output section.

6. ***Output* tab –** The output tab comprises of a list of thermodynamic properties which calculable by the CEA code. The user may also create PLOT files by selecting the caloric properties of their interest.



Figure_Apx 2: Output Tab of NASA CEA

Appendix E Thermodynamic property tables and Combustion products of candidate fuels

JETA1

Caloric Properties

Temp	N2	O2	Ar	Ne	H2O	CO2	CO	SO2	Stoic FAR	Stoic Air	h Enthalpy	s Entropy	γ Gamma	Cp Specific Heat	μ Viscosity	R Gas Constant
200	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	-102.9	5.3821	1.3832	1.0368	0.12536	287.234
300	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	2	5.8069	1.3715	1.0605	0.17771	287.259
400	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	109.3	6.1154	1.3599	1.0853	0.22367	287.227
500	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	219.1	6.3605	1.3479	1.113	0.26525	287.271
600	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	332	6.5661	1.3355	1.1435	0.3036	287.266
700	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	447.9	6.7447	1.3235	1.1752	0.33943	287.251
800	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	567	6.9037	1.3125	1.2064	0.37324	287.238
900	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	689.1	7.0475	1.3029	1.2358	0.40538	287.300
1000	0.73064	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	814.1	7.1791	1.2945	1.2628	0.43611	287.288
1100	0.73065	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	941.6	7.3007	1.2872	1.2873	0.46556	287.222
1200	0.73064	0	0.00876	0	0.12857	0.13203	0	0	0.06802	88.536	1071.4	7.4136	1.281	1.3094	0.49392	287.230
1300	0.73064	0	0.00876	0	0.12856	0.13202	0	0	0.06802	88.536	1203.4	7.5193	1.2757	1.3293	0.52139	287.284
1400	0.73064	0	0.00876	0	0.12856	0.13202	0.00001	0	0.06802	88.536	1337.3	7.6185	1.2709	1.3481	0.54815	287.356
1500	0.73063	0.00001	0.00876	0	0.12855	0.132	0.00003	0	0.06802	88.536	1473	7.7121	1.2665	1.366	0.57429	287.437
1600	0.7306	0.00003	0.00876	0	0.12853	0.13195	0.00007	0	0.06802	88.536	1610.5	7.8009	1.2622	1.3845	0.59991	287.606
1700	0.73054	0.00007	0.00876	0	0.1285	0.13186	0.00015	0	0.06802	88.536	1750	7.8854	1.2578	1.4054	0.62507	288.052
1800	0.73044	0.00014	0.00876	0	0.12843	0.13167	0.00032	0	0.06802	88.536	1891.75	7.9664	1.2529	1.4306	0.64981	288.769
1900	0.73025	0.00026	0.00876	0	0.12831	0.13135	0.00063	0	0.06802	88.536	2036.35	8.0446	1.2473	1.4627	0.67418	290.007
2000	0.72993	0.00046	0.00876	0	0.12812	0.1308	0.00113	0	0.06802	88.536	2184.6	8.1206	1.2408	1.5041	0.69819	291.898
2100	0.72944	0.00077	0.008755	0	0.12782	0.12993	0.00193	0	0.06802	88.536	2337.58	8.1952	1.2333	1.5577	0.72186	294.666
2200	0.7287	0.00122	0.00875	0	0.12739	0.12865	0.00311	0	0.06802	88.536	2496.62	8.2692	1.225	1.6258	0.74521	298.616
2300	0.72764	0.00185	0.00874	0	0.12676	0.12681	0.0048	0	0.06802	88.536	2663.28	8.3433	1.2162	1.7103	0.76823	304.035
2400	0.72619	0.0027	0.00872	0	0.12589	0.12429	0.00712	0	0.06802	88.536	2839.26	8.4182	1.2072	1.8123	0.79094	311.057
2500	0.724	0.00379	0.0087	0	0.12472	0.12099	0.01015	0	0.06802	88.536	3026.32	8.4945	1.1984	1.9318	0.81332	319.817
2600	0.72179	0.00515	0.00868	0	0.12319	0.1168	0.01399	0	0.06802	88.536	3226.17	8.5729	1.1902	2.0677	0.83539	330.429
2700	0.7187	0.00677	0.00865	0	0.12123	0.11169	0.01867	0	0.06802	88.536	3440.32	8.6537	1.183	2.2173	0.85715	342.997
2800	0.71495	0.00863	0.00862	0	0.1188	0.10564	0.02419	0	0.06802	88.536	3669.96	8.7372	1.1768	2.3768	0.87862	357.086
2900	0.71052	0.01069	0.00858	0	0.11584	0.09874	0.03047	0	0.06802	88.536	3915.9	8.8235	1.1719	2.5417	0.89982	372.829
3000	0.70543	0.01287	0.00853	0	0.11231	0.09111	0.03737	0	0.06802	88.536	4178.3	8.9124	1.1681	2.7072	0.9208	389.590

Camelina spk

Temp	N2	O2	Ar	Ne	H2O	CO2	CO	SO2	Stoic FAR	Stoic Air	Caloric Properties: h Enthalpy	s Entropy	γ Gamma	Cp Specific Heat	μ Viscosity	R Gas Constant
200	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**-103.5**	5.4118	1.3829	1.0439	0.1252	289.037
300	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**2**	5.8394	1.3716	1.0669	0.17753	289.049
400	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**109.9**	6.1496	1.3603	1.0913	0.22358	289.050
500	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**220.4**	6.396	1.3483	1.1188	0.26527	289.014
600	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**333.8**	6.6027	1.336	1.1493	0.30373	289.046
700	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**450.3**	6.7822	1.324	1.1811	0.33967	289.031
800	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**570**	6.942	1.313	1.2124	0.37358	289.018
900	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**692.7**	7.0865	1.3033	1.2419	0.40581	289.011
1000	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**818.3**	7.2188	1.2949	1.2692	0.43662	289.047
1100	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**946.4**	7.341	1.2876	1.294	0.46615	289.030
1200	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**1077**	7.4545	1.2813	1.3164	0.49457	289.006
1300	0.72713	0	0.00872	0	0.13756	0.12658	0	0	0.066576	82.479	**1209.6**	7.5607	1.2759	1.3366	0.52211	289.026
1400	0.72713	0	0.00872	0	0.13756	0.12657	0.00001	0	0.066576	82.479	**1344.3**	7.6605	1.271	1.3557	0.54891	289.060
1500	0.72711	0.00001	0.00872	0	0.13755	0.12656	0.00006	0	0.066576	82.479	**1480.8**	7.7546	1.2666	1.3739	0.57511	289.185
1600	0.72709	0.00003	0.00872	0	0.13753	0.12651	0.00015	0	0.066576	82.479	**1619.1**	7.8439	1.2623	1.3927	0.60078	289.397
1700	0.72703	0.00007	0.00872	0	0.13749	0.12642	0.00015	0	0.066576	82.479	**1759.4**	7.9289	1.2578	1.4137	0.62598	289.753
1800	0.72693	0.00014	0.00872	0	0.13742	0.12624	0.00031	0	0.066576	82.479	**1901.99**	8.0104	1.2529	1.4391	0.65076	290.485
1900	0.72674	0.00026	0.00872	0	0.13729	0.12593	0.00061	0	0.066576	82.479	**2047.45**	8.0891	1.2473	1.4713	0.67516	291.712
2000	0.72643	0.00045	0.00871	0	0.13709	0.1254	0.00109	0	0.066576	82.479	**2196.56**	8.1656	1.2408	1.5128	0.69921	293.587
2100	0.72594	0.00075	0.00871	0	0.13678	0.12456	0.00186	0	0.066576	82.479	**2350.41**	8.2406	1.2334	1.5664	0.72291	296.415
2200	0.72521	0.00119	0.0087	0	0.13631	0.12332	0.00301	0	0.066576	82.479	**2510.32**	8.315	1.2252	1.6343	0.74628	300.395
2300	0.72417	0.00181	0.00869	0	0.13564	0.12154	0.00465	0	0.066576	82.479	**2677.82**	8.3894	1.2164	1.7186	0.76933	305.742
2400	0.72274	0.00264	0.00868	0	0.13472	0.11911	0.00689	0	0.066576	82.479	**2854.626**	8.4647	1.2074	1.8204	0.79205	312.697
2500	0.72084	0.00371	0.00866	0	0.13348	0.11591	0.00983	0	0.066576	82.479	**3042.49**	8.5413	1.1986	1.9397	0.81445	321.395
2600	0.7184	0.00503	0.00864	0	0.13187	0.11186	0.01355	0	0.066576	82.479	**3243.12**	8.62	1.1905	2.0754	0.83652	332.099
2700	0.71535	0.00661	0.00861	0	0.1298	0.10691	0.01809	0	0.066576	82.479	**3458.04**	8.7011	1.1832	2.225	0.85828	344.506
2800	0.71166	0.00843	0.00858	0	0.12723	0.10107	0.02343	0	0.066576	82.479	**3688.46**	8.7849	1.1771	2.3848	0.87974	358.804
2900	0.70729	0.01043	0.0854	0	0.1241	0.09441	0.02949	0	0.066576	82.479	**3935.2**	8.8715	1.1721	2.5504	0.90093	374.476
3000	0.70225	0.01255	0.0849	0	0.12037	0.08706	0.03615	0	0.066576	82.479	**4198.6**	8.9607	1.1683	2.7172	0.92188	391.428

Jatropha SPK

Temp	N2	O2	Ar	Ne	H2O	CO2	CO	SO2	Stoich FAR	Stoich Air
200	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
300	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
400	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
500	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
600	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
700	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
800	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
900	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1000	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1100	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1200	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1300	0.72729	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1400	0.72728	0	0.00872	0	0.13716	0.12682	0	0	0.066578	82.755
1500	0.72727	0.00001	0.00872	0	0.13715	0.1268	0.00002	0	0.066578	82.755
1600	0.72724	0.00003	0.00872	0	0.13713	0.12675	0.00006	0	0.066578	82.755
1700	0.72719	0.00007	0.00872	0	0.13709	0.12666	0.00015	0	0.066578	82.755
1800	0.72708	0.00014	0.00872	0	0.13702	0.12648	0.00031	0	0.066578	82.755
1900	0.72689	0.00026	0.00872	0	0.13689	0.12617	0.00061	0	0.066578	82.755
2000	0.72658	0.00045	0.00872	0	0.13669	0.12564	0.0011	0	0.066578	82.755
2100	0.72609	0.00075	0.00871	0	0.13638	0.1248	0.00187	0	0.066578	82.755
2200	0.72537	0.0012	0.00871	0	0.13591	0.12355	0.00302	0	0.066578	82.755
2300	0.72433	0.00181	0.0087	0	0.13525	0.12177	0.0047	0	0.066578	82.755
2400	0.7229	0.00264	0.00868	0	0.13433	0.11964	0.007	0	0.066578	82.755
2500	0.721	0.00371	0.00866	0	0.1331	0.11613	0.00985	0	0.066578	82.755
2600	0.71855	0.00504	0.00864	0	0.13148	0.11208	0.01357	0	0.066578	82.755
2700	0.7155	0.00662	0.00861	0	0.12942	0.10712	0.01811	0	0.066578	82.755
2800	0.7118	0.00844	0.00858	0	0.12686	0.10128	0.02346	0	0.066578	82.755
2900	0.70743	0.01044	0.00854	0	0.12374	0.0946	0.02954	0	0.066578	82.755
3000	0.70239	0.01257	0.00849	0	0.12001	0.08724	0.03621	0	0.066578	82.755

Caloric Properties

Temp	h Enthalpy	s Entropy	γ Gamma	Cp Specific Heat	μ Viscosity	R Gas Constant
200	-103.6	5.4105	1.3829	1.0436	0.1252	288.954
300	1.9	5.838	1.3716	1.0666	0.17754	288.968
400	109.8	6.1481	1.3602	1.091	0.22358	288.912
500	220.3	6.3945	1.3483	1.1186	0.26527	288.963
600	333.6	6.6011	1.336	1.149	0.30372	288.970
700	450.1	6.7806	1.324	1.1808	0.33966	288.957
800	569.8	6.9403	1.313	1.2121	0.37356	288.947
900	692.5	7.0848	1.3033	1.2416	0.40579	288.941
1000	818	7.217	1.2949	1.2689	0.4366	288.979
1100	946.2	7.3392	1.2876	1.2937	0.46612	288.963
1200	1076.7	7.4527	1.2813	1.3161	0.49454	288.940
1300	1209.3	7.5589	1.2759	1.3362	0.52207	288.939
1400	1343.9	7.6586	1.271	1.3553	0.54888	288.974
1500	1480.4	7.7528	1.2666	1.3735	0.57507	289.101
1600	1618.7	7.842	1.2623	1.3923	0.60074	289.313
1700	1758.9	7.927	1.2578	1.4134	0.62594	289.692
1800	1901.48	8.0085	1.2529	1.4388	0.65072	290.424
1900	2046.89	8.0871	1.2473	1.4709	0.67512	291.633
2000	2195.97	8.1636	1.2408	1.5124	0.69916	293.509
2100	2349.78	8.2386	1.2334	1.566	0.72286	296.339
2200	2509.65	8.313	1.2252	1.6339	0.74623	300.322
2300	2677.12	8.3874	1.2164	1.7183	0.76928	305.689
2400	2853.884	8.4626	1.2074	1.8201	0.792	312.646
2500	3041.71	8.5393	1.1986	1.9394	0.8144	321.346
2600	3242.31	8.6179	1.1905	2.0751	0.83647	332.051
2700	3457.2	8.699	1.1832	2.2247	0.85823	344.460
2800	3687.59	8.7828	1.177	2.3845	0.87969	358.587
2900	3934.3	8.8693	1.1721	2.5501	0.90088	374.432
3000	4197.6	8.9586	1.1683	2.7168	0.92183	391.370

Microalgae SPK

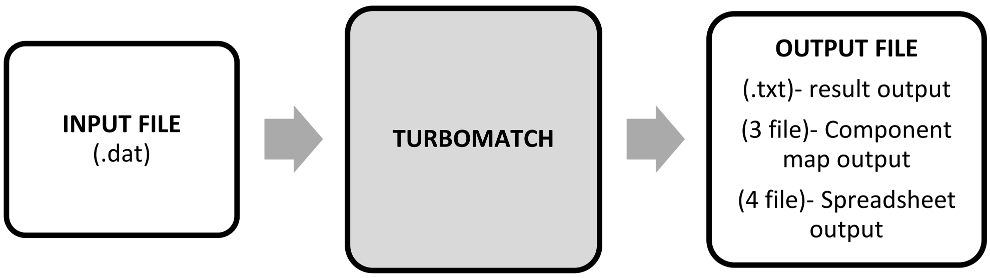
Temp	N2	O2	Ar	Ne	H2O	CO2	CO	SO2	Stoic FAR	Stoic Air
200	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
300	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
400	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
500	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
600	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
700	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
800	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
900	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
1000	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
1100	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
1200	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
1300	0.7272	0	0.00872		0.13738	0.12669	0		0.066587	84.49
1400	0.7272	0	0.00872		0.13738	0.12668	0.00001		0.066587	84.49
1500	0.72718	0.00001	0.00872		0.13737	0.12666	0.00002		0.066587	84.49
1600	0.72716	0.00003	0.00872		0.13735	0.12662	0.00006		0.066587	84.49
1700	0.7271	0.00007	0.00872		0.13731	0.12653	0.00015		0.066587	84.49
1800	0.72699	0.00014	0.00872		0.13724	0.12635	0.00031		0.066587	84.49
1900	0.7268	0.00026	0.00872		0.13711	0.12603	0.00061		0.066587	84.49
2000	0.7265	0.00045	0.00872		0.13691	0.1255	0.00109		0.066587	84.49
2100	0.726	0.00075	0.00871		0.1366	0.12467	0.00186		0.066587	84.49
2200	0.725	0.0012	0.0087		0.13613	0.12342	0.00302		0.066587	84.49
2300	0.724	0.0028	0.00869		0.13547	0.12164	0.005		0.066587	84.49
2400	0.723	0.0026	0.00868		0.13455	0.11921	0.0069		0.066587	84.49
2500	0.72091	0.00371	0.00866		0.13331	0.11601	0.00984		0.066587	84.49
2600	0.71847	0.00504	0.00864		0.13169	0.11196	0.01356		0.066587	84.49
2700	0.71542	0.00662	0.00861		0.12963	0.10701	0.0181		0.066587	84.49
2800	0.71172	0.00843	0.00858		0.12707	0.10116	0.02344		0.066587	84.49
2900	0.7055	0.01043	0.00854		0.12394	0.0945	0.02951		0.066587	84.49
3000	0.70231	0.01256	0.00849		0.12021	0.08714	0.03618		0.066587	84.49

Caloric Properties

Temp	h	s	γ	Cp	μ	R
	Enthalpy	Entropy	Gamma	Specific Heat	Viscosity	Gas Constant
200	-103.5	5.4113	1.3829	1.0438	0.1252	289.009
300	2	5.8388	1.3716	1.0668	0.17754	289.022
400	109.9	6.149	1.3603	1.0912	0.22358	289.024
500	220.3	6.3953	1.3483	1.1187	0.26527	288.989
600	333.7	6.602	1.336	1.1492	0.30373	289.020
700	450.2	6.7815	1.324	1.1809	0.33966	288.982
800	569.9	6.9412	1.313	1.2122	0.37357	288.971
900	692.6	7.0858	1.3033	1.2418	0.4058	288.988
1000	818.2	7.218	1.2949	1.2691	0.43661	289.024
1100	946.3	7.3402	1.2876	1.2939	0.46614	289.007
1200	1076.8	7.4537	1.2813	1.3163	0.49456	288.984
1300	1209.5	7.5599	1.2759	1.3364	0.52209	288.982
1400	1344.1	7.6597	1.271	1.3555	0.5489	289.017
1500	1480.6	7.7538	1.2666	1.3737	0.57509	289.143
1600	1618.9	7.8431	1.2623	1.3925	0.60076	289.355
1700	1759.2	7.9281	1.2578	1.4136	0.62596	289.733
1800	1901.76	8.0096	1.2529	1.439	0.65074	290.465
1900	2047.2	8.0882	1.2473	1.4711	0.67514	291.672
2000	2196.3	8.1647	1.2408	1.5127	0.69919	293.567
2100	2350.13	8.2397	1.2334	1.5662	0.72289	296.377
2200	2510.02	8.3141	1.2252	1.6342	0.74626	300.377
2300	2677.51	8.3885	1.2164	1.7185	0.76931	305.725
2400	2854.296	8.4637	1.2074	1.8203	0.79203	312.680
2500	3042.15	8.5404	1.1986	1.9396	0.81442	321.379
2600	3242.76	8.6191	1.1905	2.0753	0.8365	332.083
2700	3457.67	8.7002	1.1832	2.2248	0.85826	344.475
2800	3688.07	8.7839	1.1771	2.3847	0.87972	358.789
2900	3934.8	8.8705	1.1721	2.5503	0.9009	374.462
3000	4198.2	8.9598	1.1683	2.717	0.92186	391.399

Appendix F : A Brief Introduction to TURBOMATCH

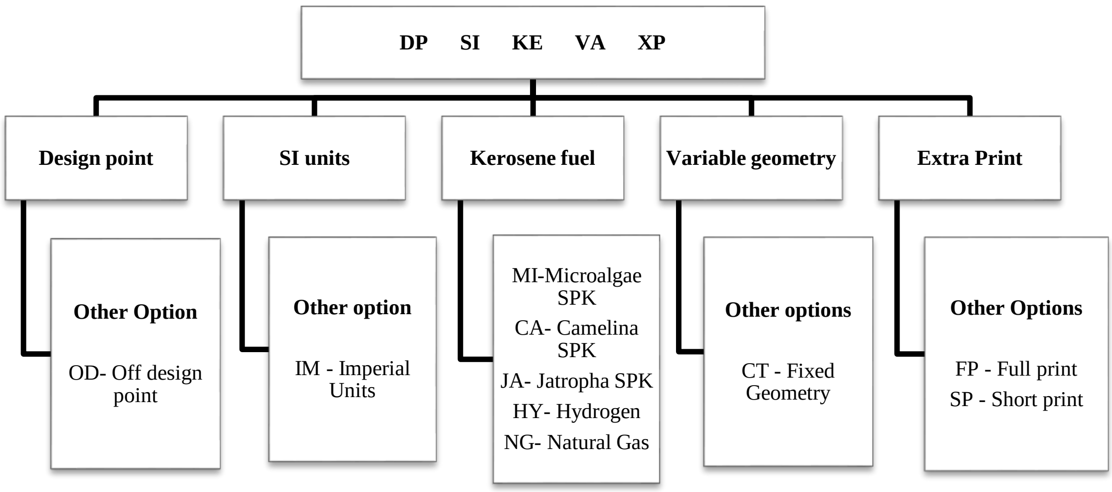
TURBOMATCH is a code that was developed at Cranfield University to facilitate digital modelling and numerical simulation of gas turbine performance. The simulations were carried out using code words termed as “BRICKS” which recognizes the various components and stations of a given engine. These Pre-programmed units called “Bricks Data” formulate the order of input into the TURBOMATCH through the **“.dat”** file and present the primary performance data either as Net thrust or Shaft power depending upon the nature and purpose of the engine. Secondary parameters include SFC, fuel flow, and thermal efficiency. Other intrinsic specifications such as individual component performance with its cycle thermodynamic parameters at each of the stations can also be extracted using TURBOMATCH. This output is provided in the **“.txt”** file.



Figure_Apx 3: TURBOMATCH SCHEME

A brief introduction to the operational selection of engine performance analysis and options available with relevance to this analysis has been illustrated in the appendix section. More detailed information on working principle behind this scheme can be obtained through the TURBOMATCH manual (Cranfield university and Theo manual).

The Operational brick provides information regarding the settings for the given engine. It is made of 5 commands each of which corresponds to a specification chosen and provided by the user. They are as follows



Figure_Apx 4: Description of operation selection and its options in TURBOMATCH ver 2.0

As mentioned earlier, pre-programmed units called Bricks facilitate the input of engine operational variables towards construction of desired engine of choice with relative ease. The Bricks assigned for the various components are as follows.

INTAKE	Intake
COMPRE	Compressor
BURNER	Combustion chamber
TURBIN	Turbine
DUCTER	Duct
NOZCON	Nozzle
PERFOR	Performance output

Table 0-1: Bricks corresponding to individual components of a Gas turbine

This program is also capable of carrying out arithmetical operations when using ARITHY command. Further information on the nature of performance calculations can be obtained by referring to the TURBOMATCH manual [37].

Appendix G Off-design performances analysis

G.1 Effect of Altitude

High Bypass Turbofan is a form of turbojet engine fitted with a large fan which has been designed to attain higher propulsive efficiency with relatively modest jet velocity (V_j) and a relatively large mass flow (W). Large quantities of mass flow are derived from the bypass and core flow, the proportions of which may vary with the design bypass ratio of the engine. In any case, relatively higher fraction of energy is required to drive the turbine component which in turn drives the fan Therefore, the core jet velocity is of modest significance to the resulting net thrust (Fn).

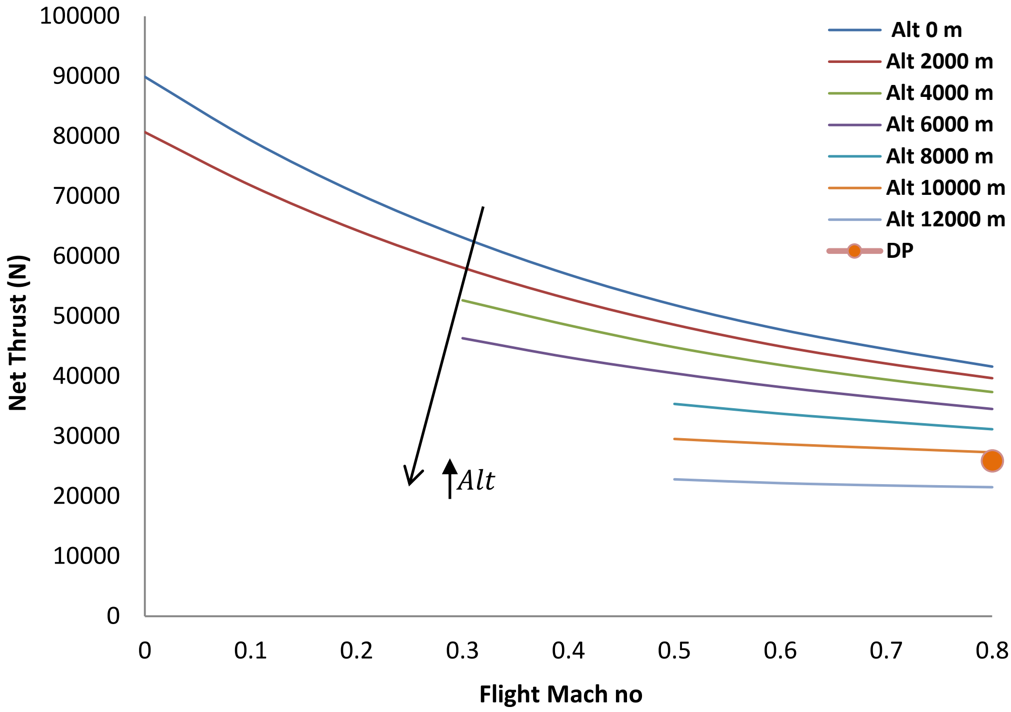
Off design analysis is conducted for a specific engine with an established design point, in order to derive its threshold limits of operation. Moreover, an off design performance analysis also enables the user comprehend and improve the level of confidence in the way TURBOMATCH performs its thermodynamic cycle calculations and performance prediction. An off-design analysis has been undertaken below to evaluate the impact of varying altitude and ambient temperature on the performance characteristics of CU-Jet. Mach no and Turbine entry temperature (TET) have been chosen as handle for each of the assessments.

G.2 Mach no as handle

This off-design analysis investigates the effect of flight altitude on the performance of CU-Jet. Mach no is used as the handle and can affect the core mass flow, compressor pressure ratio, and temperature rise across the combustor, jet velocity and eventually the net thrust or collectively summarised as affecting specific thrust. When considering operating conditions, it is in universal agreement that the temperature, pressure and density of the air reduces from seal level static conditions to the highest engine-operable altitude (12000m) chosen for this study [Table 0-2].

Altitude (m)	T_{amb} (K)	P_{amb} (kPa)	Relative density
0.0	288.15	101.32	1.0
12000.0	216.7	19.4	0.2546

Table 0-2: Altitude specific ambient conditions



Figure_Apx 5: Effect of altitude and flight Mach no on Net Thrust at constant TET (ISA conditions)

At lower altitudes and lower mach numbers, the air mass flow is higher due to intake of relatively dense air and the intake momentum drag experienced by the engine is relatively lower which eventually boosts net thrust [Eq 70]. However, gradual increase in Mach no at lower altitudes has a pronounced negative effect on the thrust which is exhibited as a linear drop in thrust with increasing Mach numbers. However, this drop is less pronounced for an engine operating at higher altitudes i.e. the degree of drop in net thrust at higher altitude is relatively lower due to the recovery of losses by ram effect (increase in mass flow aided by the increase in pressure at the intake. [Equation 72] exponential increased the intake momentum drag which has a negative impact on Net thrust as evident from.

Net Thrust = Gross Thrust – Intake Momentum Drag

$$F_n = F_g - F_d \qquad \textbf{Eq 70}$$

Gross thrust is defined as the sum of momentum thrust and pressure thrust defined in eq

$$F_g = (W \times V_j) + A\,(P_j - P_0) \qquad \textbf{Eq 71}$$

$$F_n = [(W \times V_j) + A\,(P_j - P_0)] - (W \times V_0)$$

$$= W\,(V_j - V_0) + A\,(P_j - P_0) \qquad \textbf{Eq 72}$$

[Note: $P_j = P_0$ for fully expanded nozzles (subsonic engines)]

Where,

Fn	*= Net Thrust, kN*
Fg	*= Gross Thrust, kN*
Fd	*= Intake Momentum Drag, kN*
W	*= Core Mass flow, kg/sec*
Vj	*= Jet Velocity, m/s*
A	*= Outlet Area, m^2*
Pj	*= Static pressure of the core jet stream, kPa*
P0	*= Ambient Pressure, kPa*

To elaborate on the effect of operating altitude on Net thrust, the air density decreases with increasing altitude which has been represented in Figure_Apx 6. Drop in air density further reduces the mass flow. This behaviour becomes increasingly significant with increasing altitude and is represented as an exponential drop in net thrust.

Specific Fuel consumption (SFC) is a function of Fuel flow and Net thrust which can be expressed as

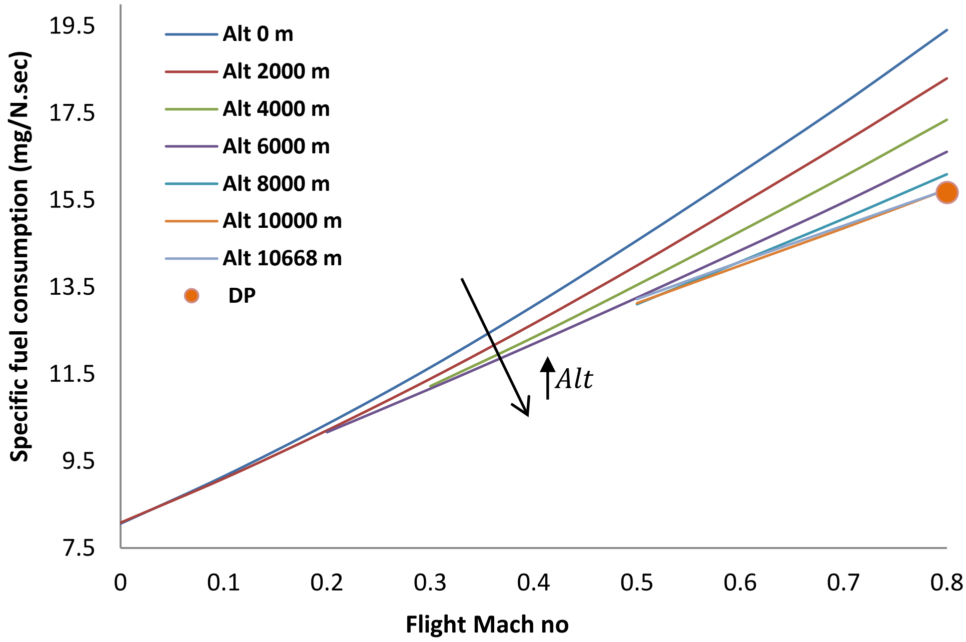
$$SFC = \frac{W_{ff}}{F_n} \qquad \textbf{Eq 73}$$

where, *SFC = Specific fuel consumption, (mg/N.s)*

W_{ff} *= Fuel flow (kg/s)*

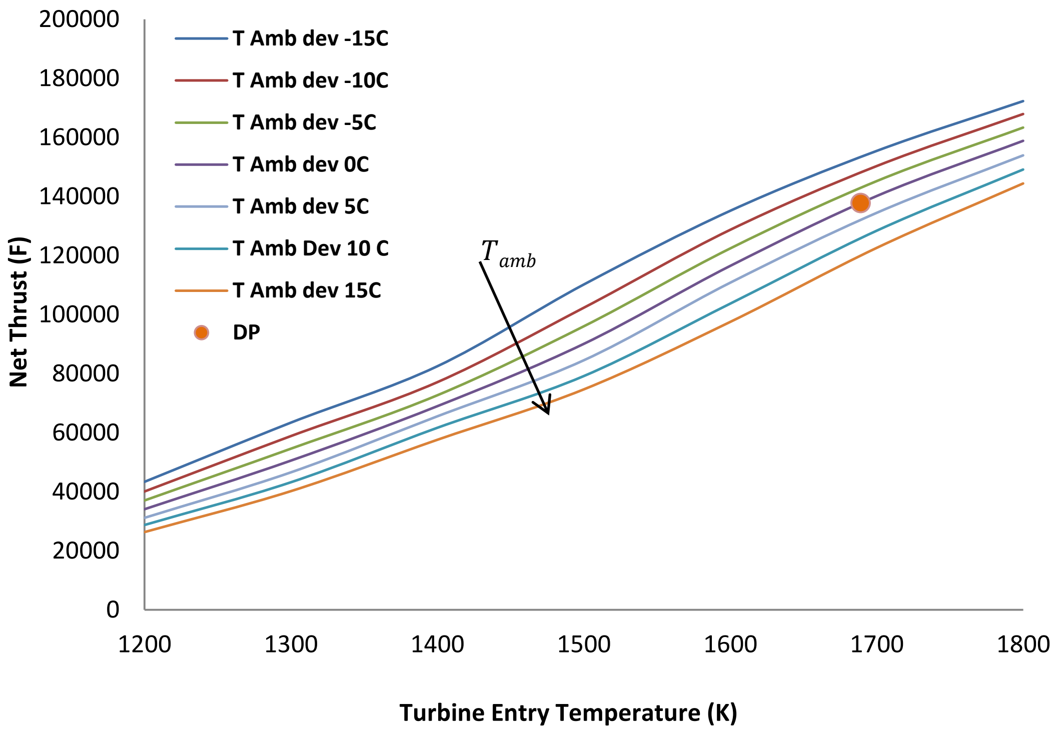
F_n *= Net Thrust (N)*

It is evident that the rate of drop in net thrust at sea level is greater than that at higher altitudes. This behaviour is due to increased momentum drag experienced at lower altitudes. At fixed thrust, the drop in mass flow (W) experienced with increasing Mach numbers is stabilised with heat addition through increasing of fuel flow (W_{ff}). This causes the jet velocity to stabilise and maintain the desired net thrust. From empirical point of view, SFC is inversely proportional to the Net thrust (Eq 33). Similar to the behaviour observed with thrust output, additional fuel flow is required when the engine is operating at lower altitude relative to that at higher altitude. Hence the SFC attributable to engine operating at lower altitude through increasing Mach number is higher than the same operating at higher Mach number. This behaviour has been diagrammatically represented in Figure_Apx 7.

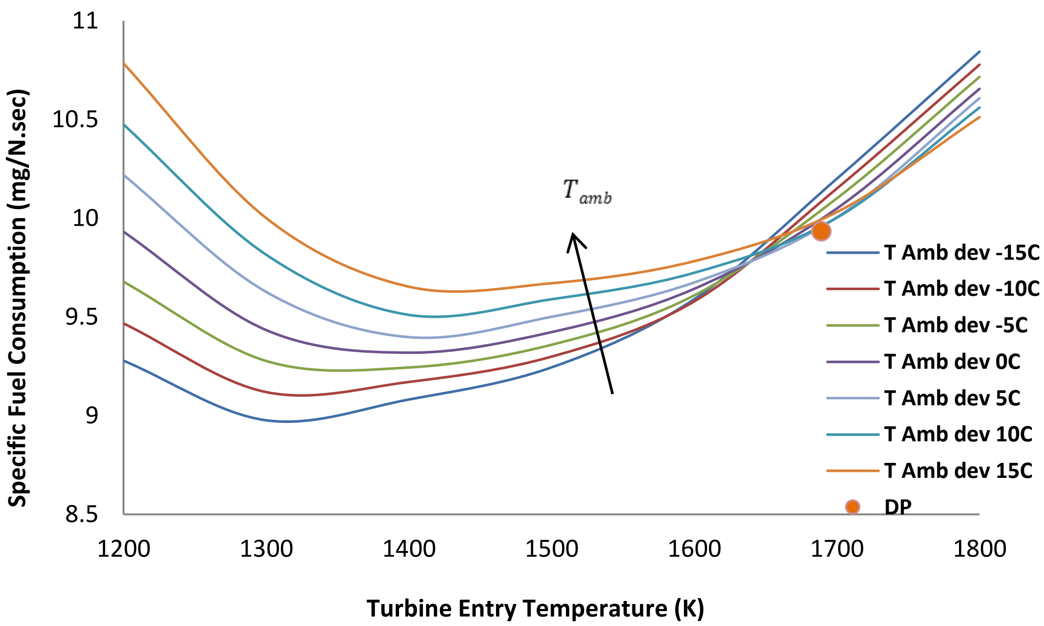


Figure_Apx 8: Effect of altitude and flight Mach no on specific fuel consumption at constant TET (ISA conditions)

6.6.3.1 Effect of Ambient temperature



Figure_Apx 9: Influence of Ambient temp and TET on Net thrust at constant Mach no and ISA conditions



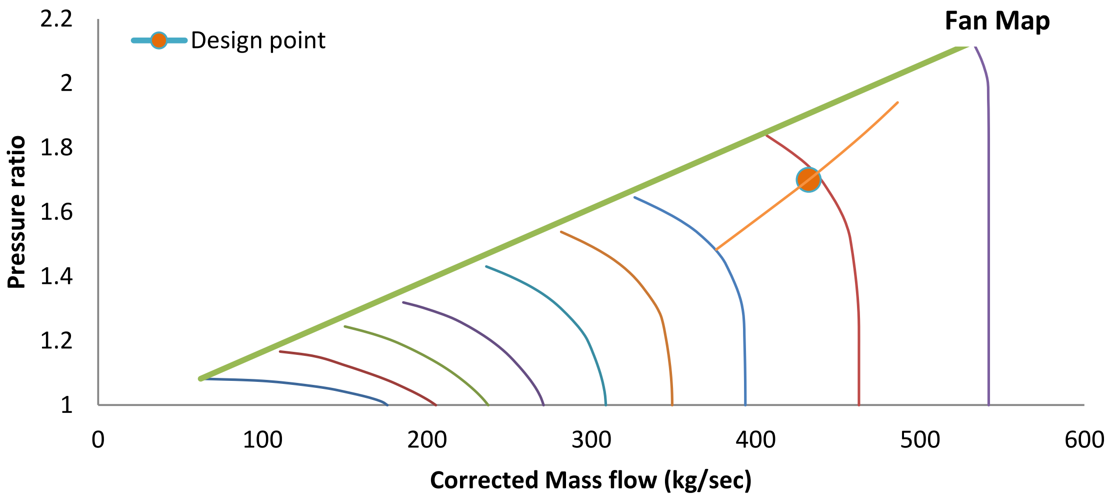
Figure_Apx 10: Influence of ambient temperature on SFC at constant Mach no and ISA conditions

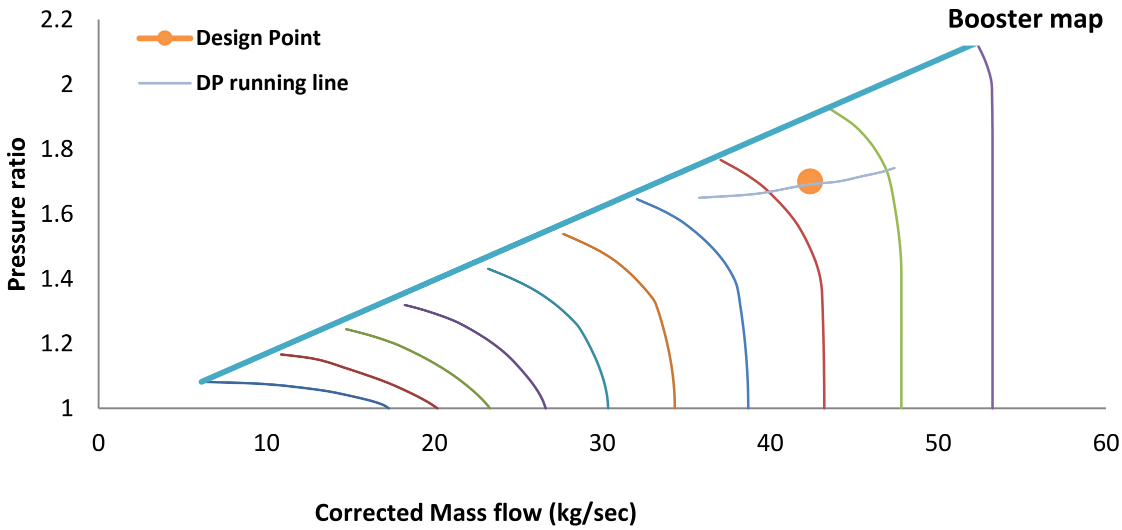
The effect of ambient temperature on engine performance at take-off condition has been analysed with the following assumptions- Mach no 0.0, and TET as handle (1200-1800K). Lower Ambient temperature aids increased thrust due to betterment of air characteristics (denser air) and air compressibility with relative ease in contrast to hotter air. This effect reasons the increase in net thrust with dropping ambient temperature. From engine lever performance perspective, increase in Turbine entry temperature (TET) of the engine is effected by heat addition i.e. increasing fuel flow (W_{ff}) which boosts the kinetic energy of the core jet stream and feeds back to the compressor speed thus increasing the compressor pressure ratios increases the shaft speed which in turn improves the compression ratios. It is essential to note that the propelling nozzle is choked. The increase in these key parameters boosts engine's net thrust thus justifying the increase in net thrust with increase in turbine entry temperature (TET). This behaviour has been diagrammatically represented in Figure_Apx 11.

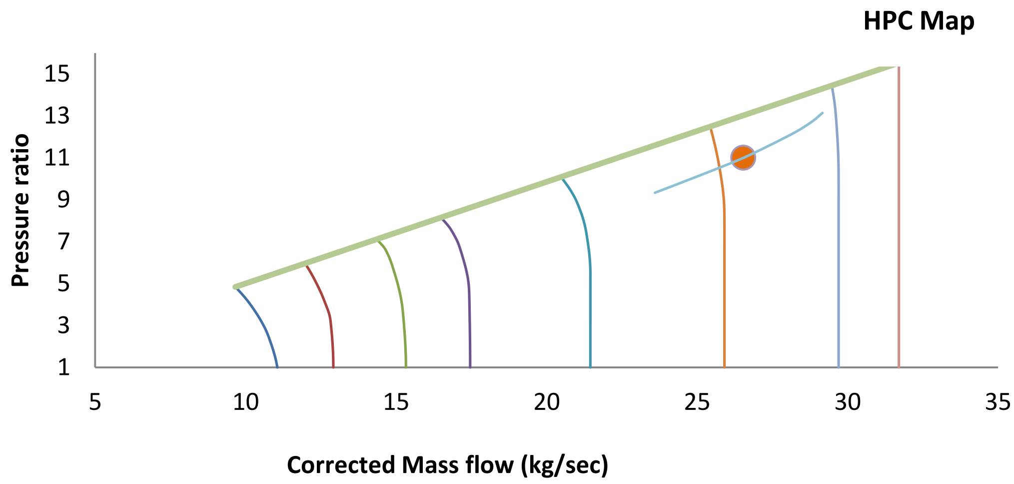
As mentioned earlier, the engine has to work harder to compress hot air (higher ambient temperature) to achieve fixed net thrust. This can be effected only through heat addition i.e. increase fuel flow which explains the increase in specific fuel consumption at hotter ambient temperatures relative to cooler ambient conditions. However, in relation to the trends followed with increase in TET as presented in Figure_Apx 12, an initial drop in specific fuel consumption is observed between the chosen temperature ranges 1200K – roughly 1400K after which it gradually increases and takes a "twist-invert" behaviour upon reaching roughly 1650K. At Low ambient temperature conditions, the mass flow are sufficiently increased relative to that the higher $T_{amb.}$ However, the overall temperature ratio across the compressor region is lower and this is compensated by increased heat addition (fuel flow) to achieve the TETs that have been chosen as the handle. The rate of heat addition required for an engine operating in a colder climate is relatively higher that that operating at a hotter climate. This behaviour creates a 3-D "twist-invert" trend and also explains why the SFC of the engine operating at SLS condition creates a "U" shaped trend.

6.6.4 Compressor Characteristics

At subsonic speeds (Mach no <1) increasing TET moves the running line up the speed lines. This behaviour is the result of increase in temperature and pressure ratios across the engine, from heat addition, leading to an increase in non-dimensional mass flow at the turbine inlet (since the propelling nozzle is choked). However, when analysing the impact of varying altitude, the running lines were determined to move to lower speed lines. Since the shaft speed is maintained constant, the amount of air inflow is likely to drop when reaching higher altitudes







Figure_Apx 13: Fan, Booster and HPC operating at design point (TET handle)

thereby creating a drop in temperature/ pressure ratios and thus corrected mass flow$\left(\frac{W\sqrt{\frac{T}{T_0}}}{\frac{P}{P_0}}\right)$.

The Booster compressor is however, more sensitive to the changes in TET (used as the handle) and displays progress towards the surge margin than that of the high pressure compressor. With increase in Mach no at constant TET, the corrected mass flow reduces exponentially. The compressor maps for each of the compressor components have been provided in Figure_Apx 14. The running lines have been plotted for off-design condition where the altitudes ranges from 12000.0m – 0.0m, TET is (1200-1800K) handled and Mach no remains constant.

Appendix H : Input Data required for Engine Emissions Index prediction using HEPHAESTUS

Fuel Type	Flight mode	Alt (m)	Amb Temp	Power setting (%)	Wf (kg/sec)	T_8 (K)	P_8 (atm)	W_8 (kg/sec)	FAR
Kerosene	Take-off	0	288.15	100	1.388	886.19	37.04	64.47	0.068
	Climb out	475	285	85	1.1137	845.79	36.56	62.63	0.068
	Approach	1650	276.15	30	0.3503	757.62	12.62	25.02	0.068
	Idle	0	288.15	7	0.124	580.09	7.84	8.549	0.068
Camelina SPK	Take-off	0	288.15	100	1.316	886.56	37.66	64.557	0.0667
	Climb out	475	285	85	0.994	818.28	36.84	62.92	0.0667
	Approach	1650	276.15	30	0.3407	700.08	12.65	25.68	0.0667
	Idle	0	288.15	7	0.1196	580.09	7.89	8.5874	0.0667
Microalgae SPK	Take-off	0	288.15	100	1.318	886.3	37.53	64.56	0.0668
	Climb out	475	285	85	0.996	820.67	36.54	62.75	0.0668
	Approach	1650	276.15	30	0.342	703.08	12.55	25.04	0.0678
	Idle	0	288.15	7	0.1204	580.5	7.86	8.514	0.0668
Jatropha SPK	Take-off	0	288.15	100	1.3155	886.55	37.74	64.84	0.0667
	Climb out	475	285	85	0.994	846.24	36.92	63.14	0.0667
	Approach	1650	276.15	30	0.3406	758.62	12.72	25.72	0.067
	Idle	0	288.15	7	0.1196	581.67	7.89	8.58	0.0667

Appendix I Input parameters required for total mission emission prediction

		Fuel burn (kg)	CO_2 emissions	Total CO_2	NOx	Total NOx	H_2O	Total H_2O
JetA	TO	157.2	3200.71	503.1	36.2	5.6	1242.26	195.2
	TOC	1946	3200.71	6228.5	26.53	51.6	1242.52	2417.9
	Cruise	11756	3200.71	37627.5	20	235.1	1239	14565.6
	Descent	2071	3200.71	6628.6	4.67	9.6	1232.97	2553.4
	Landing	549.5	3200.71	1758.7	10.58	5.81	1236.06	679.2
	Idle	161.38	3200.71	516.5	4.67	0.7	1232.97	198.9
Camelina	TO	154	3137.57	483.1	32.82	5.0	1386.31	213.4
	TOC	1861	3137.57	5839.0	23.1	42.9	1386.87	2580.9
	Cruise	11459	3137.57	35953.4	16.5	189.0	1383	15847.8
	Descent	2086	3137.57	6544.9	4.32	9.0	1376.57	2871.5
	Landing	540	3137.57	1694.2	10.43	5.6	1378.87	744.5
	Idle	156.91	3137.57	492.31	4.32	0.6	1376.57	215.9
Microalgae	TO	153.68	3139.88	482.53	33.05	5.0	1383.8	212.6
	TOC	1845.71	3139.88	5795.3	23.21	42.8	1383.84	2554.1
	Cruise	11379	3139.88	35728.6	17.5	199.1	1375	15646.1
	Descent	2066.7	3139.88	6489.1	4.32	8.9	1374.06	2839.7
	Landing	536.3	3139.88	1683.9	10.33	5.5	1376.38	738.1
	Idle	155.65	3139.88	488.7	4.32	0.6	1374.06	213.8
Jatropha	TO	153.68	3137.4	482.1	32.55	5.0	1380.7	212.1
	TOC	1845	3137.4	5788.5	23.08	42.5	1380.74	2547.4
	Cruise	11378	3137.4	35697.3	16.5	187.7	1377	15667.1
	Descent	2067	3137.4	6485.0	4.3	8.8	1370.95	2833.7
	landing	536.3	3137.4	1682.5	10.22	5.4	1373.29	736.4
	Idle	155.6	3137.4	488.1	4.3	0.6	1370.95	213.3

)t