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Estimation of GHG and pollutant emissions of supersonic aircraft with biofuels in conceptual design



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ABSTRACT

The objective of this thesis is the analysis of the environmental impact of biofuels upon supersonic passenger airplanes with a view to decarbonization target and economic sustainability.

The first part aims at examining the main features of conventional fossil fuels and at deeply analysing the various possibilities biofuels can offer in terms of different feedstocks, different production pathways and different chemical and physical properties. The goal of this part is to understand the possible advantages and disadvantages of the several types of biofuels, selecting a small number of certified sustainable aviation fuels to use for further analysis.

The second part consists in the development of a model useful to estimate pollutant emissions in a supersonic cruise, adaptable to both conventional fossil fuels and biofuels. Fuel flow method developed by Boeing for subsonic flights was taken as example and basis in order to elaborate a new methodology considering supersonic phenomenology, especially concerning supersonic air intakes. The methodology has been validated taking into exam the Concorde case study powered by fossil fuel. Only then, the methodology was modified to involve biofuels. Some estimations about biofuels' impact on emissions have been carried out, getting important data to promote further sustainable aviation fuel development because it would be an important instrument to help fighting the global environment pollution.

At the end, a graphical interface has been developed by means of a MATLAB Tool in order to let a hypothetical user visualize the effects a different choice of biofuel would have in a conceptual design process.

1.INTRODUCTION

In 2020, the global aviation market has undergone a severe decrease due to the pandemic but it is still expected to grow more and more in the next years thanks to the increasing number of passengers every year need to travel around the world. It is reported that IATA (*International Air Traffic Association*) forecast predicts 8.0 billion air travellers in 2039.

This constant growth is reflected in a constant increase of aviation fuel burnt, which is only slightly mitigated by the introduction of technology improvements allowing the airplanes to be more efficient than in the past. The large consumption of aviation fuel generates a large amount of pollutant and greenhouse gases (GHG) emissions, being responsible of atmospheric composition changes, ozone layer depletion and climate change, including the very well-known build-up of CO₂ in the atmosphere. Aviation CO₂ emissions account for around 2% of global CO₂ emissions every year [1]. The main aviation industries in the world have therefore established the target of a 50% reduction in CO₂ emissions by 2050 compared to 2005's level. This will of taking an active part in fighting against climate change involves the research of different solutions compared to the traditional technology, as well as the development of alternative and clean jet fuel.

In this framework, the interest for bio-based aviation fuels (bio-jet fuels) is arising as one of the most promising strategy to reduce aviation CO₂ emissions in the next future. Emissions can surely be reduced by improved engine efficiency, airport requalification or optimized navigation routes, but these measures could provide just a small reduction; however, a significant long-term reduction shall come from renewable and sustainable fuels. They seem to be the only real option to achieve a significant reduction of CO₂ before 2050 [2]: bio-jet fuels could be derived from sustainable sources such as plants or vegetables and they do not require modifications to the existing engines because they would be completely *drop-in*, meaning that no major changes on the on-board systems and on-ground infrastructures would be needed. Other promising technologies like cryogenic hydrogen or electric engines are unlikely to be ready in the near future, although they would be even more promising once completely settled for commercial use. However, the necessity of decreasing the short-term pollution in the atmosphere leads the aviation industries to carry on several studies about bio-jet fuels, examining the advantages and disadvantages of such a solution.

In 2012 many important aviation airliners such as United Airlines, American Airlines and Air France/KLM were already planning some flight tests and even commercial flights powered with aviation biofuels [3]. Currently, propulsion company Rolls-Royce is testing engines totally powered with aviation biofuels [4] to demonstrate that current engines for civil and business jet applications can operate with 100% sustainable aviation fuel as a full drop-in option. Furthermore, Lufthansa is promoting sustainable aviation fuel usage as first alternative to fossil jet fuels [5].

The target of decarbonisation does not just concern the existing subsonic airplanes, but also future supersonic aircraft which are currently at a conceptual design stage. Considering that a supersonic flight would imply a higher amount of fuel burnt per passenger than a subsonic one, it could be even more relevant than the case of subsonic flight due to the larger fuel consumption necessary to reach and maintain the supersonic regime. For all the reasons highlighted above, it is therefore important to develop methods and tools to estimate the emissions produced by a supersonic aircraft and the effect bio-jet fuels since the conceptual design.

Therefore, this thesis aims at analysing the most promising biofuels for aviation purposes, understanding the real effect of bio-jet fuels on the emissions of a supersonic passenger aircraft and create a simplified mathematical method to predict pollutant and green-house gases emissions during the conceptual design phase.

At first, a method to estimate the emissions of a supersonic engine using traditional fuels has been elaborated. The method is based on the already existing *fuel flow method*, but normally this method is used to estimate emission on the LTO cycle (*Landing and Take-Off cycle*) of a subsonic airplane; now the method has been adapted so that it fits with the cruise phase of a supersonic aircraft, that is the longest mission phase in terms of time. After that, the same method can be further adjusted to simulate the handling of biofuels instead of traditional fuels. At the end, the results are used to create a graphical interface to let the user see the results of the analysis, especially the total emission amount and fuel burned over a mission profile.

In this way it is possible to have a clear view of the environmental impact the airplane concept will have from the very beginning of a project, directing the choices of the conceptual design and saving efforts and time to the user.

2.TRADITIONAL FUELS

2.1 An overview of conventional jet fuels

Before introducing biofuels, it is worth reporting some considerations about conventional fuels, to prepare a solid basis for the comparison with biofuels. It is also important to stress that fuel cost covers about 30% of operational costs for subsonic aircraft [1] and are expected to play even a major role for high-speed vehicles. Therefore, a holistic approach should be adopted in the investigation of current and future fuels, to appreciate even small differences in technical, operational and management perspective.

Aviation fuel is composed by a mixture of hundreds different hydrocarbons called kerosene, extracted and distilled from crude oil. The following table shows a comparison of the important properties of the three main liquid fossil fuels: gasoline, diesel and aviation fuel (this latter covering about 10% of crude oil extraction).

Fuel properties	Gasoline	Aviation fuel	Diesel	
Density at 15°C (g/cm³)	0.72-0.78	0.75-0.84	0.82-0.85	
Kinematic viscosity (mm²/s)	0.37-0.44 (at 20°C) max. 8 (at -20°C)		2.00-4.50 (at 40°C)	
Lower heating value (MJ/kg)	43.4	43	43.4	
Flash point (°C)	-43	min. 38	min. 55	
Boiling point (°C)	max. 210	max. 300	max. 360	

Table 1: main properties of gasoline, aviation fuel and diesel (source: reference [1])

The most typical fuels used on commercial aircrafts are Jet A-1 and jet propellants (JP): they have a very similar composition, but JPs are generally used for military engines with the addition of specific additives to achieve specific requirements; JP-8 is essentially the military version of Jet A-1.

Chemical and physical properties of traditional aviation fuels are well-known and available to the public because all currently used fuels must be certified before entering the market.

In general, the data referred to density, freezing point, viscosity at -20 °C and specific energy are important to evaluate the possibility and the effects of blending conventional fuels with bio-jet fuels, whereas sulphur content, aromatics content and smoke point are crucial for emissions analysis [6]. The aromatic content is used also for blending considerations.

It is reported a table showing the collected main properties of some samples of JP-8 and Jet A-1 produced all over the world, highlighting the variation range of quantities.

Property	Minimum	Maximum
Density [kg/m³]	788.7	820.6
Freezing Point [°C]	-71	-46.2
Viscosity at -20°C [mm²/s]	2.8	6.0
Specific Energy [MJ/kg]	42.85	43.22
Sulphur Content [ppm]	7	2.423
Aromatics [vol%]	11.8	21.8
Smoke Point [mm]	19	30

Table 2: Jet A-1 and JP8 main properties (source: reference [6])

Let us examine these quantities to understand why some properties affect blending and others do not.

First, sulphur content does not limit blending: sulphur content is a property affecting emissions because a low sulphur content enables advanced emission controls and reduces air pollution; a low sulphur content is right the desired characteristic of a fuel so, since biofuels just reduce the sulphur content once blended with conventional kerosene, adding biofuels has always a positive effect from this point of view.

On the other side, viscosity is a limiting factor for blending: some biofuels are characterized by a low viscosity and this could cause large losses during fuel passage from tanks to engines and during refuelling operations.

Moreover, specific energy and density are quite related to each other: the combination of these two values affects tank volumes and it is fundamental to respect the current standards in order to have drop-in biofuels. It means that not every biofuel can be certified for aviation use, but only the ones with similar specific energy and density. A similar argument can be sustained for freezing point, because having a value outside the range would mean changing the materials, the de-icing system and the thermal system.

The aromatic content of jet fuel needs to be kept as low as possible in order to reduce swelling volume of fuel tank sealants; the maximum value according to ASTM D7566 is 25%, but it is better to stay lower. In some cases, a too low aromatic content could generate fuel leakage phenomena.

Finally, smoke point is an important property of jet fuels and other kerosene products: it is a measure of a fuel's tendency to generate smoke when burned because of some particles that do not complete combustion. It is easy to figure out how much this is relevant for emissions. The measure for smoke point is set by the flame height at which smoke begins to appear: a high smoke point is desirable.

2.2 Current Aviation Fuel Market

If aviation industries and their stakeholders want to consistently introduce biofuels in the aviation market, it is necessary to have a look on how current fuel market develops around the world so that it is possible to understand opportunities and critical issues. This brief analysis has been led on the US market, considered representative for the global aviation industry due to the large amount of air traffic every year.

Bio-jet fuels could have two major advantages compared to traditional fuels:

- the possibility of managing risks of upward fuel price trends and fuel price volatility;
- the capability to reduce greenhouse gases emissions.

Starting from these two points, it is interesting to see how biofuels could replace traditional fuels without having great disadvantages and solving instead two major problems of traditional fuels: fuel cost and atmospheric impact, precisely.

Jet fuels are classified into two types: kerosene-type (the most commonly used in commercial aviation) such as Jet A-1, Jet A and JP8; naphtha-type, such as Jet B and JP4. Biofuels target kerosene-type jet fuel.

Kerosene-type jet fuel production in United States is mainly located in the Gulf Coast, given the high refinery concentration in Texas and Louisiana. This is typical of centralized energy production strategies. On the contrary, biofuel production is spread in different territories because biorefineries are located near biomass resource bases. This is typical of new energy production concepts, aiming at setting up distributed architectures. This fact introduces a first important difference between traditional fuels and biofuels: the geographical feedstock and the consequent supply chain. The distribution system is a relevant part of the fuel "life-cycle" and logistics cannot be neglected when considering that, in all probability, biofuels should be blended with traditional fuel: all airports should be constantly supplied of both conventional and biofuels in such quantities that blending does not encounter delays. Furthermore, the distribution and cross-contamination. The first term refers to contamination derived from external sources or substances that could damage fuel properties; the second one to the problem of distributing different types of fuel that need to be kept separated without mixing.

Figure 1 shows the different geographic location of biomasses resources on the US territory. Conversely, crude oil and refineries for current jet fuel production are mainly concentrated in three main areas: Gulf of Mexico, followed by California and the Midwest. Biomass resources are extracted almost homogeneously all over the west half of the country, instead, with a prevalent concentration in Midwest anyway.



Figure 1: Refineries, airports, biomass resources in the United States (source: reference [7], public domain)

Competitiveness of bio-jet with conventional fuels is the key point for diffusion of biofuels in the aviation sector. A broader distribution of biomass resources is a first advantage of biofuels, which could face better risks associated with supply interruptions such as natural disaster or infrastructure problems. Indeed, airline companies prefer to rely on different types of fuel and different suppliers, so that they can diversify deliveries and prices.

Just the price is maybe the most important key point for bio-jet competitiveness: jet fuel prices are generally correlated to crude oil price trends, which are typically extremely volatile. This is a big problem for airline companies because they do not like large fluctuations of price, since fuel cost directly affects ticket price sales. The worst thing is that these fluctuations are caused also by geopolitical problems, which are extremely relevant right in oil producing countries. Furthermore, fuel price is estimated to grow steadily over the next twenty years, due to heavier and heavier oilfield exploitation. As crude oil reserves are dried up, fuel price will increase more and more and airline companies will desire to have another kind of fuel at their disposal and ready to be used. So, biofuels turn up as a strong solution to face volatility risks and growing costs trend.

The second mentioned advantage of bio-jet fuels was the possibility to reduce greenhouse gases emissions. In the coming years, regulations with the aim of reducing pollutant GHG emissions will increase in number and severity, especially in European Union with a specific carbon tax directed to aviation industry. If airline companies succeed in limiting emissions now, they could avoid to see costs getting higher in the future because of regulations and taxes against pollution. Bio-jet fuels should assume a key role in countering GHG emissions associated with aviation., but they could be useful also to enhance local air quality reducing particulate matter.

In conclusion, a lot of aviation companies has elected biofuels as leading player in the match against GHG emissions, not only for their potential of reducing atmospheric pollution, but also for the possibility of mitigating financial risks related to traditional fuel price volatility and fossil resources depletion.

It follows a summery table of the main characteristics and differences between conventional kerosene and biofuels.

Traditional kerosene	Bio-jet fuel		
 Growing oil price trend expected in the next 20 years Concentrated and consolidated supply chain Oil stocks will run out little by little Easy logistics Geopolitical problems in oil producing countries Prone to carbon taxation in the future 	 Reduce risks of fuel price volatility Reduce GHG and pollutant emissions Distributed supply chain Current necessity of blending with traditional kerosene Contamination and cross-contamination problems Possibility to diversify supplies Higher costs 		

Table 3: Main characteristics of traditional kerosene and biofuels

3.SUSTAINABLE AVIATION FUELS: BIOFUELS

3.1 The necessity of biofuels

A *Sustainable Aviation Fuel* (SAF) is a clean substitute for fossil jet fuels. While fossil fuel is refined from petroleum, SAF is produced from sustainable resources from a biological origin. SAF involves different kinds of fuel, of which biofuels are the most common ones. Other kinds of SAF are synfuels, exploiting electricity to produce hydrogen and combining it with carbon to achieve a kerosene-like product [8]. Every SAF type has the objective of reducing aviation environmental impact, anyway.

Many forecasts assert that CO_2 emissions would double in 2050 if no action is taken. A similar quantity of emissions in the atmosphere would cause severe global warning problems and not only because of the CO_2 quantity, but also because of the many other substances emitted by aviation engines like NO_x and HC contributing to environmental pollution.



Figure 2: Emissions from aviation in the absence of any action and emission reduction goals set by industry (source: reference [2], public domain)

Figure 2 reports the expected evolution of CO₂ emissions from 2010 to 2050: it is easy to figure out the choice of not undertaking any action would cause a constant unbearable growth, that could be reduced by future technology improvements

concerning conventional fuels and current infrastructures and operative strategies. Nevertheless, these developments are not sufficient to reverse the growing trend; the only thing they can do is the reduction of the growing line slope. The only solution to achieve a reduction compared to the current amount is the introduction of biofuels and new generation technologies like liquid hydrogen supplies or electric engines.

Clearly, the potential emission reduction depends on the fuel details because there are many different bio-jet fuel feedstocks and the choice of a type rather than another one could generate very different results. As a general feature, biofuels are produced from renewable biological resources such as plant material, rather than conventional fossil fuels like coal, oil or natural gases. The renewable origin is one of the characteristics for which many aviation companies have shifted their attention to these products, but not the only one: there is maybe another feature that could be even more relevant. Biofuels release carbon dioxide into the atmosphere when the fuel is burnt almost in the same way fossil fuels do, but the most important advantage of biofuels is in the net emissions cycle balance, considering that biofuels absorb carbon dioxide from the atmosphere as the biomass is grown.

Actually, it is not said that the GHG emissions coming out from a biofuel-powered engine are less than a fossil fuel one. The most important thing to remember when talking about biofuels is that the really great impact on emissions comes from the entire life cycle of the fuel: it is important to analyse not only the emissions coming from engine exhaust, but also to the emissions and GHG (in particular, CO₂) produced during the extraction of resources, processing, distribution and disposal phases. Therefore, analysing the lifecycle, it is possible to find out that some biofuels have higher net emissions out of engine exhaust, but they generate far less emissions during the entire life cycle or even, in the vast majority of cases, they contribute to absorb CO₂. Indeed, a target of this thesis is to make an estimation of the emissions generated from different kinds of biofuels and to understand their impact on the lifecycle.

A first generation of alternative fuels already exists and is exploited by several airlines: the most common sources of production are plants and crops, especially rich in sugar or starch in order to release their sugar content to make ethanol through fermentation. However, these first-generation alternative fuels are not really suitable for modern jet engines because of their lack of performances and safety properties [9].

Furthermore, they are subjected to additional sustainability problems related to being in competition with food supplies and requiring land changes.

Current technologies have allowed the rising of second-generation alternative fuels, which can be used for aviation. These fuels are produced from non-food biomass that are less dependent on a specific natural resource or land availability. For instance, they include municipal waste, used cooking oil and agricultural residues, but also a lot of natural plants like jatropha, algae and camelina that are not used for human or animal feeding. Second-generation biofuels have therefore two major advantages allowing them to be competitive with traditional fossil fuels:

- Providing diversified supplies and economic benefits, facing crude oil price fluctuations and supply problems. Biofuel feedstocks could be grown in several places in the world providing an important alternative to fossil fuels, mainly controlled by countries marked with political instability.
- Providing environmental benefits, reducing GHG emissions across life cycle; CO₂ absorbed by plants during the growth of the biomass is almost equal to the amount of carbon produced when the fuel is burnt. It implies the possibility to be carbon neutral over the life cycle, excluding emissions generated during production processes and distribution, giving rise to a circular phenomenon instead of a linear one, as shown in Figure 3 and Figure 4.



Figure 3: Lifecycle emissions from fossil fuels; CO₂ is emitted at every stage of the supply chain (source: reference [9], public domain)



Figure 4: Lifecycle emission from biofuels; CO₂ emitted is reabsorbed by the next generation of biomass (source: reference [9], public domain)

Of course, not all that glitters is gold! Second-generation sustainable aviation fuels have disadvantages too, first of all being completely "drop-in". The aviation industries have implemented severe safety standards regards to jet fuel and, considering an airplane normally refuels in different countries, it is necessary that new fuels can replace each other, exploiting the same already existing infrastructures, the same fuel system and the same safety standard.

The ASTM D1655 standard specification is the most widely standard used to define kerosene-type fuels for aviation engines. It presents specifications for Jet A-1 fuel setting the requirements for the fuel chemical and physical properties, but also for any additives such as antioxidants and so on. Because of the severe quality control of fuels, any fuels derived from different sources must be completely "drop-in"; it is absolutely necessary to handle the fuels together and not to generate handling problems.

The introduction of sustainable aviation fuels is therefore closely linked to the possibility to produce many different biofuels, each one being "drop-in". Currently there are a lot of biomasses to be potentially exploited to produce different SAF: the next steps are to examine the several possible feedstocks and conversion processes from biomass to biofuel.

3.2 The feedstock problem

Figure 2 has shown that a large quantity of sustainable aviation fuels is necessary to reverse the trend, but the problem is that the current production of biofuels is really small if compared to current production volumes of traditional jet fuels. Achieving a similar level of biofuel supply requires an extended campaign of efforts regarding policies and supply-chain developments only designated for bio-jet fuels: it means providing incentives for use of biofuels, developing a storage network all over the world to supply airports and promote biomass crops. However, all this could not be sufficient faced with the impossibility in scaling up production to meet demand, because the vast majority of bio-jet fuels currently available is derived from oleochemical feedstock [2]; it means they are derived industrially from animal or vegetable oils and fats. Therefore, the oleochemical production leads to "conventional bio-jets", that is the basis of the initial supply chain; in the future, when agricultural and other biomass technologies will be developed, "advanced bio-jets" will increase the offer thanks to a thermochemical production pathway. The feasibility of sustainable aviation fuels directly depends on the availability of sustainable feedstocks at competitive cost.

Nevertheless, it is clear biofuels are unable to replace traditional fuels completely, at least in the short term. The only effective strategy is the exploitation of different types of biomasses so that the sum could produce a significant quantity of biofuels.

However, it is unlikely that even the sum of all different biomasses in the world could completely replace fossil fuels. It seems so strange considering how many biomasses could be exploited in the world by means of future technologies, but it is not a crazy concern thinking to the fact that many biomasses are already exploited for alimentation or other uses: the exploitation of other biomasses for bio-jet fuel production would require more space for new crops or the replacement of existing crops. Supply is therefore a big problem that risks to compromise the introduction of biofuels in aviation market: at least, it limits the typologies of biomasses that can be used for aviation purposes.

A clear solution to solve this problem in the short term is blending biofuels with traditional fuels. This generates another problem: the compatibility of biofuels and traditional fuel. They need to have the same properties in terms of volume, freezing point, density and other similar characteristics in order to be completely *drop-in*.

Otherwise, structural changes would be needed and the advantages of using biofuels would irremediably drop drown. Furthermore, it is not said that all biofuels have exactly the same properties of conventional fuels, actually it is likely they would be at least a little bit different, so it would be necessary to control the percentage of blending in order to match the properties of biofuels with the traditional ones.

It is unlikely aviation companies will rely on just one type of biomass feedstock, because some of them are suited to grow in specific environment or climate; so, it is likely airplanes will use blends of different biofuels coming from different type of feedstock, together with conventional jet fuel. In this framework, second-generation biofuels for aviation use have the potential to provide large quantities of greener and maybe cheaper fuel; they can also grow in hostile environments such as deserts and salt water, not being this way intrusive for current crops.

Therefore, there are limits on the usage of biofuels and the possibility of using them or not depends on the production methods and the percentage of blending needed, as well as the type of biomass. The next steps consist in the analysis of different kinds of production strategies – called "pathways" – each one leading to different types of biofuels with different properties, so that some considerations about blending will be possible.

3.3 Certified pathways to produce bio-jet fuels

The knowledge of biofuel content blended with traditional jet fuel may seem irrelevant since the share of biofuel of the overall aviation fuel market is approximately few per cent, considering also the forecast for the next 5-10 years. But even so, it is important to know the biofuel content especially in early stages in order to perform the three required analysis by ASTM (*American Society for Testing and Materials*) before commercializing the type of fuel:

- an ASTM D1655 analysis of the conventional fuel before blending;
- an ASTM D7566¹ analysis of the neat biofuel before blending;
- an analysis of the blend, described in ASTM D7566.

¹ ASTM D7566: Standard Specification for Aviation Turbine Fuel Containing Synthetized Hydrocarbons

The cost of these analyses is independent of the blend ratio in the first two cases, but in the case of analysis after blending the cost will be very much affected by the blend ratio: indeed, considering using only a few per cent of blend ratio, the cost per ton of the analysis will be very high because just few tons of tested biofuel will be sold. This argument assumes more value when taking into account that each one of these analyses takes even more than 20-man hours to be performed and requires specialized and expensive equipment.

As of May 2016, ASTM had certified 4 different technology pathways [1] to produce bio-jet fuels and has defined 5 types of synthetized paraffinic kerosene (SPK) as blending components for conventional jet fuel to make up bio-jet fuels. The main production pathways of certified SPKs are listed in the Table 4 [1].

Pathways	SPK	Descriptions			
Gas-to-jet	FT-SPK	Gasification through Fischer-Tropsch method (FT), using municipal solid waste (MSW) or woody biomass as feedstock; thermochemical conversion process.			
	FT-SPK/A	The aromatic content is intentionally increased compared to FT-SPK, adding bio-based aromatics.			
Oil-to-jet	HEFA-SPK	Hydroprocessed Esters and Fatty Acids, using oleochemic feedstock such as oil and fats; oleochemical conversion process.			
Sugar-to-jet	SIP-SPK	Synthetised Iso-Paraffinic fuels, formerly known as the direct sugar-to-hydrocarbon route. Hydrolysis to obtain fermentable sugar; fermentation of sugars for farnesene production, followed by hydroprocessing and fractioning; biochemical conversion process.			
Alcohol-to-jet	ATJ-SPK	"Hybrid" thermochemical or biochemical conversion process: hydrolysis to obtain fermentable sugar; fermentation of sugars for iso-butanol and ethanol production.			

Table 4: The certified production pathways of synthetized paraffinic kerosene (source: reference [1] and [2], public domain)

Up to May 2016, the vast majority of currently available commercial bio-jet fuels are HEFA bio-jet. HEFA was proved in 2011 with up to a blending ratio of 50%. The same blending ratio of 50% is allowed for FT-SPK and ATJ-SPK. Instead, SIP was allowed to be blended with conventional fuel as well, but only up to 10% [1]. The first certified conversion process was FT-SPK, approved in 2009. HEFA-SPK was approved in 2011 and SIP in 2014. The last one to be approved is ATJ-SPK, certified in 2018 [10].

In general, introducing a new jet fuel blending component in aeronautics requires a long approval process and it may take from 5 up to 10 years. This is the reason why the next analysis deals with the mentioned production pathways, which are the most probable pathways to be considered for supplying aviation market.

A fuel production pathway is generally made by a sequence of stages as showed in the following flow chart.



The pathway starts from the feedstock production, that is the production of the chosen biomass; it continues with a pre-treatment to achieve the requirements of the conversion process; at the end, the conversion process itself that provides the aviation fuel. The economic sustainability of a pathway is strictly linked to the characteristics of the pathway as well as the transport from a phase to the next one.

Four types of feedstock can be used for the conversion process, as shown in Figure 5: it is a more detailed scheme referred to the previous flow chart where each step is associated with the different feedstocks and the approved conversion processes.



Figure 5: General outline of SAF pathways (source: reference [10], public domain)

Figure 5 will be the reference point for the following analysis that will deal with the different feedstock options at first and the conversion processes right after.

3.3.1 Feedstock selections

Sugar/Starch feedstock

Both sugar and starch plants provide fermentable feedstock, easily transformable into alcohol such as ethanol or butanol; then, sustainable aviation fuels can be easily produced from alcohols.

The main difference between sugar and starch plants is that the former ones directly provide fermentable sugars (obtained by mechanical process), whereas the latter ones the sugars are not available immediately, but they need to be obtained through chemical reactions.

The most common sugar plant is sugarcane of which Brazil is the major producer; it is generally exploited to produce sugar and ethanol. The most cultivated starch plant is maize, instead, of which USA are the major producer. Brazil and USA together produce over 85% of ethanol in the world by means of sugar obtained from sugarcane and maize [10].

Oil feedstock

Talking about oil feedstocks, we are referring to vegetable oils and oil residues that can be used for HEFA process. The main plants producing oil feedstocks are oil palm and soybean, but both are used for food and biodiesel production and the production request is already high. Even in this case US and Brazil are the main producers especially about soybean, while Indonesia and Malaysia are the main suppliers of oil palm [10]. Furthermore, oil palm crops are perennial, in contrast to annual soybean crops.

Some innovative plants included in second generation biofuel feedstocks have been identified as possible alternatives for SAF production thanks to some important advantages such as the possibility to be grown also in marginal lands, although some of them have high costs limiting large scale production. Hereafter some examples of these innovative plants: • Jatropha (*Jatropha curcas*) is a plant whose seeds contain 30-40% of lipid oil to convert in oil; it can be grown in a vast range of hostile lands such as arid soils. This characteristic is very useful because jatropha does not limit food crops. Furthermore, Jatropha's seeds are not edible.



Figure 6: Jatropha plant (source: reference [9], public domain)

• **Camelina** (*Camelina sativa*) has a high lipid content, so it is used for its high energy content to produce green fuels. Camelina is used as a rotational crop when the land would be unused otherwise. It would be an important resource to diversify the crops because a unique crop would degrade the soil.



Figure 7: Camelina plant (source: reference [9], public domain)

 Algae may be the most promising second-generation feedstock to implement a large-scale production for biofuels thank to the capability of be grown in salt water and hostile places. Furthermore, they flourish in a high concentration carbon dioxide environment and they can absorb CO₂ helping decarbonization goals. Other important advantages are the growth speed of this feedstock with the consequent possibility to produce far more oil than other feedstocks and, of course, not being a plant reserved to food.



Figure 8: Algae (source: reference [9], public domain)

• **Halophytes** are grasses typical of salt marshes and can grow in salt water and other habitats where plants do not normally grow.



Figure 9: Halophytes (source: reference [9], public domain)

Lignocellulosic feedstock

Another important alternative to produce biofuels is the exploitation of lignocellulosic resources which can be converted into SAF through thermochemical or biochemical process, as shown in Figure 5. Several types of wood can be used for this purpose, for instance willow, poplar and eucalyptus, but other feedstocks can be useful such as sawdust, miscanthus and switchgrass [10]. These feedstocks are characterized by low costs, high energy potential and the possibility to grow on lands that have not been turned into food crops.

Concerning to lignocellulosic feedstock, an explored solution is the use of biological waste, especially such as wood products, paper, forestry waste and municipal solid

waste [9]. This would be an important factor with a dual purpose: producing biofuels and disposing of waste.

3.3.2 Conversion processes

The conversion processes will be presented in order of year of certification, starting from FT-SPK (related to lignocellulosic feedstock), moving then to HEFA (linked to oil feedstock) and ending with ATJ and SIP (dedicated to sugar and starch feedstock). Each process is preceded by a pre-treatment with the aim of preparing the feedstock to be converted into SAF.

Thermochemical conversion process: Fischer-Tropsch technology

The thermochemical pathway is dedicated to lignocellulosic feedstock and the main technology is the Fischer-Tropsch process (FT), which is the first approved production pathway for synthetic kerosene. Here is already suggested a clue of the necessary pretreatment before the conversion into SAF: it deals with a treatment that allows the lignocellulosic feedstock to become synthetic material, in particular a "syngas". It follows the four-step list characterizing this pathway:

- The lignocellulosic feedstock is converted into a syngas composed by a mixture of CO and H₂ [6], involving partial oxidation and steam gasification. Gasification involves the heating of small biomass particles at high temperatures in a controlled-oxygen environment in order to produce synthesis gas [2].
- After purification, the syngas is synthesized into a mixture of gases and liquids which contain hydrocarbon chains of different sized [10]; this is the right Fischer-Tropsch process.
- 3) Other treatments such as hydrocracking and isomerization are applied.
- 4) Distillation and separation of the raw products into single products: kerosene is one of them.

This process has already existed before the advent of biofuels, when it was employed to convert coal and natural gas into fuel. The process has been proved to be suitable also for biomasses and it has been certified after some changes of process due to the different necessary treatment of biomasses, but there are no facilities in the world producing bio-jet fuel from biomass [6].



In Figure 10 is reported the scheme of the FT process using wood as starting biomass.

Figure 10: Scheme of the Fischer-Tropsch process for wood (source: reference [6], public domain)

In the scheme it is possible to notice the kerosene as one of the process outputs and the several treatments preceding the proper FT synthesis.

The major problems of thermochemical routes to biofuels regard the process efficiency and the technology risk [2]. For instance, an efficient syngas production should generate a mixture of CO and H₂ only, without any contaminants; instead, gasification of biomass often results in a product that need to be cleaned up. The final result is a fuel with less energy density than fuels derived from natural gas and it needs to be enriched in H₂, also. Cleaning the syngas is certainly possible, but it would require higher costs [2]. The only way to make this approach economically viable is to scale up the plants but this would require larger storage, more efficient supply chain, and shall be properly justified and supported by an increase in demand. Some experts believe FT costs could considerably decrease as the technology is improved, especially if municipal solid waste (MSW) is used as feedstock [2].

The FT fuels described so far do not contain aromatic compounds, but a certain percentage of aromatic content (8%) is required to fuel in order to ensure seal swell and tightness of valves [6]. This is the main reason why the FT-SPK fuel can be blended with conventional fuel with a maximum blend ratio of 50%. A variation of FT-SPK called FT-SPK/A has been certified by ASTM: it includes aromatic compound. However, ASTM approved this pathway only for a 50% blend with traditional kerosene at the moment, although it would constitute a fully synthetic kerosene at principle.

Oleochemical conversion process: HEFA kerosene

The oleochemical conversion process is used when the feedstock involves oil and fats and it is also called "lipids conversion process". The final products of this technology are HEFA (*Hydroprocessed Esters and Fatty Acids*), which have similar characteristics to traditional fuels. Until ASTM certification in 2011, this pathway was known as HVO (*Hydrotreated Vegetable Oils*), but a new acronym was introducing to include solid fats as feedstock, in addition to oils [6]. Now HEFA is the dominant pathway for producing SAF and currently operates at commercial scale [2].

The HEFA process is similar to refining petroleum ad it consists in a reaction of vegetable oils in the presence of hydrogen and come catalysts to produce different fuels such as aviation fuel, diesel, gasoline and naphtha, where each one needs to be separated.



Figure 11: Scheme of oleochemical conversion process (source: reference [2], public domain)

The first step is the pre-treatment of the biomass so that it is made ready for the production. The prepared material is submitted to hydrotreatment by means of a reaction with hydrogen: this step removes the oxygen (deoxygenation) and converts the substance into hydrocarbon chains. After that, the material is hydrocracked and isomerized to give the right properties to the fluid. The final step is the distillation during which the fluid is separated into different fuels [6]. The process is the same for all feedstocks, except for pre-treatment that could be different.

Nevertheless, there are some problems and challenges that should be solved to make HEFA competitive with conventional fuel:

- Large hydrogen supplies required for the process; this in not only a logistic problem but also a cost challenge.
- High heat generated during the reaction that must be kept under control.
- Vast supply chain to establish an economy of scale; specifically, HEFA cost directly depends on feedstock costs, which represent 70% of the final cost of the fuel [10].
- Evaluation of pre-treatment costs because of the vegetable oil impurities reducing fuel efficiency; considering the necessity of discarding low quality oil feedstock.

Like FT-SPK biofuels, HEFA does not contain aromatics; therefore, it was approved in 2011 with a maximum blend ratio of 50%. Some studies are being carried out by some aviation companies like Boeing to realise an HEFA kerosene that could be able to be approved without the necessity of blending with tradition fuel: it means the airplane would be powered with 100% SAF.

Many HEFA facilities already exist worldwide, but they mainly produce biofuels for road transports at the moment.

Biochemical conversion process: ATJ and SIP

In this category there are two approved pathways: ATJ (*Alcohol-to-jet*) process and SIP (*Synthetic Iso-Paraffins*) process.

In the first case, SAF is produced from ethanol or isobutanol molecules, mainly derived from sugar or starch plants. ATJ is composed by two independent steps: the production of the alcohol and the conversion process from alcohol to fuel. The first step and the choice of the alcohol source is important to evaluate the sustainability of the process, whereas the second step is the relevant step for certification and it represents the proper ATJ process, made of the following steps [6, 10]:

- Dehydration: water within material is removed, entering this way the process as a gas
- Oligomerization: small molecules are converted into complex ones.
- Hydrogenation: hydrogen is added to the mixture.
- Fractionation: the mixture is distilled into the types of fuel.

The aspects that could make this pathway more competitive regards mostly oligomerization. ATJ is the last approved pathway and there are few data about chemical composition of products and their characteristics. However, like the others, ATJ biofuels do not contain aromatics and this is the reason why the maximum approved blend ratio with conventional fuel is 50%. ATJ-SKA is the version with aromatic compounds, but it has not been approved by ASTM yet.

The feedstock of the alcohol bound to ATJ process can be highly variable, but in general preference is for lignocellulosic residues [6].



Figure 12: Simplified scheme of ATJ process (source: reference [3], public domain)

In the second case, SIP employs OGM to convert sugar into hydrocarbons or lipids, through fermentation. Instead of producing ethanol, the process produces a substance called farnesene – a renewable synthetic iso-paraffin -, which in turn can be converted into a fluid very similar to jet fuel: *farnesane*, gained by means of hydroprocessing [2]. At the moment SIP is used with sugarcane as feedstock, but it can be potentially used with all kinds of sugar plants [6]. The major problem of this pathway is the low conversion yield. It is also known as DSHC (*Direct Sugars to Hydrocarbons*) and it has been approved for a maximum blend ratio of 10%, far lower than the 50% of the other pathways, because of the really different chemical composition and carbon chain,

which makes the standard specification. Indeed, the long carbon chain makes the fuel very viscous and with low combustion performances in jet engines [1]. Despite of this, SIP pathway may overcome the typical biofuels problems like biomass availability and economic competitiveness; for instance, SIP process seems to has lower costs than FT process.

3.4 General properties of biofuels

Reminding that the final target is the comparison between emissions and performances of traditional fuels and biofuels, it is the moment to examine the physical and chemical properties of sustainable aviation fuels just like it was done for traditional fuel. The characteristics of SAF are very important when judging the feasibility of "drop-in" biofuels and the effects of blending. The final mixture must fulfil the regulation requirements regarding fuel performances and safety. Since density and blend ratio generally displays a linear trend, properties can be evaluated as weighted mean on the percentages of mixture's compounds.

Now a general analysis of the main properties is carried on.

Low temperature fluidity

Low temperature fluidity is very important to ensure fuel fluidity at the low typical temperatures of high altitudes. It depends on freezing point and kinematic viscosity.

- Freezing point is a key property of aviation fuels. The maximum value for FT-SPK, FT-SPK/A, HEFA and ATJ-SPK is -40°C, whereas it is -60°C for SIP [1]. The main factors that could affects biofuel freezing point are the iso-paraffins content, the aromatic content and the hydrocarbon chain length. High iso-paraffins and aromatic content make freezing point low, whereas long carbon chains make freezing point high. Therefore, the hydrocracking step is important to reduce carbon chain length.
- **Kinematic viscosity at -20°C** is the other important parameter about low temperature fluidity. The kinematic viscosity limit is not specified in regulation about biofuels, but the value of the blended jet fuel must be lower than 8 mm²/s. If the mixture is very viscous, there could be problems to

pumps or incomplete combustions. In general, the values of the different biofuels quite fulfil the requirement, except for SIP fuel, which has a high viscosity and it must have a low blend percentage. The kinematic viscosity of bio-jet fuels seems to have the same behaviour of fluids, varying with temperature. Short carbon length leads to low kinematic viscosity. In general, all biofuels have good viscosity properties, except for SIP because of the carbon chain length [1].

Combustion characteristics

Combustion characteristics are maybe the most important properties for bio-jet fuels because of their target of decarbonization and pollutant emission reduction.

- Smoke point is typically a property of conventional fuels (for which the flame height must be higher than 25mm without smoke) and a high smoke point is related to a low tendency of producing smoke. Currently, there are no limits for biofuel smoke point in regulations, but it is demonstrated that the smoke point of FT-SPK and HEFA is far higher than fossil fuel ones: even higher than 40 mm. The reason is the low aromatic content of biofuels. The effect of this would be a reduction of pollutant emission, especially as far as unburned hydrocarbons (UHC).
- **Particulate matter (PM) emissions** have the same behaviour of smoke point because they depend on the aromatic content. It means that a reduction of 40-60% is reachable, depending on the biofuel.
- Gaseous emissions refer to CO, CO₂ and NO_x emissions and they depend on the flight operative condition. In general, some studies [1] showed that a 10% NO_x reduction is possible for pure FT-SPK, whereas a 5% for a 50/50 blend with traditional fuel. Instead, CO emission were also 10-20% lower for both FT-SPK and HEFA. The reason is always the same: the poor aromatic content of biofuels allows a complete combustion. Nevertheless, other studies showed that HC emissions were a bit higher than traditional fuel because of the different flight conditions and the fuel rate. In conclusion, biofuel gaseous emission should be a bit lower, or at least comparable, than fossil fuel ones.

Fuel density and aircraft range

This part is mainly referred to the energy density of fuel, because it is a very important parameter affecting fuel consumption and, consequently, costs. Once the tank volume is fixed, an aircraft gets better performances when the fuel has a high energy density for two reasons: the aircraft travels for longer range or the aircraft consumes less fuel.

- Fuel density at 15°C should be comprised in a range of 730-770 kg/m³ for FT, HEFA and ATJ, whereas SIP should have a density of 765-780 kg/m³, probably because of the longer chains in farnesene [1]. It is even possible to reach a density of 800 kg/m³ for FT-SPK/A fuel thanks to the aromatic content included. It means the aromatic content strongly affects the fuel density.
- Net heat of combustion (also known as lower heating value) is regulated by ASTM and its value must be higher than 42.8 MJ/kg for traditional fuels and blended mixtures. Biofuels on their own does not have limits, except for SIP which has a minimum value of 43.5 MJ/kg [1]. In general, blending biofuels with traditional fuels reduces the net heat of combustion, but of course this is influenced by aromatic content.

3.5 A table of the most characterizing and promising biofuels

In this subchapter a table of the main chosen biofuels is shown. Each biofuel is representative of a category that could be a feedstock or a production pathway. The properties are the main interesting characteristics from emissions' point of view, instead. Not all properties are included, but only the ones that could affect the following analysis.

Fuel	Fuel Fuel point [°C]		Smoke point [mm]	Fuel density at 15°C [kg/m³]	Net heat of combustion [MJ/kg]
Jet A-1	-1 -47 4.27		27.1	804	43.15
Shell FT-SPK	-55 2.6		40	737	44.1
Sasol FT-SPK	< -77	3.8	> 40	762	44.2
Camelina HEFA	< -77	3.3	> 50	751	44.1
Coconut HEFA	-18.5	6.94	92.7	759	42.48
SIP-SPK (farnesane)	-90	14.1	> 50	773	43.93
ATJ-SPK	-50	4.795	23	757.1	44

Table 5: General important properties for emission calculation of different types of fuel (sources: reference [1], [6])

Except for Jet A-1 which is a fossil fuel, all the others ones are bio-jet fuels of different species and produced by means of different pathways. The various types have already been examined; the only thing to specify is the difference between Shell and Sasol FT-SPK: they are only FT-SPK biofuels produced by two different companies (Shell and Sasol) and it is significant to look at the differences in values of these two types that show that biofuels are not the same for every company, even if the same pathway is used; there could be differences also using the same feedstock, because

maybe it is different the geographical origin, so the feedstock properties as consequence.

In the following analysis there will be a comparison among the emissions generated by the different fuels especially using the last column, which values will be used to implement a method to compare emissions of traditional fuels with biofuels' ones. The penultimate column will be use to estimate the impact on fuel tank volumes, instead.

Another table is here presented to show which results one can expect from the analysis of emissions: it is reported the expected percentage variation of emission index of the main production pathways, on the basis of existing references.

Estimated Δ (EI) for different pollutant substances							
CO Reference HC Reference NOx Refer							
FT-SPK	-10%	[1]	-	-	+-10%	[28]	
HEFA	-5/10%	[1]	-10%	[27]	+15/20%	[27]	
SIP-SPK	0	[5]	0	[5]	-	-	
ATJ-SPK	2%	[26]	-	-	+10/15%	[26]	

Table 6: Estimated $\Delta(EI)$ for different pollutant substances

3.6 How to create a SAF market

After having examined the general characteristics of the different types of biofuels, ones could wonder how to choose a biofuel, how to understand the environmental sustainability and how to evaluate the economic feasibility. All these questions regard the introduction of biofuels into the global aviation market and the choice of a supply rather than another one.

It has been seen that, in general, performance properties of biofuels are satisfactory and they represent an important alternative to fossil fuels by now. However, there are still a lot of challenges to face, starting with the life cycle costs: biofuels have a higher price if compared to traditional fuels, sometimes even 2-3 times higher [1], depending on the feedstock. It would be very important for the planet having the possibility to introduce some economically viable biofuels because pollutant GHG emissions could be reduced thanks to them.

So, if it is possible to examine the pros and the cons of different types of biofuels during a commercial aviation mission, it would be easier to understand which biofuels could be more promising and government policies could be more focused on giving incentives to SAF development. Indeed, taxes and incentives could be the only factor to reduce life cycle SAF costs, but anyway it is necessary to understand the benefits of each biofuel during a mission. This is the reason why a list with the most characterizing biofuels and their properties has been prepared, so that it will be used to simulate an aviation mission: the amount of fuel used and the total emissions will be estimated.

Analysing the total LCC impact is very difficult and expensive, so in this thesis the analysis consists of general considerations and observations about the environmental impact and the related costs, in order to make a deeper investigation about biofuels: the analyses should not just stop at technical considerations, but they should always take into exam the economic feasibility, otherwise one risks to make analyses whose outputs are not useful in the real world. The analyses about biofuels properties have to be matched with some considerations about costs and Figure 13 shows a resume of the order of magnitude of some possible biofuels.
Conversion process	Feedstock	Cost (feedstock contribution)	Reference	
HEFA	Camelina oil	\$0.80/L	(Natelson and others 2015)	
	Palm oil	\$0.70–0.79/L (75% of OPEX)	(Hilbers and others 2015)	
	Soybean oil	\$1.01–1.16/L (up to 70%)	(Pearlson and others 2013)	
	Yellow grease Tallow	\$0.88–1.06/L (MSP)* \$1.05–1.25/L (MSP)* (65%–76%)	(Seber and others 2014)	
	Waste oil	\$1.03/L (70%)	(De Jong and others 2015)	
FT	Corn-stover (gasification)	US\$ 0.90/L	(Agusdinata and others 2011)	
	Switchgrass (gasification)	US\$ 1.10/L	(Agusullata and others 2011)	
	Lignocellulose (gasification)	US\$ 1.96/L (MSP)*	(Diederichs and others 2016)	
	Wood (gasification)	US\$ 1.14-1.22/L (MSP)*	(Zhu and others 2011)	
	Wood (gasification)	US\$ 1.13/L	(Ekbom and others 2009)	
ATJ	Sugarcane (ethanol) Corn (ethanol) Switchgrass (ethanol)	US\$ 1.56/L (MSP)* US\$ 1.75/L (MSP)* US\$ 2.30/L (MSP)*	(Staples and others 2014)	
	Lignocellulose (syngas)	US\$ 1.80/L (MSP)*	(Atsonios and others 2015)	
	Lignocellulose (syngas)	US\$ 2.00/L (MSP)*	(Diederichs and others 2016)	
	Sugarcane (ethanol)	US\$ 2.76/L (MSP)*	(Diederichs and others 2016)	

MSP = Minimum Selling Price

Figure 13: Results from techno-economic analyses of SAF (source: reference [10], public domain)

Looking at this table it is clear how HEFA and FT are far more convenient than ATJ pathway. Remembering that SIP had much lower costs than FT, it is intuitive to consider SIP as the most convenient biofuel from a cost point of view. No precise public data are available at the moment about SIP costs, but they could easily be around \$0.60-0.70/L. Now another element has been added to complete the analysis and to understand which biofuels could be the best ones to promote. It is useful to report in a table all advantages and disadvantages of the types examined before, so that a conclusion can be drawn.

From this table it is possible to indicate which biofuels could be more worthy to be promoted from an economical point of view, or better, which biofuels have more possibilities to success.

	Advantages	Disadvantages
FT-SPK	 Large availability of feedstock Efficient and widely tested conversion process High smoke point 	 Realisation of production facilities needed Contamination risk High demand needed to cut costs
HEFA	 Low costs Possibility to grow feedstocks in hostile environment Currently operative at commercial scale High smoke point 	 Needs large scale production Large hydrogen supplies Heat control problem during conversion process Variable costs depending on feedstock quality
SIP-SPK	 Very low costs High availability of feedstock Low freezing point High density 	 Certified blend only up to 10% Low conversion yield Low combustion performances High viscosity
ATJ-SPK	 Good availability of feedstock 	 High costs Last conversion process to be approved and few data available

Starting from the last one, ATJ-SPK is the last certified pathway: for this reason, it is already in delay because the aviation field needs biofuels in few years and there is limited time to catch up the others pathways; furthermore, it seems to have high costs and it would be very inconvenient unless great efforts are made.

On the other hand, SIP-SPK is very promising because it has very different properties that make it outstanding, like the far lower costs and the higher density. However, it has some problems to be solved to get approval for a larger percentage of blending, otherwise it has not the possibility to substitute fossil fuels, but it will be only complementary.

At the end, indicating a better pathway between FT and HEFA is really difficult at this stage and it depends on many factors; they can be both worthy to be promoted, because they offer good peculiarities in terms of costs, availability and process efficiency. On one side, HEFA is already used and it promises lower costs, but it has some conversion process problems and feedstock cultures have to be created and developed in the world. On the other side, FT needs the realisation of production facilities and it will have high costs until the scaling-up of the production.

The economic analysis stops here because there are no other public data at the moment to deepen the investigation, but it exists another important discriminating factor to go on with examining biofuels: the pollutant emissions have a key role in deciding which biofuel is worthy to be used and the next chapters will try to estimate which pathways guarantee less emissions.

What is sure is that all biofuels' advantages are not sufficient at the moment to substitute fossil fuels alone without the help of incentives and specific policies of governments, because average kerosene cost in the world is around \$0.70/L [11] in February 2021 and it offers a sure supply chain. However, through a wide promotion, some types of biofuels can really be competitive on every front.

4. REVISED FUEL FLOW METHOD FOR SUPERSONIC CRUISE CONDITIONS

4.1 General description

In this chapter the methodology developed in this thesis for the estimation of emissions of a supersonic flight is described: an already existing methodology developed by *Boeing* for subsonic airplanes has been taken as a basis and a new method has been developed to try to do the same thing for supersonic aircrafts; supersonic flight requires some important changes on the method, especially concerning the phenomenology of shock waves.

The most used method to estimate aircraft engine emissions of HC, CO and NO_x is the so-called "P3T3 method", which depends on the engine performances. However, it would be useful to have a valid method for estimating emissions without having access to aircraft performance models. This is why "fuel flow method" has been developed and it owes its name to the fact that engine fuel flow is the basic parameter of this method. While the P3T3 method is adopted for emissions certification [12], fuel flow method is not so much rigorous and, for instance, it can give reasonable approximations of emissions on the order of \pm 10-15% for NO_x. Variations of HC and CO have not been studied, but the limited data suggest larger differences on the order of 20-30% [12]. Therefore, fuel flow method can be an important methodology to estimate emissions in the phase of conceptual design: it gives the designer the possibility to evaluate the project environmental impact and the fulfilment to emission requirements; it can also be an instrument for the designer to choose the type of fuel the aircraft will be powered with.

It is very important the capacity to estimate HC, CO and NO_x emissions in project phase because they have a real impact on people life:

• HC (*Hydrocarbon*) are unburned particles derived by unburned and wasted fuel. The action of sunlight and the presence of other air pollutants generate a reaction which result is the formation of compounds that are considered being a major contributor to smog [13].

- CO (*Carbon Monoxide*) is a colourless, odourless, toxic air pollutant produced when the combustion of carbon in the fuel is incomplete; if the reaction is completed, CO burns to form CO₂. Inhaling high concentrations of CO can cause health hazards such as headaches and heart diseases.
- NO_x (*Nitric Oxide*) gases involve NO and NO₂ and are formed by the combination of nitrogen and oxygen in the combustion air due to the dissociation of nitrogen N₂ in the air. NO_x gases cause smog and acid rain and are relevant to fine particulate matter (PM) formation.

Before approving a project, the environmental impact must be approved and certified. At the moment, emission certification concerns only the area nearby airport facilities, where the pollutant emissions would have the strongest impact on local air quality for human life; however, emissions at altitude are not less important because they affect environment, meteorology and global warming. So, having a method allowing to estimate emissions at altitude right in conceptual design would be important also in view of future likely regulations concerning the cruise phase. Moreover, the cruise phase is also the most lasting phase over a mission and it has a great impact about emissions. It assumes even more significance when talking about long-haul flight, where cruise lasts many hours. These are the main reasons standing behind the aim of this thesis, which does not look only at the current situation of commercial aviation, but thinks about the future and the possible future challenges. Thus, since it is likely according to many studies that supersonic flights will come back in vogue in the next years, it is important to extend the current methods about subsonic flights to supersonic ones, to understand the advantages and the opportunities. Even more so if considering that biofuels are currently less known and their relevance in aviation market could grow fast in the future; there are no data about their exploitation to power supersonic aircrafts and thesis will try to understand the impact. So, this thesis will develop a way to adapt the methodology to supersonic biofuel-powered airplanes' cruise phase.

4.2 P3T3 method

The P3T3 method is the most used methodology to certificate emissions generated by jet engines and it requires knowledge of gas parameters at combustor inlet. Specifically, one needs to know P₃ (flow pressure at combustor intake), T₃ (flow temperature at combustor intake) and the fuel flow. In addition, atmospheric humidity is needed for NO_x estimation. The temperature T₃ at altitude is used to estimate an emission index at sea level, then it is applied a pressure correction to shift ground level measurements to an altitude condition, by means of some correlations about emission developed from testing [12]:

$$\circ EICO_{alt} = EICO_{SL} \left(\frac{p_{3SL}^{0}}{p_{3alt}^{0}}\right)^{x} \qquad \left[\frac{g CO}{kg fuel}\right]$$

$$\circ EIHC_{alt} = EIHC_{SL} \left(\frac{p_{3SL}^{0}}{p_{3alt}^{0}}\right)^{x} \qquad \left[\frac{g HC}{kg fuel}\right]$$

$$\circ EINO_{x_{alt}} = EINO_{x_{SL}} \left(\frac{p_{3alt}^{0}}{p_{3SL}^{0}}\right)^{y} e^{H} \qquad \left[\frac{g NO_{x}}{kg fuel}\right]$$

The EI is the *emission index* of a species of pollutant substances like CO, HC or NO_x and expresses how many grams of pollutant substance is emitted every kilogram of fuel burned. It is the most important parameter to understand the environmental impact of a jet engine and it is immediate to see that, in order to know emissions at altitude, it is necessary to know the emissions at sea level condition. This fact is remarked by the ratio of total pressure that express the correlation between altitude condition and sea level condition. It is important to notice that the correlation for NO_x is the reciprocal of CO and HC. It suggests an important behaviour: NO_x have an opposite trend compared to CO and HC. In particular, NO_x rises with increasing engine power, whereas the opposite happened for CO and HC.

The exponents x and y depend only on the engine, more specifically on the combustor, and they are derived in empirical way. The value of x is assumed to be 1. The value of y is assumed to be included between 0.2 and 0.5, with a most probable value of 0.4 [12]. The higher the exponent x the lower CO and HC emissions will be: it is a very important parameter and, doubling the exponent, EICO and EIHC are reduced of about four times. Instead, the opposite happens for y: the higher y, the higher EINO_x

will be. In this case, doubling the exponent, $EINO_x$ doubles, so *y* seems to be less important than *x*, even if very relevant anyway.

It is very complex to estimate these exponents for supersonic flights: there are no clues helping understand if x and y get higher or lower in supersonic regime and it is possible that even the answer is not unique, changing according to the engine. The only thing to do in conceptual design, when the engine specifications are not completely known yet, is to assume the same exponents for subsonic flights and remembering their importance on the estimation. Further studies on the exponents can improve the accuracy of the estimation.

4.3 Fuel Flow Method: derivation process

4.3.1 The original "Fuel flow method2" by Boeing for subsonic aircrafts

The fuel flow method for subsonic cruise starts trying to find a correlation of pressures that allow to use the EI formulas without requiring sensitive data of the engine from the manufacturer, which is the main problem of P3T3 method. An alternative method based on fuel flow can be used to correlate emissions to engine power without using sensitive data. In addition to fuel flow, it is necessary the correlation between P₃ and T₃, as well as in P3T3 method, formulating it as a function of ambient or freestream conditions. Therefore, it is necessary to examine the compression process between freestream and combustor inlet: it is assumed to be isentropic, so the relations for isentropic flow are valid [12].

$$\frac{T_3}{T_1} = \left(\frac{p_3}{p_1}\right)^{\frac{\gamma-1}{\gamma}} \qquad \rightarrow \qquad T_3 = T_1 \left(\frac{p_3}{p_1}\right)^{\frac{\gamma-1}{\gamma}}$$

It is possible to write the last equation at altitude and at sea level, following the assumptions that the temperature T_3 is the same at altitude and at sea level because it represents the conditions at combustor's inlet and it must be fixed to get an optimal combustion.

Defining

$$\delta_1 = \frac{p_1}{101325}; \qquad \qquad \theta_1 = \frac{T_1}{288.15}$$

it easy to get the following relationship

$$\frac{p_{3_{alt}}}{p_{3_{SL}}} = \frac{\delta_1}{\theta_1^{\frac{\gamma}{\gamma-1}}}$$

Now this equation shall be modified to express the ratio of total pressures, necessary to use the EIs' equations. Using the following expressions

$$\circ \quad \delta_{amb} = \delta_1 \beta^{\frac{\gamma}{\gamma-1}};$$

$$\circ \quad \theta_{amb} = \theta_1 \beta;$$

one gets

$$\frac{p_{3_{alt}}^{0}}{p_{3_{SL}}^{0}} = \frac{\delta_{amb}}{\theta_{amb}^{3.5}}$$

This is the fundamental equation of the subsonic pressure correction, that allows to estimate EI at altitude knowing EI at sea level. The equation is very simple and is based on two assumptions: the isentropic process before combustor and the same T₃ at sea level and altitude. While the latter is still valid for supersonic flights because the requirements for the combustor are the same, the former hypothesis falls when considering the shock wave characterising supersonic regime.

Another correction is necessary to have a method that does not require sensitive data of the engines. The other correction deals with the fuel flow rate into the combustor because it allows to calculate the emission indexes at sea level. It is reported here the final equation of the correction, that will be explained deeper when the supersonic correction will be described.

$$w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} (1 + 0.2M^2)$$

By means of the two equations, it is possible to estimate the emission indexes at altitude just knowing the fuel flow rate at the same altitude, through the following procedure.



Using this method just as it is, it implies that is not possible to do any estimations about biofuels because the equation does not involve the type of fuel. Some modifications are needed to extend the methodology to the supersonic regime and different kinds of fuel.

In particular the new method will be founded on:

- new hypothesis about the process ongoing between freestream and combustor;
- a strategy to include biofuels based on lower heating value (LHV).

Elaborating these two aspects it will be possible to widen the fuel flow method to supersonic regime and biofuels, allowing new conceptual designs of supersonic aircrafts to involve the environmental impact.

4.3.2 Supersonic pressure correction

Differently from the subsonic case, the process between freestream and combustor inlet cannot be considered isentropic in the supersonic case. The compression process needs to be split in two parts: the first part is the compression from freestream to compressor inlet, the second part goes from compressor inlet to combustor inlet. In this way it is possible to analyse a first non-isentropic compression characterized by shock waves and a second isentropic compression separately.

The starting point is the T_3/T_1 ratio, representing the ratio between the combustor inlet temperature T_3 and the ambient temperature T_1 . This ratio is expanded this way:

$$\frac{T_3}{T_1} = \frac{T_3}{T_2} \frac{T_2}{T_1}$$

where T_2 is the compressor inlet temperature. So, between the freestream and compressor, through the air intake, the compression is not isentropic; it is isentropic through the compressor, instead. The T_3/T_2 ratio can be expressed with the following isentropic relation:

$$\frac{T_3}{T_2} = \left(\frac{p_3}{p_2}\right)^{\frac{\gamma-1}{\gamma}} \longrightarrow \frac{T_3}{T_1} = \left(\frac{p_3}{p_2}\right)^{\frac{\gamma-1}{\gamma}} \frac{T_2}{T_1}$$

Now it is necessary to develop a model representing the shock wave conditions through the air intake; in this way the ratios of pressures and temperatures through the shock waves can be expressed.

Concorde engine's *Rolls Royce/Snecma Olympus* 593 provides a good evidence concerning to supersonic inlets. Figure 14 represents a section of the entire engine, a turbojet class with afterburner, but the focus is on the variable geometry inlet. The air intake allows the flow to decrease its speed from Mach 2 to Mach 0.5 [24] through four shock waves: the first three shock waves are oblique waves, whereas the fourth wave is a normal one. The aim of the first three shocks is to reduce the speed of the supersonic flow so that the flow impacting the normal wave generates just a weak shock. In this way, the total energy dissipation of the waves' set is lower if compared to having only a strong normal shock. It is also possible to notice a bleed which has the purposes of collecting a cold air flow for pneumatic system and mixing with the hot air outgoing from turbine.



Figure 14: Concorde engine section (public domain)

The air intake is unique for each engine, whose geometry mainly depends on cruise speed and compressor requirements. It means that the shock waves might have different angles and different intensities, in addition to the fact that the variable geometry might be different for each engine. Since the model should be able to be applicable for this wide range of supersonic air intakes and for all flight conditions, it has been considered convenient to represent sequence of shock waves as a combination of an oblique shock and a reflection shock. Otherwise, it would have been necessary to analyse different models for the different deflections of the walls and there would have been infinite possibilities. This approximation seems strange at first sight, but it assumes meaning looking at the structure of the first three shock waves, which have almost a point in common.



Figure 15: Mach reflection (source: reference [14])

Near the wall, however, the reflection shock is almost a normal shock, this is why it is possible to represent the entire process with a normal shock and a correction factor considering the difference from an oblique shock, the further subsonic compression before the compressor and the air bleed between the shock and the compressor. It is demonstrated that multiple oblique shock waves before a normal shock wave are more efficient about pressure loss [14]. It means that the pressure p_2 would be underestimated with the normal shock approximation and the correction factor is needed to achieve the higher value. For supersonic regime, it is estimated that a 20-40% efficiency gain is realistic for Mach 2-3 [14], so it is possible to consider a correction factor k_P≈1.3 in order to increase the pressure ratio of the air intake.

The truthfulness of this theory can be demonstrated considering the pressure data of Concorde engine's air intake, in which the flow passes from Mach 2 to Mach 0.5 during the process before entering the compressor [24].

At the same time, the temperature ratio undergoes an opposite effect because of the approximation: the temperature T₂ would be overestimated because the normal shock is more dissipative. So, it is necessary to apply a similar corrective factor. Analysing the effects of such an approximation, it is possible to see that it is necessary to reduce the temperature ratio after the approximation [14] and a corrective factor $k_t \approx 0.77$ for Mach 2 is definable.

In this way it is possible to express the p_2/p_1 and T_2/T_1 as a function of the freestream Mach M₁, in which the corrective factors k_p and k_t have been added:

$$p_{2} = k_{p} p_{1} \frac{p_{2}}{p_{1}} = k_{p} p_{1} \left(1 + \frac{2\gamma}{\gamma + 1} (M_{1}^{2} - 1) \right)$$
$$\frac{T_{2}}{T_{1}} = \left[1 + \frac{2\gamma}{\gamma + 1} (M_{1}^{2} - 1) \right] \frac{2 + (\gamma - 1)M_{1}^{2}}{(\gamma + 1)M_{1}^{2}}$$

Using the above T_3/T_1 ratio, T_3 is going to be expressed this way:

$$T_{3} = T_{1} \left(\frac{p_{3}}{k p_{1} \frac{p_{2}}{p_{1}}} \right)^{\frac{\gamma - 1}{\gamma}} k_{t} \frac{T_{2}}{T_{1}}$$

The above equation should be written at a flight condition:

$$T_{3_{alt}} = T_{1_{alt}} \left(\frac{p_{3_{alt}}}{k_p \ p_{1_{alt}} \frac{p_{2_{alt}}}{p_{1_{alt}}}} \right)^{\frac{\gamma - 1}{\gamma}} k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}$$

At the same time, it can be written at sea level on the basis of an isentropic condition because the flight at sea level is subsonic:

$$T_{3_{SL}} = T_{1_{SL}} \left(\frac{p_{3_{SL}}}{p_{1_{SL}}}\right)^{\frac{\gamma-1}{\gamma}}$$

where

$$T_{1_{SL}} = 288.15 \text{ K}$$

 \circ P1_SL = 101325 Pa

The method is based on the correlation between the T_3 at sea level and the T_3 at altitude: they have the same value because T_3 represents the temperature of the flow entering the combustor; that T_3 has to be a fixed parameter in order to generate a good combustion.

$$T_{3_{alt}} = T_{3_{SL}}$$

$$T_{1_{alt}} \left(\frac{p_{3_{alt}}}{k_p \ p_{1_{alt}} \frac{p_{2_{alt}}}{p_{1_{alt}}}} \right)^{\frac{\gamma - 1}{\gamma}} k_t \frac{T_{2_{alt}}}{T_{1_{alt}}} = 288.15 \left(\frac{p_{3_{SL}}}{101325} \right)^{\frac{\gamma - 1}{\gamma}}$$

At this point, two new parameters will be defined; they are useful to simplify the equations and to express the ratio with the values at sea level:

$$\delta_1 = \frac{p_1}{101325}; \qquad \qquad \theta_1 = \frac{T_1}{288.15}$$

Proceeding in this way:

$$\left(\frac{p_{3_{alt}}}{k_p \ p_{3_{SL}} \frac{p_{2_{alt}}}{p_{1_{alt}}}}\right)^{\frac{\gamma-1}{\gamma}} = \frac{288.15}{T_{1_{alt}}} \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}}\right) \left(\frac{p_{1_{alt}}}{101325}\right)^{\frac{\gamma-1}{\gamma}}$$

$$\left(\frac{p_{3_{alt}}}{p_{3_{SL}}}\right)^{\frac{\gamma-1}{\gamma}} \left(\frac{1}{k_p \frac{p_{2_{alt}}}{p_{1_{alt}}}}\right)^{\frac{\gamma-1}{\gamma}} = \frac{1}{\theta_1} \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}}\right) \delta_1^{\frac{\gamma-1}{\gamma}}$$
$$\left(\frac{p_{3_{alt}}}{p_{3_{SL}}}\right)^{\frac{\gamma-1}{\gamma}} = \frac{\delta_1^{\frac{\gamma-1}{\gamma}}}{\theta_1} \left(k_p \frac{p_{2_{alt}}}{p_{1_{alt}}}\right)^{\frac{\gamma-1}{\gamma}} \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}}\right)$$

Through some passages the resulting equations is derived:

$$\frac{p_{3_{alt}}}{p_{3_{SL}}} = \frac{\delta_1}{\theta_1^{\frac{\gamma}{\gamma-1}}} \left(k_p \ \frac{p_{2_{alt}}}{p_{1_{alt}}} \right) \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}} \right)^{\frac{\gamma}{\gamma-1}}$$

At this point we are going to use some relations to pass from static to total quantities:

$$\circ \quad \beta = 1 + \frac{\gamma - 1}{2} M^{2};$$

$$\circ \quad \frac{p_{0}}{p} = \left(1 + \frac{\gamma - 1}{2} M^{2}\right)^{\frac{\gamma}{\gamma - 1}};$$

$$\circ \quad \frac{T_{0}}{T} = 1 + \frac{\gamma - 1}{2} M^{2};$$

The equation becomes this one:

$$\frac{p_{3_{alt}}^0}{p_{3_{SL}}^0} = \frac{\delta_1 \beta^{\frac{\gamma}{\gamma-1}}}{(\theta_1 \beta)^{\frac{\gamma}{\gamma-1}}} \left(k_p \ \frac{p_{2_{alt}}}{p_{1_{alt}}}\right) \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}}\right)^{\frac{\gamma}{\gamma-1}}$$

Using the following expressions

$$\circ \quad \delta_{amb} = \delta_1 \beta^{\frac{\gamma}{\gamma-1}};$$

$$\circ \quad \theta_{amb} = \theta_1 \beta;$$

and assuming γ =1.4, it becomes

$$\frac{p_{3_{alt}}^{0}}{p_{3_{SL}}^{0}} = \frac{\delta_{amb}}{\theta_{amb}^{3.5}} \left(k_p \ \frac{p_{2_{alt}}}{p_{1_{alt}}} \right) \left(\frac{1}{k_t} \frac{T_{1_{alt}}}{T_{2_{alt}}} \right)^{3.5}$$

The polytropic efficiency is used to describe the compression from the freestream to the combustor inlet:

$$\frac{T_3}{T_1} = \left(\frac{p_3}{p_1}\right)^{\frac{\gamma-1}{\gamma\eta_p}} \longrightarrow \frac{p_{3_{alt}}^0}{p_{3_{SL}}^0} = \frac{\delta_{amb}}{\theta_{amb}^{\frac{\gamma\eta_p}{\gamma-1}}}$$

where

 $\circ \gamma = 1.38$

$$\circ \eta_{\rm P} = 90\%$$

The final equation:

$$\frac{p_{3_{alt}}^{0}}{p_{3_{SL}}^{0}} = \frac{\delta_{amb}^{1.02}}{\theta_{amb}^{3.3}} \left(k_p \left(\frac{p_{2_{alt}}}{p_{1_{alt}}} \right)_{f(M_1)} \right) \left(\frac{1}{k_t} \left(\frac{T_{1_{alt}}}{T_{2_{alt}}} \right)_{f(M_1)} \right)^{3.3}$$

In this equation a small empiric modification is added to the exponent of δ_{amb} to achieve better results. This last equation can be used in the relation of the emission estimated with the P3T3 method:

$$\circ EICO_{alt} = EICO_{SL} \left(\frac{p_{3SL}^{0}}{p_{3alt}^{0}}\right)^{x} = EICO_{SL} \left[\frac{\theta_{amb}^{3.3}}{\delta_{amb}^{1.02}} \left(\frac{1}{k_{p}\frac{p_{2alt}}{p_{1alt}}}\right) \left(k_{t}\frac{T_{2alt}}{T_{1alt}}\right)^{3.3}\right]^{x}$$

$$\circ EIHC_{alt} = EIHC_{SL} \left(\frac{p_{3SL}^{0}}{p_{3alt}^{0}}\right)^{x} = EIHC_{SL} \left[\frac{\theta_{amb}^{3.3}}{\delta_{amb}^{1.02}} \left(\frac{1}{k_{p}\frac{p_{2alt}}{p_{1alt}}}\right) \left(k_{t}\frac{T_{2alt}}{T_{1alt}}\right)^{3.3}\right]^{x}$$

$$\circ EINO_{xalt} = EINO_{xSL} \left(\frac{p_{3alt}^{0}}{p_{3SL}^{0}}\right)^{y} e^{H} = EINO_{xSL} \left[\frac{\delta_{amb}^{1.02}}{\theta_{amb}^{3.3}} \left(k_{p}\frac{p_{2alt}}{p_{1alt}}\right) \left(\frac{1}{k_{t}\frac{T_{2alt}}{T_{1alt}}}\right)^{3.3}\right]^{y} e^{H}$$

If the coefficients x and y are not available, it is assumed that x=1 and y=0.4 [12]. The coefficient e^{H} represents the humidity factor [12], where

- H = humidity correction = $-19^*(\omega 0.00634)$
- o $\omega = \text{humidity ratio} = \frac{0.62197058*RH*p_{sat}}{p_1*0.00014503773800722*68.9473 RH*p_{sat}} \left[\frac{kg \ water}{kg \ dry \ air}\right]$
- o RH = relative humidity (es. 0.5 = 50%) [15]

- o $P_{sat} = saturation \ pressure = 6.107 * 10^{\frac{7.5 * T_{ambc}}{237.7 + T_{ambc}}}$
- o $T_{ambc} = T_1 273.15 [°C]$

These equations above can be used to estimate the emission indexes of the various species of pollutant substances only knowing just a few parameters: it necessary to know the cruise Mach, the cruise altitude and the emission indexes at sea level. Just with these three elements, it is possible to derive the emission indexes at altitude for the following reasons:

- Ambient conditions are derived by cruise altitude by means of an atmospheric model, that allows to derive also the relative humidity RH.
- The emission indexes at sea level must be calculated at the same percentage of power that would be used at altitude.
- The other quantities depend only on cruise Mach and can be derived from shock wave tables of reference [14].

So, this method will be used to estimate the total emissions of a supersonic cruise phase, if the duration of the cruise phase is known.

4.3.3 Supersonic fuel flow rate correction

At this point, a correlation concerning the fuel flow is necessary to avoid achieving the values of emissions indexes at sea level; this can be done by means of an energetic balance through the combustor [12], using the fuel flow:

$$\eta_b w_f LHV = (w_f + w_a)c_P(T_4 - T_3)$$

- η_b: burner efficiency [adimensional]
- wf: engine fuel flow rate [kg/s]
- LHV: fuel lower heating value [J/kg]
- w_a: engine air flow rate [kg/s]
- cP: specific heat at constant pressure $[J/(kg \cdot K)]$
- T₃: total temperature at combustor inlet [K]
- T4: total temperature at combustor exit [K]

Since the fuel flow rate w_f is typically about 4-5% of the airflow rate, it is possible to make the assumption that the temperature T₃ is the same for both flows and the same reasoning can be made about specific heats. Therefore, the equation can be approximated in the following way:

$$\eta_b w_f LHV = (1.05w_a)c_P (T_4 - T_3)$$

Using this equation at altitude and at sea level it comes:

$$w_{f_{SL}} = w_{f_{alt}} \frac{w_{a_{SL}}}{w_{a_{alt}}} \frac{\eta_{b_{alt}}}{\eta_{b_{SL}}}$$

At this point the airflow ratio will be expressed as pressure ratio considering the airflow rate into the combustor at sea level:

$$w_{a_{SL}} = k \frac{p_{3_{SL}}^0}{\sqrt{T_{3_{SL}}}} f(M_3)_{SL} \quad \text{where} \quad k = \frac{\sqrt{\gamma}}{\sqrt{RT_3}} \quad and \quad f(M_3) = M \left(\frac{1}{1 + \frac{\gamma - 1}{2}M^2}\right)^{\frac{\gamma + 1}{2(\gamma - 1)}}$$

A similar expression can be written at altitude:

$$w_{a_{alt}} = k \frac{p_{3_{alt}}^0}{\sqrt{T_{3_{alt}}}} f(M_3)_{alt}$$

The combustor exit is choked and the total temperatures T₃ supposed to be the same at sea level and altitude, so

$$f(M_3)_{SL} = f(M_3)_{alt} \quad \rightarrow \quad w_{f_{SL}} = w_{f_{alt}} \frac{p_{3_{SL}}^0}{p_{3_{alt}}^0} \frac{\eta_{b_{alt}}}{\eta_{b_{SL}}}$$

At this point it is easy to use the energetic balance through the combustor to express the burner efficiency in function of fuel-air ratio:

$$w_{f_{SL}} = w_{f_{alt}} \frac{p_{3_{SL}}^0}{p_{3_{alt}}^0} \frac{\left(\frac{W_f}{W_a}\right)_{SL}}{\left(\frac{W_f}{W_a}\right)_{alt}}$$

in which the total pressure ratio con be substituted with the relation found in the pressure correction process, expressed for γ =1.4:

$$w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.5}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{3.5} \frac{\left(\frac{w_f}{w_a}\right)_{SL}}{\left(\frac{w_f}{w_a}\right)_{alt}}$$

Following the process explained in reference [12] it is easy to express

$$\left(\frac{w_f}{w_a}\right)_{SL} = \left(\frac{w_f}{w_a}\right)_{alt} \theta_1^{x-1} \longrightarrow w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.5}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{3.5} \theta_1^{x-1}$$

Where the exponent x is unique for each engine but it can be assumed equal to 2 as a first approximation, remembering we are in a conceptual design phase:

$$w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.5}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{3.5} \theta_1$$

Using the compressible relationships for total to static pressure and temperature:

$$\begin{aligned} \theta_{1} &= \theta_{amb} (1 + 0.2M^{2}) \rightarrow w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.5}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_{p} p_{2_{alt}}} \right) \left(k_{t} \frac{T_{2_{alt}}}{T_{1_{alt}}} \right)^{3.5} \theta_{amb} (1 + 0.2M^{2}) \\ w_{f_{SL}} &= w_{f_{alt}} \frac{\theta_{amb}^{4.5}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_{p} p_{2_{alt}}} \right) \left(k_{t} \frac{T_{2_{alt}}}{T_{1_{alt}}} \right)^{3.5} (1 + 0.2M^{2}) \end{aligned}$$

The experimental methods on different subsonic engines show that an exponent of 3.8 instead of 4.5 is better in order to match data. The problem is that the exponent 4.5 involves the same 3.5 present in the temperature ratio exponent; this means that, if the 4.5 exponent has been corrected, the same correction shall be made to the temperature ratio exponent. A hypothetical way is used: knowing that the exponent 4.5 has been reduced by 15.6% to 3.8, the same percentage is applied to the 3.5 of the temperature ratio, obtaining an exponent equal to 2.95.

$$w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p \, p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{2.95} (1 + 0.2M^2)$$

The process is not ended yet because the equation above lets the user to estimate the fuel flow, but one needs to know how to correlate this equation with emissions.

First of all, until now the fuel flow is calculated bleed off, but when the engine really operates there is a bleed flow that influences the calculation and an installation correction factor "r" is needed, depending on the thrust. The less the thrust, the higher the correction factor will be.

Thrust (%)	100%	85%	30%	7%
LTO mode	Take-off	Climb-out	Approach	Idle/Taxi
Fuel flow factor	1.010	1.013	1.020	1.100

Table 7: Bleed fuel flow factor (source: reference [12], public domain)

The equation becomes as it follows:

$$w_{f_{SL}} = r * w_{f_{alt}} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p \, p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{2.95} (1 + 0.2M^2)$$

As far as cruise phase is concerned, a discussion is needed to understand which correction factor has to be chosen. Since the formula correlates the fuel flow at sea level with fuel flow at altitudes, the first thought could be to compare the engine power at sea level and at altitude: it is clear that the thrust provided in cruise phase is far lower than at low altitudes; more specifically it is about 30% of the maximum power [16] and one could think to use the approach correction factor. However, it is to be considered that the maximum thrust decreases with altitude and in cruise phase the engine works at maximum continuous in order to travel fast and reach the final destination. This is why the real thrust in cruise phase is about 85% of the maximum thrust that can be generated at cruise altitude. So, the question is the next one: emissions depend on the net value of thrust or on the percentage of thrust compared to the maximum in every operative condition? The answer is the second one, because the percentage of thrust establishes the amount of fuel to be injected into combustor, so the emissions. Therefore, it is reasonable to pick an installation correction factor equal to 1.013 that corresponds to 85% of thrust.

However, it was still about fuel flow and the emissions have not been appointed yet. Once again, engine characteristics come out: there are some experimental graphs correlating emission indexes with fuel flow, with some limits established by thrust performances of the engine. In general, the engine manufacturers test the engines from minimum to maximum power, gaining the emissions and the fuel flow for each operative condition. Public data are limited, instead, to four points of the LTO cycle, which are the same four points of the installation correction factor said above. These data can be found on the *ICAO Emissions Databank* of reference [17], where there are the data of almost all engines used for subsonic flight since 1982. In this databank there are data about fuel flow and EI at four points of LTO cycle (take-off, climb, approach, taxi/idle). So, it possible to represent a correlation between fuel flow and emission index for each point of the LTO cycle in a graph, interpolating somewhat the four points and using a logarithmic scale because of the different order of magnitude from low power to high power. An example is reported, choosing the *Kuznetsov NK-86*, just to show how it works:



Figure 16: Kuznetsov NK-86 ICAO datapoints for fuel flow method (example)

So, knowing the fuel flow from fuel flow method it is possible to enter the diagram from the x axis and discover the EI of the desired (or likely undesired) pollutant species. In this diagram it is important to highlight a fact that was supposed in previous passages. The NO_x behaviour is opposite to CO and HC ones, as supposed in

P3T3 equations: the higher the power, the higher EINO_x because the combustion has a tendence to be complete, whereas the lower the power, the higher EICO and EIHC because combustion will be incomplete.

In conclusion, this is a powerful instrument to estimate emissions because it uses only public data, but it has a great problem as far as supersonic flight is concerned: availability of turbojet engine data. The ICAO databank regards turbofan engines indeed and there are no complete data for supersonic engines, although some data about Concorde's emissions are available. This is the reason why for further supersonic emissions estimation the data about Concorde will be used, assuming those data as sufficiently representative of the class of supersonic passenger aircrafts flying between Mach 1.5 and 3.

4.3.4 Introduction of SAF into fuel flow method

At this point it is time to introduce SAF into fuel flow method, in order to understand the advantages of using such a fuel instead of traditional fuel. SAF can be implemented into the methodology through an important parameter that appears in fuel flow correction and that was previously emphasized when talking about the important general characteristics of biofuels: the lower heating value LHV (or net heat of combustion).

The lower heating value is present in the energetic balance through the combustor, so it is a clue that it affects the fuel flow. Indeed, the lower heating value is an energetic index that express the energy the fuel is able to release. It is immediate to understand that the higher the heating value, the larger the energy released per kg of fuel, the less the fuel to burn. Since the emissions directly depend on the amount of burned fuel, a minor amount of fuel involves less pollutant substances emitted.

If one remembers there were some differences in LHV values for the various species of SAF, it is interesting to know how much these variations affect the emissions. So, it is necessary to find a way to correlate LHV with emissions. Instinctively, one could think to directly use the energetic balance through the combustor of the fuel flow correction, but looking at the process it can be seen that LHV is elided when the ratio between sea level condition and altitude condition is done. So, how implementing biofuels?

The solution comes from the previous consideration: if it is true that a higher LHV implies less fuel burnt, so there is proportionality between these two quantities that assumes even more meaning remembering we are dealing with conceptual design. So, it is possible to indicate with LHV the lower heating value of traditional fuel (Jet A-1, for example) and with LHV' the lower heating value of the particular biofuel which one wants to compare. The same apostrophe is used to designate the fuel flow of the specific biofuel. A proportionality relation can be developed as it follows:

$$\frac{LHV'}{LHV} \propto \frac{W_f}{W'_f}$$

Thus, the LHV ratio can be used to correct the fuel flow correction equations this way, so that it can be applied to the 4-point LTO map.

Fuel flow correction equation for SAF:

$$w_{falt}' = w_{falt} \frac{LHV}{LHV'}$$
$$w_{fsl}' = r * w_{falt} \frac{LHV}{LHV'} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} \left(\frac{p_{1alt}}{k_p p_{2alt}}\right) \left(k_t \frac{T_{2alt}}{T_{1alt}}\right)^{2.95} (1 + 0.2M^2)$$

Now it is possible to use all this methodology to make evaluation on advantages of biofuels in supersonic flights, always reminding that the analysis is done for a conceptual design study and that supersonic data are very few.

However, all these equations are valid only if the aircraft is powered with 100% SAF but, as said in the previous chapter, there are still certification limits to the amount of SAF to use to power the engines and a blending with traditional fuels is mandatory for various reasons. It would important to find a way to consider the blending percentages into the equations, operating on the parameter LHV', that would change depending on blending.

Luckily, the dependence of LHV from blending is linear [6] and it is easy to implement a weighted average to modify LHV'. Indicating with z (%) the blending

percentage and with LHV" the final LHV that consider blending, the formula is modified this way:

$$LHV'' = \frac{LHV' * z + LHV(100 - z)}{100}$$

As consequence, the previous equation about fuel flow has to be modified.

Fuel flow correction equation for SAF with blending:

$$w'_{falt} = w_{falt} \frac{LHV}{LHV''}; \qquad LHV'' = \frac{LHV' * z + LHV(100 - z)}{100}$$

$$w_{f_{SL}}' = r * w_{f_{alt}} \frac{LHV}{LHV''} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{2.95} (1 + 0.2M^2)$$

EI correction for SAF:



In addition, it seems that a correction for biofuel is necessary also as far as sea level EI is concerned: if biofuels are used, the curves of the EI-w_f map translate down of a certain percentage, but the amount of translation depends on both the production pathway and the specific feedstock of the biofuel and it is very difficult to predict how much the curve goes down. This is why this aspect has not been treated in this thesis, but can be further explored in other studies. However, without considering this additional correction, the methodology is still valid because it would overestimate the emissions, so it is a conservative methodology regarding the emissions of biofuels.

5. VALIDATION AND RESULTS

5.1 Methodology validation: Concorde case study

The first step of this chapter is the validation of the methodology previously presented through the case study of the most representative supersonic passenger airplane ever realised: the Concorde. It is the only supersonic passenger airplane of which a large base of data exists.

The Concorde may be considered as the most representative supersonic passenger airplane not only for the large amount of available data, but also for its technical peculiarities: above all, the cruise speed at Mach 2.02, which is representative of the entire supersonic regime, analysed between Mach 1.2 and Mach 3; then, the maximum cruise altitude at 60'000 ft, far above the standard altitude of current subsonic airplanes; finally, there are many data allowing to model the engine air intake, as done in Chapter 4.

Here after are two tables where Concorde data used for the analysis are listed.

Concorde data for validation of fuel flow method				
Quantity	Value	Source		
Maximum cruise altitude [ft]	60000	Reference [25]		
Cruise Mach number	2.02	Reference [25]		
EINO _x (54000 ft) [g/kg fuel]	20.97	Reference [22]		
Fuel burnt (LTO cycle) [kg]	6420	Reference [20]		
Fuel flow rate (cruise) [kg/s]	1.5	Reference [22]		

Concorde LTO data at sea level					
Production	Mf (kg/h)	Comb. Ineff.	EICO	EIHC	EINOx
Idle	1140	0.0584	118	36	2.5
Descent	2360	0.0380	82	22	4.0
Approach	4550	0.0201	55	8.5	6.5
Climb-out	9100	0.0059	20	1.5	12.5
Take-off	12700	0.0003	1.1	0*	22.3
Afterburner	10000	0.0207	64.5	6.6	0

Table 8: Concorde LTO data at sea level (source: reference [29])

These data will be used to run a MATLAB simulation to estimate emissions in supersonic regime and they will be compared to the official data of tests carried on when the Concorde was still operative. The MATLAB code will follow the fuel flow method previously presented, of course. The exception is the starred value of EIHC in take-off: a value of 0.1 will be used to avoid problems of the logarithmic diagrams, because the zero value cannot be represented in a logarithmic scale.

First of all, an atmospheric model is necessary to establish the ambient conditions in which shock relations are calculated. A standard atmospheric model in which pressure and temperature depend only on altitude is used [18].



Figure 17: Earth Atmospheric Model (source: reference [18], public domain)

The unit of measurement are the Metric units. It is unlikely supersonic airplanes will fly above 25.000 m in the near future, but the atmospheric model is complete in case of some analysis at those altitudes.

The second step is the definition of the relative humidity starting from the chosen altitude, because it affects the NOx emissions. The humidity model has been taken from a series of conditions [15] concerning troposphere and stratosphere, so the hypothesis is that humidity changes only with altitude in a standard day. Therefore, some bands of relative humidity (*RH*) values have been established to simply the calculations in the following way:

• RH = 0.75 for altitudes lower than 3000 meters;

- RH = 0.66 for altitudes within 3000 and 7000 meters;
- RH = 0.6 for altitudes within 7000 and 12000 meters;
- RH = 0.7 for altitudes within 12000 and 16000 meters;
- RH = 0.5 for upper altitudes;

These bands have been determined through the mean of values of some atmospheric models among which the following is the main one.



Figure 18: Profile of relative humidity of tropical atmosphere (source: reference [19], public domain)

Then, other important values to set are the coefficient factors relative to the engine air intake: in Chapter 4 it has been already set $k_p = 1.3$ and $k_t = 0.77$ for Concorde; now it is discussed how to change them in function of the Mach. Indeed, Mach variation creates some problems because the behaviour is linked also to the peculiarities of the air intake. Essentially, cruise Mach number causes variations in the flow reaching the combustor, but inlet geometry changes at the same to adapt the flow to combustor's requirements. In Chapter 4 all this phenomenology was included in two corrective factors k_p and k_t that were fixed for Concorde's cruise conditions, but they should change in function of the Mach. However, the behaviour of kp and k_t is very complex to estimate, because it depends not only on Mach number, but also on the inlet geometry, the percentage of bleeding and the isentropic pre-compression the flow undergoes before entering the compressor itself. Therefore, through aerodynamic considerations [14], since *k* factor is an indicator of how much useful work can be done by the gas, an estimation of k_p behaviour has been done with the following assumptions and calculations:

- At Mach 1, k_p=1 because there are not any positive effects coming from the inlet geometry, that makes its job when the Mach is higher and it is necessary to make the flow to enter smoothly.
- At Mach 2 the Concorde cruise speed it was calculated k_p=1.3 because the inlet provides about 30% of positive effects.
- At Mach =3, k_P=1.76 [14], instead, for the same reasons.

By means of these three points, it is possible to approximate k_p behaviour through a trend line of second order passing by the points. In this way it is possible to evaluate the evolution of k_p in function of Mach number.

$$k_p = 0.08M^2 + 0.06M + 0.86$$

The corrective factor k_t is evaluated in a similar way, knowing that the approximation of normal shock wave makes the T₂ temperature higher than it would be through multiple oblique shock waves:

- At Mach 1, k=1 because there are not any effects coming from the inlet geometry.
- At Mach 2 the Concorde cruise speed it was calculated k=0.77 because the T₂ temperature has to be reduced of about 23%.
- At Mach =3, k_t=0.65 [14], instead, for the same reasons.

By means of these three points, it is possible to approximate *k*^{*t*} behaviour through a trend line of second order passing by the points.

$$k_t = 0.055M^2 - 0.395M + 1.34$$

At this point, almost all data are available for the application of the fuel flow method. So, following the procedure, the first step is the passage from fuel flow rate at altitude (1.5 kg/s) to fuel flow rate at sea level, by means of the equation

$$w_{f_{SL}} = w_{f_{alt}} \frac{\theta_{amb}^{3.8}}{\delta_{amb}} \left(\frac{p_{1_{alt}}}{k_p \, p_{2_{alt}}}\right) \left(k_t \frac{T_{2_{alt}}}{T_{1_{alt}}}\right)^{2.95} (1 + 0.2M^2) = 4.986 \, kg/s$$

At this point it is necessary the EI-w_f sea level map for Concorde, designed from reference [29] and reported in Figure 19.



Figure 19: Concorde's El-wf map

This map is a bit different compared to the classical 4-point ICAO map, showed for instance in Figure 16. There are 6 points because there is a distinction between approach and descent and there is an additional segment regarding the afterburner, not present in subsonic engines. So, there are two lines dividing after the climb's point: the upper line is related to the use of the afterburner, whereas the lower one is linked to an engine regime without afterburning. It is remarkable the fact that the afterburner does not affect the EINO_x.

At this point, having the w_f value at sea level, the corresponding EI values are derived in a graphical way.

- EICO_{SL} = 1.1 g/kg fuel;
- EIHC_{SL} = 0.1 g/kg fuel;
- $EINO_{x_{SL}} = 22.3 \text{ g/kg fuel.}$

Having the EI values at sea level, the pressure correction is applied to get the EI values at altitude.

$$\circ EICO_{alt} = EICO_{SL} \left[\frac{\theta_{amb}^{3.3}}{\delta_{amb}^{1.02}} \left(\frac{1}{k_p \frac{p_{2alt}}{p_{1alt}}} \right) \left(k_t \frac{T_{2alt}}{T_{1alt}} \right)^{3.3} \right]^{\chi} = 1.9 \text{ g/kg fuel}$$

$$\circ EIHC_{alt} = EIHC_{SL} \left[\frac{\theta_{amb}^{3.3}}{\delta_{amb}^{1.02}} \left(\frac{1}{k_p \frac{p_{2alt}}{p_{1alt}}} \right) \left(k_t \frac{T_{2alt}}{T_{1alt}} \right)^{3.3} \right]^{\chi} = 0.17 \text{ g/kg fuel}$$

$$\circ EINO_{x_{alt}} = EINO_{x_{SL}} \left[\frac{\delta_{amb}^{1.02}}{\theta_{amb}^{3.3}} \left(k_p \frac{p_{2alt}}{p_{1alt}} \right) \left(\frac{1}{k_t \frac{T_{2alt}}{T_{1alt}}} \right)^{3.3} \right]^{\chi} e^H = 20.2 \text{ g/kg fuel}$$

It is important to remember that

$$x = 1; \quad y = 0.4$$

The emissions indexes at altitude (orange columns) are calculated by means of this MATLAB code, which generates a bar graph showing the resulting values of the three species taken into exam for the Concorde, comparing them with the starting values at sea level (blue columns).



Figure 20: Concorde emission indexes at Mach 2, absolute values (source: MATLAB code)

It is interesting to see how CO and HC emissions become higher passing from sea level to altitude, whereas the opposite happens for NOx. This is effect of the characteristics of the pressure correction's equations.

The bar diagram in Figure 20 shows the absolute values, but it is worthy to get the relative values to understand how much large the variations are. Figure 21 shows the percentage variation for the different species. It is clear that CO and HC emissions increase of more than 70%, whereas NO_x emissions get reduced of about 10%. This is the effect of the different exponent - CO and HC had the same exponent *x*, whereas NO_x had the exponent *y* – and the humidity factor present only for NO_x. However, in general, the differences are very pronounced, especially for CO and HC, due to the high Mach reached in a supersonic flight.



Figure 21: El percentage variation of the different species (source: MATLAB code)

Now it is necessary to validate these results in order to extend the method to different flight conditions and different fuels. In 1994 the Concorde exhaust was tested near the coast of New Zealand in cruise conditions [22] at Mach 2 and 53000 ft of altitude, without afterburners operating. Looking at the values of tests, it is noticeable that only NO_x an CO data are available among the species taken into consideration,

but it is sufficient to validate the method because if NO_x and CO are well estimated, also HC will have reasonable values. It is said that the average EINO_y (that is the sum of NO_x and all the other species derived from NO₂) is 23.3 g/kg fuel with an uncertainty of $\pm 20\%$ [22]. But the average ratio of NO_x/NO_y is 0.87 [22], thus the average EINO_x is equal to 20.27 g/kg fuel. Comparing the tested value (20.27 g/kg fuel) with the resulting value of the calculation (21.85 g/kg fuel) at 53000 ft, the difference between the two values is only equal to $\pm 7.8\%$ that is absolutely acceptable in a conceptual design. Indeed, it is proved that fuel flow method for subsonic airplanes can give results differing from real values of about 10-15% [12], so in this case the difference is far smaller, which makes the methodology validated for NO_x. Moreover, it has been estimated the EINO_x value if the original method would have been applied without the supersonic correction and the result is an underestimated value of 25%, that is unacceptable.



Figure 22: EINOx comparison for validation

It is also reported that EICO should be lower than 3.5 g/kg of fuel [22]; the estimated value in cruise phase is 1.9 g/kg of fuel, that is absolutely acceptable.

It is very important to remember that it is not sure the difference is so small in every flight condition and every aircraft. This is an estimation based on many standard assumptions, mostly established as average of the characteristics of subsonic aircrafts. It is possible that having the true values of supersonic aircrafts - especially regarding the experimental exponents used in the equations -, the results could change.

5.2 Results gained varying flight conditions

Once the methodology is validated for supersonic flight conditions, it is worthy to extend the analysis to different flight conditions, especially to different Mach numbers and different altitudes. The objective is the representation of the variations by means of diagrams showing the behaviour of emission indexes in function of altitude or Mach.

First, Mach number is kept fixed equal to 2 and the altitude changes from 0 to 80000 ft (about 24 km). Higher altitudes are not taken into exam at the moment because it is really unlikely supersonic flights will fly above 24 km of altitude in the near future, but it is still possible changing the parameters. Figure 23 represents the resulting diagram for each type of pollutant emission. It is important to notice the trend discontinuity at 11 km of altitude due to the passage from troposphere to lower stratosphere (or tropopause): in this atmospheric layer the temperature stops decreasing and the model assumes it fixed at about -56°C. This causes a change of behaviour of the quantities because the exponential trend of the pressure becomes overwhelming.



Figure 23: Diagram EI-Altitude at Mach 2 (source: MATLAB code)

Having a deeper glance to the trend, it is to see once more the different behaviour of NO_x compared to HC and CO. HC and CO trends are somewhat worrying because

they are the beginning of an exponential trend that should be limited. Luckily, the values are naturally limited by the fact that airplane will not fly at higher altitudes. It is interesting to plot the diagrams of EI in function of ambient temperature and pressure to understand which one is most influent on EI.



Figure 24: Diagram EI-Temperature at Mach 2 (source: MATLAB code)

The diagram has a different behaviour compared to the "original" one in function of the altitude. First, the *x* axis has been set in reverse direction so that sea level conditions are in the left side and the reader can look from left to right with increasing altitude. However, it seems that temperature mitigates the EI variation with altitude because the trends are different.

This suspect is confirmed by the EI-Pressure diagram, which shows a very similar behaviour of Figure 23, except for the different scale due to the exponential decreasing of pressure with altitude. Therefore, pressure has a primary effect on EI and temperature just a secondary effect that mitigates pressure outcomes. It is possible to observe some fluctuations of the NO_x at high altitudes, probably due to variation of the humidity that is not correlated to a temperature variation anymore.



Figure 25: Diagram EI-Pressure at Mach 2 (source: MATLAB code)

Secondly, as far as Mach variation is concerned, it is possible to applicate the same approach used for altitude in order to generate an EI-Mach diagram with Mach number varying from 1.2 to 3.5.



Figure 26: EI-Mach diagram (60000 ft) - absolute scale

Figure 26 is the resulting diagram and it is clear that Mach number has a great importance on the estimation. When the Mach number become higher than 3, it seems that trend changes direction, but this is not so much true because it is probably due to

the weakness of the model for high supersonic regime. It is safer to apply the model just to Mach number between 1.2 and 3.

It is interesting to try to create a map with both Mach and altitude, knowing that it would be a map applicable only for a defined engine. Hereafter some results.



Figure 27: EICO-Mach-altitude diagram (engine fixed)



Figure 28: EIHC-Mach-altitude (engine fixed)



Figure 29: EINOx-Mach-altitude (engine fixed)

Of course, the most important part of these maps is the main diagonal coming from Mach 1.2 at 7 km of altitude to Mach 3 at 24 km of altitude because it is the most probable path followed by supersonic airplanes.

It is also possible to overlap the three maps to compare the orders of magnitude: EINO_x is the one above the others, EICO in the middle and EIHC below.



Figure 30: EI-Mach-altitude (engine fixed)
5.3 Results over a hypothetical mission profile

Knowing that it is possible to evaluate the emissions at different altitudes and Mach, it is interesting to try to make an estimation over a hypothetical mission profile. A typical mission profile of the Concorde has been chosen as example and it has been simplified just to make easier the calculation, but a more complex mission can be absolutely studied.

In Figure 31 the mission profile taken as example is showed in terms of altitude and Mach number, by means of a double *y*-axis diagram. The take-off and landing phases have been strongly simplified.



Figure 31: Concorde mission profile for estimation of emissions

It is important to remark that the revised fuel flow method is valid only for supersonic regime, so the original fuel flow method has been used for the subsonic phases of the mission. Moreover, there is also a transonic phase where both methods are not valid, even if they have been used for continuity over the mission. This is why there are some important fluctuations nearby the flight times corresponding to Mach 1, that is the critical value determining the passage from the original method to the revised one.



Figure 32: Estimation of emissions over a mission profile

The three different orders of magnitude of the three species of pollutant emissions in cruise phase are very clear in this diagram. CO and HC emissions are very high during taxi phases (because of the inefficiency of combustion) and take-off phase (because of the activation of the post-combustor).

5.4 Results of SAF analysis

All previous analysis has been carried out considering a conventional fuel such as Jet A-1 was used. Now biofuels come on stage: the effects of different biofuels on EI will be examined through a range of different blending mixtures, keeping Mach and altitude fixed. Biofuels listed on Table 5 will be taken into exam.

A series of bar diagrams will be derived from fuel flow method estimations: each bar diagram will show the percentage variation of emissions the engine will have using different types of biofuels with different blending. Every estimation will be made at Mach 2 and 60000 ft of altitude; it is somehow an estimation of emissions Concorde would have had if it were powered with biofuels. However, the fuel flow rate at altitude has been supposed equal to 1 kg/s instead of 1.5 kg/s. The reason behind this choice is that a fuel flow rate of 1.5 kg/s would generate a fuel flow rate at sea level that would fall in a flat segment of the EI map; it would cause no differences between traditional and biofuel, so a different value has been chosen to have an estimation in more meaningful conditions.

The first diagram has been achieved supposing a 10% of blending for each SAF type.



Figure 33: SAF blend emissions variation compared to Jet A-1 (Mach 2, 60000 ft, 10% blend)

The first evidence catching the eye is the opposite behaviour of Coconut HEFA compared to all other biofuels. It means that not all SAF have the same behaviour and the choice of Coconut HEFA has been made right in this direction, right to show that not all biofuels have the same effects. More specifically, it is clear that 5 biofuels out of 6 cause an apparent little increase of CO and HC and a little reduction of NO_x, the opposite for Coconut HEFA as just discussed. Soon it will be discussed why the variations are just apparent: indeed, at the end of the analysis, the result will be a reduction of CO and HC and an increase of NO_x. Assuming a 10% blend, the global variation is very small anyway, but it should not be worrying: the percentage represents the variation of just a 10% blend on the EI, that is weighted for each kg of fuel. Actually, many tons of fuel are burned by each airplane for each flight and small quantities per kg of fuel will become large quantities of emissions reduction if

calculated on a large scale. Further analysis will be made about this. For the moment, let us focus on the differences among SAF types:

- Sasol FT-SPK results to be the biofuel that undergoes the largest variations, even more than Shell FT-SPK, demonstrating that some differences can exist also within the same typology of production pathway if a different feedstock is chosen. Sasol FT-SPK results to be the most efficient biofuel, but it is natural because FT-SPK is the first certified production pathway in chronological order and Sasol is maybe the company that made more efforts to develop a good biofuel.
- Camelina HEFA is another biofuel that manifest large variations, as well as Shell FT-SPK, and it proves how HEFA SAF may be the most subject to fluctuations on behaviour depending on the selected feedstock.
- SIP-SPK is the biofuel which causes the lower variations of GHG emissions, but it very understandable because of the different peculiarities of SIP such as lower costs and good feedstock availability. Nonetheless, SIP is able to give positive effects anyway and this makes SIP a good concurrent of the other biofuels, even more so considering that the technology is more recent.

Now let us see the bar diagrams for other percentages of blending, passing now to a 50% blend. SIP-SPK is present just to make easier the realisation of the diagrams, although it has been certified only for a maximum blend of 10%.



Figure 34: SAF blend emissions variation compared to Jet A-1 (Mach 2, 60000 ft, 50% blend)

The values increase linearly in proportion to the blending percentage increase. The percentages of variation are now more significant, even if still low, but they can cause important variations on a large scale. Of course, all previous considerations are still valid because in this model the augmentation is linear.

It is interesting to report as final diagram the estimation with a blend equal to 100% that means powering an airplane 100% SAF, just to see the maximum potential forecast by this model.



Figure 35: SAF blend emissions variation compared to Jet A-1 (Mach 2, 60000 ft, 100% blend)

Figure 35 shows the maximum possible variations thanks to the introduction of SAF into aviation engines at the aforementioned flight conditions. It is a more relevant variation than that with a 10% blend, which could cause great effects in GHG emissions impact. It is important to remember two things:

• Fuel flow method is a model to estimate subsonic emissions which has been modified to be applied to supersonic flights and to involve biofuels, but one of the premises of the entire methodology was that a difference of about 10% could exist compared to real values of traditional fuels, so the same can be assumed for biofuels. It means that these estimations should not be taken as data for certification but as instrument to decide a direction at the beginning of a project. It is an analysis to be summed to all other studies related to

biofuels that proves the opportunities SAF can offer to aviation. It is likely that the results are underestimated looking at other scientific studies, but they demonstrate the possibility to have an impact on GHG emissions. The benefits could be even higher then 2-3% of variation compared to traditional fuel, but fuel flow method cannot establish that variation without having access to experimental data and engine characteristics. It is not just that. These results are an average among all the possible peculiarities of the engine existing in the world because the target of this analysis is a general method to estimate the effect of biofuels on emissions in supersonic flight, no matter which engine is used, as far as possible, even if the model is mostly based on Concorde's engine.

• The results shown in the bar diagrams are only the values about the emission indexes EI, which unit of measurement is *g* emissions/kg fuel. It means that even a reduction of 2% is applied to every kg of fuel, but a current passenger airplane burns many tons of fuel every flight. Multiplying the EI variation by the tons burnt per flight by the flights undertaken by every commercial airplane in the world, it is immediate to see the huge effects biofuels can bring to the aviation companies and to the environment. This argument assumes even more meaning considering that some mixture of biofuels would have a lower LHV than a pure conventional fossil fuel: this means a lower quantity of fuel burnt on equal terms of energy provided.

The second point is exactly the key reason for which the increase of CO and HC was just apparent. Actually, the emission indexes EICO and EIHC really increase, but the value refers to *g emissions/kg fuel*, so the less fuel is burnt, the less the emissions will be. It is necessary to think on a large scale to better understand the argument.

It is assumed to pick a blend mixture of 100% SA and the results about EICO are extended to 1000 kg of fuel consumed, deriving how many kilograms of CO are saved every 1000 kg of fuel burnt. It is done multiplying the EICO by the fuel burnt and dividing it by 1000 to get the kilograms of pollutant substance.



Figure 36: CO emissions reduction every 1000 kg of fuel

The resulting diagram in Figure 36 is a bundle of straight lines - each one representing a different biofuel – ending near 1000 kg of fuel. It seems strange at a first sight because the lines do not end at the same value of fuel, but some lines are longer and others are shorter. The explanation lies on the second point of the previous considerations. This diagram involves two effects:

- 1) the emissions variation directly due to the exploitation of biofuels;
- 2) the variation of fuel burnt due to the different LHV of the blended mixture compared to pure Jet A-1.

Therefore, there is an important advantage that is fuel saving, which is able to overturn the effect number 1. Indeed, for many biofuels, the straight line ends before 1000 kg of fuel burnt and this fact contributes to emissions reduction. The most advantageous biofuel is now Sasol FT-SPK: it has the most pendant straight line, but it stops first because it can provide more energy; so, looking at the amount of CO emissions, Sasol FT-SPK is the biofuel that has the lowest value, immediately followed by Camelina HEFA and Shell FT-SPK.

This observation may sound strange because in general comparisons are made at the same quantities; for instance, one wants to know how many grams of CO are emitted every 1000 kg of fuel burnt. This information is already included in the percentage variation above mentioned because it is the percentage value itself. Now the analysis goes deeper: one wants to know how many grams of emitted CO are saved using biofuels instead of pure Jet A-1 on equals terms of energy generated. So, the reasoning is made on a performance basis: one assumes that the blended mixture generates the same performances of pure Jet A-1.

So, how should one read the diagram?

First, one takes note of the *y* value corresponding to 1000 kg of Jet A-1, at the end of the straight line. The comparison shall be made with the *y* value of the end the other lines and only with that one. Actually, the entire argument can be resumed using the "equivalent fuel", but the previous diagram is useful to visualize the idea behind.

Equivalent fuel permits to express the desired quantity – EI for instance - in function of the same amount of fuel considering the energy differences among different fuels; it allows to equalize the performances and the relative diagram is reported in Figure 37, where the lines have been zoomed near to 1000 kg of equivalent fuel.



Figure 37: CO emissions reduction every 1000 kg of equivalent fuel

Anyway, it is interesting to fill in a table showing CO savings for different quantities of Jet A-1 burnt in relation to different types of biofuels. Three example quantities have been chosen:

- 1 kg of Jet A-1, to compare this value with the one derived from bar diagrams;
- 1000 kg of Jet A-1, to write explicitly the values resulting in Figure 36 and to show the progression;

• 404[.]000 kg of Jet A-1, that is the quantity of fuel burnt every day by all Concorde in the world in 1992 [21].

Every quantity of fuel has two columns: the first one shows the absolute value of CO reduction, whereas the second one the relative value. It is interesting to observe how the relative value remains almost constant increasing the fuel.

	CO savings on 1 kg of Jet A-1 [g]		CO savings on 1000 kg of Jet A-1 [g]		CO savings on 404 [.] 000 kg of Jet A-1 [kg]	
Shell FT-SPK	0.9964	0.76%	996.4	0.76%	399.4	0.75%
Sasol FT-SPK	0.1101	0.84%	1100.7	0.84%	442.3	0.83%
Camelina HEFA	0.9964	0.76%	996.4	0.76%	399.4	0.75%
Coconut HEFA	-0.6630	-0.50%	-663.0	-0.50%	-271.6	-0.51%
SIP-SPK	0.8149	0.62%	814.9	0.62%	326.8	0.62%
ATJ-SPK	0.8937	0.68%	893.7	0.68%	356.7	0.67%

Table 9: CO savings from small to large scale

Looking at absolute values, instead, it is important to highlight that the values in the last column are kilograms. Except for this, passing from the first to the last column, it becomes more and more evident the impact of biofuels on the reduction of CO. Furthermore, the last column considers only a 100% blend and only Concorde flights per day in 1992, but air traffic is incredibly growth in the following years. Imaging to use biofuels for many more airplanes, maybe with engine 100% SAF, it is easy to see the great impact biofuels could have on decarbonization targets. Moreover, it was said that a great advantage of biofuels is the circular path of lifecycle emissions (*cf.* Figure 4): this means that if it is demonstrated that exhaust emissions are at least the same for both biofuels and conventional fuels, so the largest impact on emissions comes from the possibility of biomasses to reabsorb the GHG emitted by aviation.

To conclude the chapter, these results have to be involved in the economic analysis, where greater possibilities to success were prerogative of HEFA and FT. That two typologies of pathway are more advantageous also from emissions point of view, especially the biofuel produced by Sasol with FT-SPK. These results confirm the fact that HEFA and FT are probably the most promising biofuels, but the small differences between them does not allow to establish which is the best one. Both can be competitive with traditional kerosene and both can contribute to reduce pollutant emissions significantly.

6.A GRAPHICAL INTERFACE FOR ESTIMATION OF EMISSIONS

This chapter deals with the realisation of a graphical interface created with a MATLAB Tool. The aim is to give an instrument to estimate emissions and to make decisions in the conceptual design phase. Indeed, at *Politecnico di Torino* a software called ASTRID-H has been developed for conceptual design of high-speed aircrafts [23]: it allows the user to manage high-level requirements about configuration and performances, but an environmental requirement is not present yet. The graphical interface will not allow to establish if the environmental requirement is respected or not, but it will be useful to have an overview about the environmental problem so that the user is aware about the characteristics of the aircraft he is going to design.

The graphical interface is realised by means of *MATLAB App Designer*, that is a recent interactive development environment for designing an app layout and programming its behaviour. The environment is divided in two parts:

- a *Design View* allows the programmer to project the interface just like it will appear to the final user; the programmer can insert spaces where the user can modify or select the inputs and the parameters, giving advices at the same time about the limits of the procedure;
- a *Code View* allows the programmer to write the code with the same language of *MATLAB Editor*, except for some differences about a variables' names and how to use functions.

Firstly, the Design View is projected: it is not only a space to choose parameters, but also to visualize images and diagrams, as well as the results coming from the App usage. It has been decided to divide the interface in three pages: the first one, called *Aircraft settings* and showed in Figure 38, is composed by several elements (or components in MATLAB language) through which the user can manage his analysis. He can choose the flight conditions, some parameters related to the engine and the time of cruise phase. Why just cruise phase and not the entire mission? Because it is possible to divide the mission in LTO cycle and cruise phase, keeping the LTO cycle almost standard for a determined type of vehicle. In this case, dealing with conceptual design, it was thought that the user does not have all information about LTO cycle yet and it was preferable to use a mean of the LTO cycle data of existed supersonic airplanes. Instead, cruise phase is linked to aircraft range and it is an information necessary in conceptual design, therefore already available.

Aircraft settings	Fuel and emission settings	Simulation results	+
User is called to a	set the data looking at limits	and advices	
Cruise Mach	number 2	Supersonic field, s	set in the limits: [1.2, 3.5]
Cruise Alti	titude [ft]	Set in the preferre	d limits: [0, 90000 ft]
Cruise phase	e time [h]		
Corrective fa	factor kp 1.3	Push the c	question mark button for explanations
Corrective	factor kt 0.76	i ?	
Exp	ponent x	?	
Exp	ponent y 0.4	• ?	

Figure 38: MATLAB App Designer, Design View, Aircraft settings



Figure 39: MATLAB App Designer, corrective factor's question mark

The corrective factors k_p and k_t and the exponents x and y are the same parameters presented in Chapter 4 and some starting values are suggested to facilitate the procedure. The user has anyway the possibility to change the values.

The question mark components give some advices to the user whenever he passes the cursor over the button. Pushing on the question mark linked to the corrective factor k_p , an additional window (Figure 39) pops up showing the instructions to set a reasonable value. This is one of the most important and delicate parameters, as well as k_t , and the user shall pay much attention to change it, otherwise the simulation will not be meaningful anymore.

The second page is called *Fuel settings* and asks the user to set some parameters related to the fuel and the emissions indexes at sea level, providing information to be aware of the choices. It is showed in Figure 40.



Figure 40: MATLAB App Designer, Design View, Fuel settings

As far as fuel choice is concerned, the user can select all biofuels analysed in the thesis with the addition of *Jatropha HEFA* for compatibility requirements with the corresponding interface related to subsonic flights. There is also a description of the main chrematistics of the biofuels displayed by a window which appears pushing the button on the right.

	Advantages	Disadvantages	
Shell FT-SPK	Large availability of feedstock, efficient conversion process	Realisation of production facilities needed, contamination risk, high demand to cut costs	
Sasol FT-SPK	Large availability of feedstock, efficient conversion process, already successfully tested and produced	Contamination risk, high demand to cut costs, facilities needed to increase production	
Camelina HEFA	Low costs, possibility to grow feedstock in hostile environment, currently operative at commercial scale	Needs large scale production, large hydrogen supplies, heat control problems in production	
Coconut HEFA	Low costs	Poor feedstock, poor reduction of pollutant emissions	
Jatropha HEFA	Low costs, possibility to grow feedstock in hostile environment, it does not limit food crops	Needs large scale production, large hydrogen supplies, heat control problems in production	
SIP-SPK	Very low costs, high availability of feedstock, low freezing point, high density	Certified blend only up to 10%, low conversion yield, low combustion performances, high viscosity	
ATJ-SPK	Good availability of feedstock	High costs, last biofuel to be approved, few data available	

Figure 41: MATLAB App Designer, App View, Biofuels

The last element of this second page is the *Start simulation* button, that is maybe the most important component of the entire interface because it hides the function needed to run the simulation. Before examining the function, it is necessary to understand how the third page is structured. For the moment it is sufficient to know that, clicking on the button, the simulation starts and the results will be displayed in the third page, called *Simulation results* and showed in Figure 42.

In the third page a window to show the results has been prepared: there are a bar diagram showing the EIs on a logarithmic scale and the numeric values aside for precision; then, there are the quantities of fuel burnt and volume occupied during the entire mission, divided into traditional fuel and biofuel. The values depend on



blending, as well as on flight conditions. Of course, if Jet A-1 is chosen, biofuel's quantities are zero.

Figure 42: MATLAB App Designer, App View, Simulation results

Now it remains to be seen how the three pages are linked, especially where the results come from. It is in this circumstance that the Code View comes into play: it is necessary to run the simulation and the Code View contains the code to generate results. For a simple graphical interface like this one, the code is almost entirely automatically generated: the programmer sets the limits or the specifications of each elements - just like one does with MATLAB Property Editor – and the code turns up in Code View screen. It is possible to create call-backs of the components to connect them and to use the values for calculations. In this interface the only really necessary call-back is linked to the "Start simulation" button, because it runs the simulation and it is necessary to recall a function containing the code for calculation.

```
% Callbacks that handle component events
methods (Access = private)
% Button pushed function: StartsimulationButton
function StartsimulationButtonPushed(app, event)
app=emissions_simulation(app);
end
end
```

Figure 43: MATLAB App Designer, Code View, call-back example

Figure 43 shows how the "Start simulation" button's call-back appears in Code View. The white line is the only modifiable line, but of course can be expanded if necessary. However, this call-back requires just a line to recall the MATLAB function *emissions_simulation.m* that contains the code.

The *emissions simulation* function is simply a MATLAB function modified to be suited to App Designer. The modifies concern the way to recall the variables, which are given by the call-backs of the app. It is possible to rename a variable so that the code is easier to read, but anyway at the end the outputs have to be put into the app components through the call-back name, instead of direct output of the function as it happened for MATLAB Editor.

So, this function is sufficient to make the App run and to gain results, as showed in Figure 42. Other two functions are involved: they are intended to show pictures for explanations to the user, in particular they are used to show Figure 39 and Figure 41.

7. CONCLUSIONS

Bio-jet fuels can really become a real alternative of traditional fossil fuels. Under the same performances, they can provide a great contribute to decarbonization target of aviation agencies. Until now, tests have proven undeniable advantages for subsonic flights. This thesis has shown that also supersonic models forecast GHG emissions reduction if biofuels are used. The model is a simple generic strategy to estimate emissions out of aircraft engine exhaust and it has been thought to encompass the possible engines for supersonic regime, without considering the internal differences among the engines. The results are actually little poor if considering the benefits of a single engine, but they acquire much more meaning if one sees the big picture of aviation transports: indeed, a small percentage of emissions reduction is multiplied by the huge number of flights carried on every day and the effects are much larger. This could be the road to follow to promote biofuels in the aviation market: aiming at scaling-up the offer, because the strategy works only at a large scale. Otherwise, if used in small quantities, biofuels are not worthy because they would have higher costs than conventional kerosene and an unconsolidated supply chain. This is a problem because, like any other product, it has to enter the market before being scaled-up and the first stage is absolutely the most expensive. Therefore, policies and incentives are necessary to encourage industries to invest in biofuels to sustain the economy. Instead, the environmental benefits are already proven and some companies could choose biofuels just to avoid higher taxations for fossil fuels in the future: taxation is indeed a key to reduce the current cost gap between traditional kerosene and sustainable aviation fuels.

Along this thesis, different kinds of biofuels have been talked about. Each biofuel is based on different biomass resources and different production pathways. It is a very different situation compared to fossil kerosene that has almost the same properties no matter the origin and the production technology has only small differences depending on the country. Therefore, there are really several factors affecting the convenience of a biofuel rather than another one and this thesis tries to evaluate the best biofuels under two aspects: the main factor is environmental and the other one is economical. Four production pathways, all certified for aviation usage, have been analysed and the results attest that two out of four are currently more promising: FT and HEFA. They can offer a greater GHG emissions reduction and lower costs at the same time than the other kinds of production process. Of course, the underlying assumptions are very generic because they are high-level hypothesis to be appliable to the entire supersonic regime from Mach 1.2 to Mach 3.5 more or less. Furthermore, the analyses have been carried on exclusively with public data about biofuels; no private data from production companies have been used. Therefore, the results should not be taken as accurate certifying data, but they can point a way and help designers to decide for biofuels exploitation or not. It is a study that can be added to all others studies which prove the effectivity of biofuels in reaching the environmental targets given by aviation authorities as well as the economic needs of aviation industries. In addition, it has been developed a method that looks to the future of commercial airplanes and shows how biofuels could provide great advantages also for supersonic flights. The methodology for supersonic regime has much more problems than the subsonic equivalent, but it is sufficient to understand the potential of sustainable aviation fuels in a conceptual design phase. The final goal is to encourage further studies and research to promote the introduction of biofuels in the aviation market, that is still anchored to fossil kerosene but it is undergoing more and more impulses to rely on biofuels, especially from supersonic flights' world that could take advantage of SAF to come back on top: if great results about pollutant emissions reduction are confirmed and costs are kept low, biofuels could represent a succeeding strategy for supersonic airplanes.

Of course, there are still a lot of challenges and problems to solve before sustainable aviation fuels can really substitute conventional kerosene, but studies and research like this thesis can undoubtedly enhance the efforts to promote biofuels as reliable key to reduce environmental impact of aviation field and make the Earth a better and less polluted place to live.

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