



2nd ECATS Conference

Making Aviation Environmentally Sustainable



ECATS International Association



PROCEEDINGS

7-9 November 2016, Titania Hotel, Athens - Greece

Monday November 7th, 2016

12.00 - 13.30 Registration – Welcome Coffee

13.30 - 13.45 Welcome

13.45 - 15.00 **Alternative Fuels for Aviation**
Chairperson: **Joanna Bauldreay**

Sustainable HEFAs for Aviation
Stella Bezergianni

Alternative fuels for aviation. Beyond ITAKA
Inmaculada Gomez Jimenez

Alternative aviation fuels - Lifecycle emission and energy profiles
Laura Lonza

15.00 - 15.40 Coffee Break

15.10 - 15.40 Poster Session

PP01: Cost-effective and sustainable decarbonisation of aviation fuels
Stella Bezergianni

PP02: Experimental and computational study of reciprocal interactions of O-Nitrile elastomer and alternative aviation fuel chemical constituents
Ehsan Alborzi

PP03: Heat release markers for the combustion of alternative aviation fuels in gas turbines
George Skevis

PP04: Methodologies for automatic hydrocarbon autoxidation mechanism generation
Matthew Dwyer

PP05: Camelina oil - A possible biofuel for terrestrial application
Ionut Porumbel

PP06: Intercooled recuperated aero engine: Early development stages and optimization of recuperation based on conventional heat exchangers
Dimitrios Misirlis

15.40 - 17.40 **Alternative Fuels for Aviation** (continuing)
Chairperson: **Christopher Lewis**

US Perspective - Alternative fuel research and the ASCENT program
Mohan Gupta

Smart fuels for aviation: The SMARTCATS cost action
George Skevis

Quasi automated approach for construction of reduced chemical kinetic mechanism for autoxidation of blend of conventional and alternative fuels
Ehsan Alborzi

A study on the emissions of alternative aviation fuels
Marina Braun-Unkhoff

Wrap-up
Christopher Lewis, Joanna Bauldreay

18.00 Conference Reception at the Olive Garden of the Titania Hotel

08.30 - 09.00 Registration – Coffee

FORUM–AE Workshop on Climate Impact

09.00 - 10.15 **Climate Impact and Mitigation Concepts**

Chairperson: **Sigrun Matthes**

Intro: Climate impact of aviation

Sigrun Matthes

Future aviation CO2 emissions impact on climate

Etienne Terrenoire

Seasonal analysis of contrail and contrail cirrus

Margarita Vazquez Navarro

10.15 - 10.45 Coffee Break

10.45 - 12.15 **Climate Impact and Mitigation Concepts** (continuing)

Chairperson: **Sigrun Matthes**

Climate impact of contrail and contrail cirrus

Lisa Bock

Chemical impacts of aviation emissions

Volker Grewe

Alternative routing: Climate impact mitigation studies

Sigrun Matthes

Wrap-up

Etienne Terrenoire

12.15 - 13.15 Lunch Break at the Olive Garden Restaurant

13.15 - 15.00 **Climate Impact and Mitigation Concepts** (continuing)

Chairperson: **Didier Hauglustaine**

Intro: Greener by design

John Green

Emission and mitigation concepts

Paul Madden

Flame stabilization aerodynamics and emissions performance at stratified or fully premixed inlet mixture conditions

Panayiotis Koutmos

Intercooled recuperated aero engine: Development and optimization of innovative heat exchanger concepts

Dimitrios Misirlis

15.00 - 15.30 Coffee Break

15.30 - 17.25 **Climate Impact and Mitigation Concepts** (continuing)

Chairperson: **Didier Hauglustaine**

Assessment of PM emission from engines

Olivier Penanhoat

The expected impact from the introduction of a new Strut-Braced Wing aircraft configuration on global air traffic emissions and climate - results from the WeCare project

Florian Linke

Drag reduction in aircraft wings using dielectric barrier discharge

Zinon Vlastosergios

Aircraft level assessment of contrail mitigation

Jean-Charles Khou

Wrap-up

Ling Lim

19.00 Conference Dinner at The Acropolis Museum (meeting point at the hotel lobby)

08.30 - 09.00	Coffee
09.00 - 11.00	<p>Green Flights - Climate Optimal Flight Trajectory Florian Linke</p> <p>Chairperson:</p> <p>A note on how to internalize aviation's climate impact on Non-CO2 effects Robin Ghosh</p> <p>Feasibility of climate-optimized air traffic routing for trans-Atlantic flights Volker Grewe</p> <p>Simulation of air traffic using weather-based climate cost functions – Feasibility analysis Tanja Luchkova</p> <p>US Perspective - ASCENT program and FAA studies on Interdependency and climate modeling Mohan Gupta</p> <p>Wrap - Up Florian Linke</p>
11.00 - 11.40	Coffee Break
11.10 - 11.40	Poster Session
	<p>PP07: Environmental impact functions: Linking environmental impact information for planning environmentally-optimal trajectories Sigrun Matthes</p> <p>PP08: Eco-efficient aviation: An overview on first results from the WeCare project Volker Grewe</p> <p>PP09: Identifying climate optimal trajectories in under different synoptical situations Sigrun Matthes</p>
11.40 - 12.55	<p>Interdependency and aviation environmental Modelling Dominique Collin</p> <p>Chairperson:</p> <p>Assessing trends in aviation noise and emissions in Europe using advanced modeling capabilities Laurent Cavadini</p> <p>Modelling of aircraft emissions in the airport area Kateryna Synylo</p> <p>Modelling airport air quality at high resolution Claire Sarrat</p>
12.55 - 13.55	Lunch Break at the Olive Garden Restaurant
13.55 - 15.00	<p>Interdependency and aviation environmental Modelling Dominique Collin</p> <p>Chairperson:</p> <p>The aircraft emissions model: Future Aviation Scenario Tool (FAST) Ling Lim</p> <p>An Integrated Modelling Approach for Climate Impact Assessments in the Future Air Transportation System – Findings from the WeCare Project Robin Ghosh</p> <p>Wrap-up Paul Brok</p>
15.00 - 15.20	Coffee Break
15.20 - 15.50	<p>Early Career Researcher Award Ceremony Wrap-up and closing remarks Simon Blakey</p>



ORAL PRESENTATIONS

Alternative Fuels for Aviation

SUSTAINABLE HEFAS FOR AVIATION

S. Bezergianni, L.P. Chrysikou

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Abstract. There are several technological pathways for the production of alternative and high sustainable aviation fuels, aspiring to mitigate GHG emissions. Hydrogenated Esters and Fatty Acids (HEFAs) are ASTM-certified aviation biofuels with no technical or safety consideration during the numerous demonstration applications, with only limitation their production cost. In this work, the sustainability potential of HEFAs for aviation applications is examined, considering the cultivation/transportation and hydroconversion of different lipid sources/feedstocks (plant oils and microalgae). The hydroconversion of each lipid source is evaluated with respect to the individual quality characteristics (fatty acids content type, chain length, saturation degree) providing a theoretical evaluation protocol for different potential feedstocks. The results indicate that lipid sources consisting of saturated fatty acids of close-to-jet carbon-chain length (C12-C14) are the most promising feedstocks for aviation HEFAs production.

Keywords: HEFA, hydroconversion, lipids, microalgae, LCA

INTRODUCTION

Aviation transport has specific climate impacts compared to other transport modes mainly because most air-transport emissions occur at a high altitude. Air transport currently accounts for a small share (10%) of global energy consumption but its growth rate is one of the largest ones (5% annually according to IATA), rendering an expected 1.5-3% growth in aviation fuels consumption, and subsequent increase of GHG emissions. In order to mitigate the corresponding climate change effects attributed to the aviation sector, a 1.8 billion tons reduction of the equivalent CO₂ emissions is required by 2050. This target can be partially achieved by improving fleet rollover, aircraft infrastructure as well as engine performance, while a 25-50% CO₂ emission reduction is expected by the use of renewable aviation fuels. Thus, the technology development of new alternative and high sustainable aviation fuels that can mitigate GHG emissions is of outmost importance.

At present there are several technological pathways leading to aviation biofuels, based on thermochemical and/or enzymatic conversion of biomass (ex. lipids, sugars, and lingo-celulosic material). The available technological pathways and produced aviation biofuels offer different advantages and disadvantages with regards to the production costs, quality characteristics, and feedstock flexibility/availability. Hydrogenated Esters and Fatty Acids (HEFAs) are ASTM-certified (D7566) biofuels that have demonstrated no technical or safety problem in flights, while their production is already supported by several plants in operation. Nevertheless, the dependence on plant oil contained lipids and high production costs (1700-2400\$/t) limit HEFAs market growth and sustainability potential. A simplified process diagram of HEFAs production is given in Figure 1.

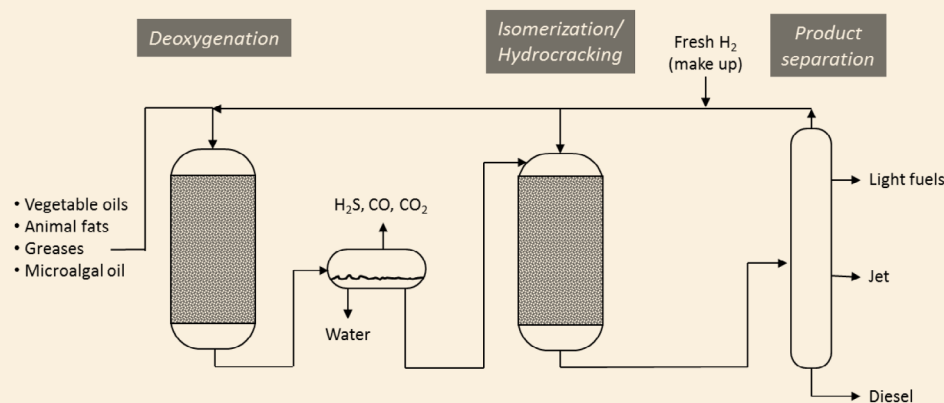


Figure 1. HEFA biofuels production simplified schematic

In this paper, HEFAs sustainability optimization potential is evaluated with respect to the lipids feedstock type, taking into consideration the cultivation/harvesting costs and the hydrogen consumption associated with the underlying conversion reactions.

AVIATION HEFAS SUSTAINABILITY

HEFAs sustainable production is strongly related with the lipid sources cost and the downstream catalytic hydroconversion process operating cost. Regarding the later, over 77% is attributed on the H₂ utilized according to Lehmus (2011), as H₂ consumption affects both the operating cost and the final fuel carbon footprint.

The hydrogen consumption during the catalytic hydroconversion of lipids into aviation biofuels (biojet) involves a reaction network series including saturation, oxygen removal, isomerization and cracking, which is described in Figure 2. In particular the first reaction involves the hydrogenolysis of the triglyceride molecules into fatty acids and propane. For plant oil lipids, consisting mainly of triglycerides, this reaction has to take place before any other reaction and is associated with a large amount of hydrogen consumption. In the case of microalgae lipids, however, this reaction does not occur, as free fatty acids are mainly constituting microalgae-based feedstocks. Saturation is the second type of reaction that takes place (Eq.2), but for this reaction step, the hydrogen consumption depends on the type of fatty acids contained in the feedstock, i.e. plant oils with a large percentage of unsaturated fatty acids such as sunflower consume larger amounts of hydrogen for saturation. For this reason the hydrogen consumption during the saturation step varies significantly for different plant oils. The third group of reactions is deoxygenation, which leads to the removal of oxygen from the fatty acid molecules. There are three different possible routes including hydrogenation (Eq. 3a), decarbonylation (Eq. 3b) and decarboxylation (Eq. 3c). The last two routes are definitely the most desired ones as they only consume 1 mol of hydrogen per mol of fatty acid. However, the current commercial hydrotreating catalysts are not as selective towards the last two routes and they are mostly activating the hydrogenation step which consumes a lot of hydrogen. The fourth reaction step is isomerization, which is required in order to convert n-paraffins to iso- and cyclo-paraffins, improving the cold flow properties, and is not associated with significant hydrogen consumption. Finally, hydrocracking is the reaction that is required in order to crack C-C paraffin bonds to produce smaller carbon-chain length molecules, which are within the desired C9-C13 range.

Reaction type	Reaction mechanism	H ₂ /oil (mol/100mol)
Triglyceride hydrogenolysis	$\begin{array}{c} \text{O} \\ \parallel \\ \text{CH}_2\text{-O-C-R} \\ \\ \text{CH-O-CO-R} \\ \\ \text{CH}_2\text{-O-C-R} \\ \parallel \\ \text{O} \end{array} + 2\text{H}_2 \longrightarrow 3\text{R-CH}_2\text{COOH} + \text{CH}_3\text{-CH}_2\text{-CH}_3 \quad (1)$	2·100
Saturation	$\text{R-(CH=CH)}_n\text{-COOH} + n\text{H}_2 \longrightarrow \text{R-CH}_2\text{-CH}_2\text{-COOH} \quad (2)$	$\frac{3 \cdot n}{n=50-225^*}$
Deoxygenation	$\left\{ \begin{array}{l} \text{R-CH}_2\text{COOH} + 3\text{H}_2 \longrightarrow \text{R-CH}_2\text{CH}_3 + 2\text{H}_2\text{O} \quad (3\text{-a}) \\ \text{R-CH}_2\text{COOH} + \text{H}_2 \longrightarrow \text{R-CH}_3 + \text{CO} + \text{H}_2\text{O} \quad (3\text{-b}) \\ \text{R-CH}_2\text{COOH} + \text{H}_2 \longrightarrow \text{R-CH}_3 + \text{CO}_2 \quad (3\text{-c}) \end{array} \right.$	3·100
Isomerization	$\text{R-CH}_2\text{-CH}_2\text{-CH}_3 \longrightarrow \begin{array}{c} \text{R-CH-CH}_3 \\ \\ \text{CH}_3 \end{array} \quad (4)$	0
Hydrocracking	$\text{R-CH}_2\text{-CH}_2\text{-CH}_3 + \text{H}_2 \longrightarrow \text{R-H} + \text{CH}_3\text{-CH}_2\text{-CH}_3 \quad (5)$	3·(78-95)**

*Based on range of content of unsaturated fatty acids of each vegetable oil

**Based on range of content of large-carbon chain fatty acids of each of each vegetable oil

Figure 2. Main catalytic hydroconversion reaction mechanisms of lipid feedstocks

Based on the detailed examination of the aforementioned reaction network for HEFAs production, the fraction of long-chain fatty acids, degree of saturation and the free fatty acids (that require no hydrogenolysis) varies with the type of lipid source as it was presented in Winayanuwattikun *et al.* (2008), rendering some lipids more demanding than others in terms of the hydrogen consumption associated with the different reactions. In fact, based on the aforementioned analysis, hydrogen consumption and thus the overall production cost would significantly decrease if the lipid source consisted of saturated fatty acids of close-to-jet carbon-chain length (C12-C14).

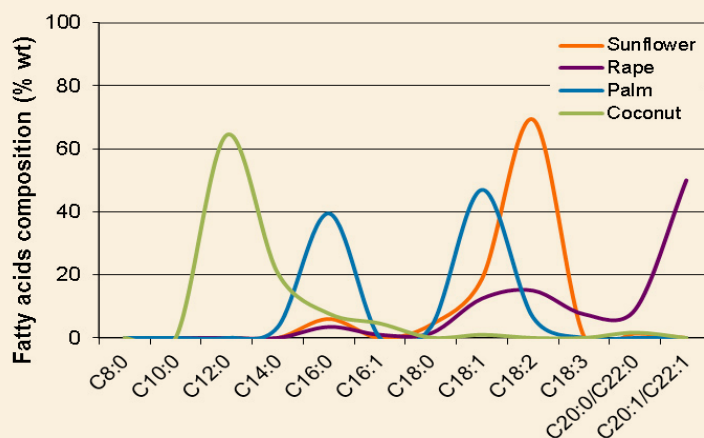


Figure 3. Fatty acid composition of four plant lipids examined

Nevertheless, nature renders great variability with respect to the consistency of various lipids sources (see Figure 3), which is reflected in the theoretical H_2 consumption during their hydroconversion to jet fuel, as shown in Table 1. Sunflower oil contains triglycerides consisting of C18 fatty acids which are mostly (89%) unsaturated, therefore its conversion to jet molecules would require significant H_2 for both saturation and hydrocracking reactions. While the other two widely used plant oils (rape and palm) do not render significant savings on H_2 consumption, coconut oil exhibits significant improvement as 92% of each contained fatty acids are saturated and 85% are within the desired C12-C14 range. Microalgae based lipids have the advantage of containing free fatty acids, therefore not requiring hydrogenolysis, which are mostly saturated. However, with the exception of *Strichodesmium erythraeum sp.* which consists of C10-C14 molecules, all other well established species render C14-C16 hydrocarbons, thus requiring hydrocracking.

It is significant to note that plant lipids containing triglycerides demand H_2 during hydrogenolysis (Figure 2-Eq.1) but render triple volume yields on the produced jet molecules (1 mole plant-oil contained triglycerides renders around 3 moles of jet), while microalgae lipids consisting of free fatty acids may not require hydrogenolysis but have no volume increase (1 mole microalgae-oil fatty acids renders 1 mole jet). For this reason H_2 consumption difference is less significant when it is presented in mol H_2 per mol of jet produced (see Table 1).

When the sustainability of different lipid sources is compared, one has to take into account the energy and other inputs demand during all the steps prior to the biofuels conversion plant, i.e. cultivation and transportation costs. Based on a recent study by Edwards *et al.* (2014), the GHG emissions of the four plant lipid sources examined range between 16.4-26.7g CO_2 -eq/MJ_{oil} which according to the expected volume yield increase discussed above corresponds to 185.1 – 301.3 g CO_2 -eq/lit jet produced, while microalgae lipid sources render a 50-80% reduction of the GHG emissions per lit of jet fuel produced, based on Patil *et al.* (2007) and Benemann (2012) data.

Table 1. Theoretical H₂ consumption and GHG emissions for aviation HEFAs production from different lipid sources

	Plant oils				Microalgae oils			
	Sunflower	Rape	Palm	Coconut	<i>Dunaliella</i> sp.	<i>Chlorella</i> sp.	<i>Nannochloropsis Oceanica</i>	<i>Strichodesmium erythraeum</i> sp.
1. Hydrogenolysis	2.0	2.0	2.0	2.0	0.0	0.0	0.0	0.0
2. Saturation	6.3	1.4	0.6	0.1	0.0	0.0	0.0	0.5
3. Deoxygenation	6.0	6.0	6.0	6.0	2.0	2.0	2.0	2.0
4. Isomerization	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5. Hydrocracking	2.6	2.6	2.5	0.5	0.9	0.8	0.7	0.4
Total (mol H ₂ /mol oil)	16.9	12.0	11.1	8.5	2.9	2.8	2.7	2.4
Total (mol H₂/mol jet)	5.6	4.0	3.7	2.8	2.9	2.8	2.7	2.4
GHG (g CO₂-eq/l jet)	6.0	4.3	3.9	3.0	3.1	3.0	2.9	2.6

CONCLUSIONS

The sustainability potential of aviation HEFAs was evaluated in terms of the cultivation/transportation and hydroconversion requirements of different lipid sources/feedstocks (plant oils and microalgae). Based on this study, the microalgae originating lipids had favourable carbon footprint vs. the plant lipids. Particularly for the plant lipids, it was shown that their cultivation/transportation steps were the main contributors to the overall jet production carbon footprint, due to the excessive input demands of their cultivation steps. The microalgae lipids had a significantly lower demanding cultivation steps, favouring the overall footprint. The hydroconversion energy requirements (H₂ consumption) were much lower as compared to those of the cultivation steps for all types of lipid sources. In fact the hydroconversion energy inputs of some plant oil contained lipids (palm and coconut) were comparable with the microalgae ones per unit volume of the jet produced.

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ALTERNATIVE FUELS FOR AVIATION. BEYOND ITAKA

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Abstract. The ITAKA project aimed to demonstrate the development of biojet in an economically, socially, and environmentally sustainable manner, improving the readiness of European technology and infrastructures. ITAKA has performed research and demonstration activities along the biojet value chain from production to its final use by the airlines in commercial operations, using conventional airport infrastructures and dedicated supply for testing flights.

Progress has been achieved for camelina and UCO as feedstocks, improving their readiness for Europe. At the refining phase, results show that there is potential to better adjust the parameters of the fuel to the needs of the aircraft. At aircraft-fuel systems level, tests on engine, APU and flights have provided information about performance and emissions, delivering interesting potential benefits as the reduction of frequency of maintenance or the mitigation of local pollutants.

Particularly relevant, ITAKA has provided the first worldwide demonstration of comingled use of biojet at an airport, providing key elements for the discussions about emissions trading, other than demonstrating the drop-in characteristics of the biojet and generating public awareness about the use of biojet at airports.

Interesting results have been gathered about the technical, operational and performance challenges and opportunities of using alternative fuels. Also, some gaps have been identified, especially related with the market situation that should be discussed to continue promoting the use of alternative fuels.

As a result, ITAKA outputs can be used by the scientific community as a basis for further research and for strategic decision making about alternative fuels for aviation agendas.

Keywords: Biojet, alternative fuels, deployment, sustainability.

INTRODUCTION

The Initiative Towards sustainable Kerosene for Aviation (ITAKA) is a collaborative project framed in the implementation of the European Union policies, implementation of European Industrial Bioenergy Initiative (EIBI) and specifically aims to contribute to the fulfilment of some of the short-term (2015) EU Advanced Biofuels Flight Path objectives.

The ITAKA project supports the development of aviation biofuels in an economically, socially, and environmentally sustainable manner, improving the readiness of existing technology and infrastructures. This has been achieved through a first of its kind collaborative project in the EU, which has developed a full value-chain in Europe to produce sustainable drop-in Hydroprocessed Esters and Fatty Acids at large scale.

The value chain was fully demonstrated by testing the use of the biojet fuel produced in existing logistic systems and in normal flight operations in the EU. ITAKA linked supply and demand by establishing a relationship under specific conditions between feedstock grower, biofuel producer, distributor and final user (airlines), encompassing the entire supply chain.

ITAKA links supply and demand by connecting the full value-chain: feedstock grower, biofuel producer, distributor and airlines.

ITAKA addressed challenges in two main areas:

- Development of commercial scale production and study implications of large-scale use.
- Research on sustainability, economic competitiveness and technology readiness.

The overall objective of ITAKA was to produce sustainable Synthetic Paraffinic Kerosene (SPK) at large scale in order to allow testing and demonstrating its use in existing logistic systems and in normal flight operations in Europe. The generated knowledge is aimed to identify and address barriers to innovation and commercial deployment.

Development and validation of biojet full value chain, starting from camelina oil provider to production plant, testing, blending, distributing and storing the fuel until the delivery to the end-user.

Sustainability, competitiveness and technology assessments have been performed, studying economic, social and regulatory implications of large-scale use.

Beyond these technological and research objectives, ITAKA also contributes to the achievement of a further EU objective: the need to coordinate efforts and complementarities among European initiatives on sustainable aviation fuels, as highlighted during the Flight Path definition and identified in SWAFEA recommendations: "Setting up a knowledge and test capability network within the EU to provide an EU based fuel evaluation capability". ITAKA has been built aiming to engage key stakeholders and to make a first significant step in the establishment of such a European network; ITAKA is connected and collaborated with the main biojet fuel initiatives in Europe and worldwide.

WORK PLAN

The ITAKA workplan covers all phases of the value chain for the implementation of the biofuels, from feedstock to final users:

1. Feedstocks: focused on camelina oil, this phase delivers adapted camelina varieties and crop protocols for its cultivation in Europe.
2. Energy: includes the production of biojet fuel, the innovations for the production in existing refineries, the assessment on waste oils and a model for the collection and elaboration of economic and financial data related to the refining technologies.
3. Logistics: this phase tackles all the issues regarding the delivery of the fuel, from the refinery to the final use, including the segregated distribution for specific tests but also the use in normal airports systems.
4. Aviation: this phase is focused in analyse the different effects and differences of the biojet fuel use in the aircraft fuel systems, but also to interact with the airlines to knowing their requests and needs regarding alternative fuels.

Finally, all these four blocks are integrated to improve the coordination and interfaces and also to assess the technological and sustainability performances.



Figure 1. Structure of the ITAKA work plan. The central element of the project is linking the different elements of the value chain for its integration under sustainability conditions.

RESULTS

All the experiences and research carried out have contributed to optimize the value chain performance in Europe. For clarity sake, the main results are showed in the Table 1.

Table 1. Main ITAKA results per value chain step

Value chain step	Description of key result
Camelina oil production	<ul style="list-style-type: none"> • 4 camelina large plantations deployed in Spain + 2 in Romania • Selected and new camelina varieties adapted for Europe and with increased oil content • Optimized camelina growing protocols • new techniques for pre-processing UCO (Used cooking Oil)
Refining	<ul style="list-style-type: none"> • Improved refining facilities (new circulation line) • Adapted protocol for in house quality testing
Logistics	<ul style="list-style-type: none"> • Better knowledge of the fuel logistics infrastructure: different systems, owners and operators and solutions for biojet, including new procedures for agreements and traceability. • 1st worldwide use of biojet on an airport hydrant system (Oslo airport) demonstrating normal use. • Blending accountability: to be tracked based on chain of custody documentation on mass-balance basis for carbon trading and other mechanisms.
Aviation use	<ul style="list-style-type: none"> • 18 flights AMS-AUA-BON [A330-200]: no detrimental effects on operation, similar or slightly better fuel consumption • 2 APU tests for pollutant emissions: reduction in fuel flow, reduction in the SAE smoke number and possible reduction in PMs. No changes NOx or UHC. • 80 flights OSL-AMS [E190]: no detrimental effects on operation, similar or slightly better fuel consumption
Sustainability	<ul style="list-style-type: none"> • GHG savings estimated to achieve 60%, (66% as a standard value). EU RED RSB and RSB certification for the CCE camelina oil plantations. • Low ILUC risk assessment: as camelina is produced in fallow land under rotation, no demand of additional land or substitution of crops. • Several sustainability checks: RFS2 and SkyNRG sustainability board passed.

CONCLUSIONS

The main conclusions out from the ITAKA project are:

- There is potential for production of camelina oil as feedstock for sustainable biojet fuel in Europe, not enough to covering all the targets, but as a significant contributor.
- There are absolutely no negative effects from the use of the biojet in operations, including some main maintenance operations like in flight generated water drainage.
- The results indicate that greenhouse gases savings can go over 80% when using UCO and over 60% when using camelina oil as feedstock. While, some other pollutants like particulates (nvPMs) can be improved using synthetic fuels with a lower content in aromatics as the biojet.

Biojet production in the European Union faces some barriers and limitations, particularly regarding the market and the price gap, but it is technologically ready to produce and use biojet from the HEFA pathway.

ACKNOWLEDGMENTS

The ITAKA Consortium was composed by companies from 9 countries and coordinated by SENASA, representing the actors involved in the full production and value chain: Airbus Group (FRA, UK), Biotehgen (RO), Camelina Company España (ES), CLH (ES), Embraer (BR), EPFL (CH), Manchester Metropolitan University (UK), Neste (FI), RE-CORD (IT), SkyNRG (NL).

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REFERENCES

The detailed results summarized in this article can be found at www.itaka-project.eu.

ALTERNATIVE AVIATION FUELS - LIFECYCLE EMISSION AND ENERGY PROFILES

Laura Lonza
European Commission

Abstract. The results are presented of a study carried out at the European Commission's Joint Research Centre providing insights on the GHG emissions profiles and the energy efficiency of representative options for the supply of alternative aviation fuels. Such insights are expected to be of interest to and – ideally – use by decision-makers when considering investment options.

When assessing alternative options – not a simple task due to varied levels of technology maturity – it is important to consider whether the energy efficiency of each alternative fuel option is justified by the benefits in terms of emissions' reductions within a reasonable timeframe.

The energy and GHG savings of drop-in biofuels for aviation are critically dependent on manufacturing processes and the fate of co-products. Methodology choices are therefore crucial to determine results. For purposes of reporting or accounting, emissions from combustion biofuels are often considered as being zero as the fuels are produced from biomass (i.e., the emissions are biogenic). However, non-biogenic emissions associated with biofuels result from the cultivation, harvesting and transport of the biomass, as well as from its conversion into biofuel. The scope of the analysis is focussed on alternative drop-in jet fuels.

The results indicate that fuels made from wastes and residues exhibit much lower GHG emissions per MJ of final fuel when compared to aviation fuels produced from the range of vegetable oils analysed. Of the vegetable oils investigated, a large effect on emissions was seen in palm oil pathways due to two factors; namely the type of land used for cultivation and whether or not methane capture was employed at the oil mill.

SMART FUELS FOR AVIATION: THE SMARTCATS COST ACTION

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Abstract. The successful introduction of sustainable alternative fuels (including biofuels and synthetic fuels) in the aviation sector requires a thorough collaboration of academic, industrial and policy actors covering all aspects of fuel production, distribution and utilization. The SMARTCATS COST Action (Chemistry of Smart Energy Carriers and Technologies, CM1404, www.smartcats.eu), aims to create a Europe-wide network of world leading academic and research institutions and key industries to promote the use of Smart Energy Carriers, SECs (fossil, unconventional and renewable) on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies. The approach to accomplish this aim is twofold. On the one hand, academic/research organizations will devote strong efforts to bring together fundamental/advanced numerical and diagnostic tools to improve the understanding of combustion kinetics and by-products formation of SECs at micro/meso-scale levels. On the other hand, the intended exchange between academic and industrial partners will support the optimization of tools developed in the Action exploiting the way that SECs could be utilised at the macro-scale in advanced combustion technology devices. This interaction will lead to the identification of standards and criteria for the development of a searchable database and internet tool devoted to integration of experimental and numerical combustion chemical/physical data which will provide easy access to information relevant to SECs components. The current paper provides a detailed description of SMARTCATS work programme and illustrates examples of its application to the development and utilization of alternative aviation fuels.

Keywords: Smart energy carriers, Alternative aviation fuels, Academia/Industry Symbiosis

INTRODUCTION

A safe, secure and environmentally-friendly energy supply is among the highest priorities and concerns of contemporary society. Currently, combustion of conventional and alternative fuels accounts for about 80% of total gross energy production in Europe. The greatest challenge that the combustion community has to face in the coming years is the urgent need for maximum fuel flexibility of combustion technologies, the minimization of greenhouse gas (GHG) emissions and the adjustment of distributed energy production, the so called Combustion Trilemma, Fig. 1. Fuel flexibility is a prerequisite to exploit a fast changing fuel market and an increasing number of energy carriers available. Mitigation of GHG emissions is a central priority of the EU Framework Programme for Research and Innovation Horizon 2020 and it is clear that a multifaceted approach, encompassing highly efficient low- carbon technologies coupled with medium-term emission containment (e.g. Carbon Capture and Storage/Utilization), will have to be pursued in order to avoid potentially catastrophic climatic consequences. The realization of a new energy production and distribution system based on smart grid concepts is often seen as a possible straightforward option for developed countries.

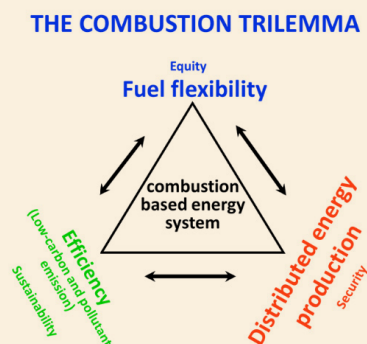


Figure 1. The Combustion Trilemma

These three needs derive from a complex geo-political situation with multiple influences on fuel availability and perspectives as well as from the long term objective of build up a low carbon society in the EU, the opportunity offered by the growing of cyber-physical applications and their reflection on smart energy distribution and utilization grids and the ecological drives.

The scope, objectives and outcomes of the Action are of primary relevance to the aviation sector. Aviation is one of the strongest growing transport sectors and this trend is expected to continue. Advanced biofuels constitute the only viable and sustainable alternative to kerosene. The comprehensive assessment of alternative biofuels properties and their integration with propulsion devices are crucial issues for the aviation industry and can be addressed in the context of SMARTCATs.

DEFINITION OF SMART ENERGY CARRIERS

All these factors call for the characterization, specification and proper utilization of new Smart Energy Carriers (SECs). This category includes conventional and novel energetic molecules from alternative or conventional (re)sources, selected on the basis of their best available production and/or utilization technologies. Accordingly, to be considered "smart" an energy carrier and related technologies must be energetically and CO₂ efficient and able to provide the most suitable energy mix to exploit varying and locally diverse sources and to satisfy the requirements for eco-compatibility and sustainability. SECs are strong candidates as possible solutions for energy storage, transfer and transformation from renewable (wind, solar, biomass, wastes) and unconventional sources (e.g. shale gas). SECs include a wide range of compounds like aliphatics, oxygenates (alcohols, esters, ethers) as well as olefins, naphthenes and their mixtures with diluents (CO₂ and H₂O). As a consequence, energy conversion systems have to face an increasing variety of smart carriers that change their characteristics depending on the available source. Even though tailor-made fuel technologies are under development, feedstock and fuel processing variability influences fuel properties in a complex and sometimes unpredictable way. To meet these needs, advanced combustion technologies for energy and power generation in the industrial, domestic and transport sectors are required. Such technologies have to be fuel-flexible and able to achieve high efficiencies, often operating under conditions that are significantly different from those of conventional combustion modes. A new knowledge has to be built to make SECs and new combustion technologies usable in an efficient and sustainable way.

THE SMARTCATS COST ACTION

The approach to accomplish this aim is twofold. On the one hand, academic/research organizations will devote strong efforts to bring together fundamental/advanced numerical and diagnostic tools to improve the understanding of combustion at micro/meso-scale levels. On the other hand, the exchange between academic and industrial partners will support the optimization of tools developed in the Action exploiting the way that SECs could be utilised at the macro-scale in advanced combustion devices. This interaction will lead to the identification of standards and criteria for the development of internet tools devoted to integration of experimental and numerical physico-chemical combustion data.

According to this methodology the SMARTCATs work programme is structured in five Working Groups (WG), as outlined in Fig. 2.

WG1. Smart Energy Carriers gas phase chemistry: from experiments to kinetic models that aims to improve the knowledge on detailed chemistry and thermochemistry for the combustion, pyrolysis, and oxidation of fuels, such as natural gas mixtures (compressed natural gas, liquefied natural gas, syngas natural gas, bio- methane), simple molecules (large normal and iso-paraffins, alcohols, esters, saturated and unsaturated cyclic ethers) that can be present in 1st and 2nd generation biofuels and complex mixtures of molecules actually found in 1st and 2nd generation biofuels or in the proposed surrogates.

WG2: Chemistry for control of by-products in Smart Energy Carrier conversion that aims to increase knowledge on the formation of organic and inorganic combustion by-products. The pollutant tendency of smart energy carriers will be studied by tracing pollutant species typically formed in combustion (carbon monoxide, unburned hydrocarbons (UHC), polycyclic aromatic hydrocarbons (PAH), aldehydes, NO_x soot and nano-particles) as well as other classes of pollutants possibly originating from SECs.

WG3: Chemical and optical advanced diagnostics for Smart Energy Carriers conversion monitoring that aims to improve the knowledge on advanced combustion diagnostics, with a strong focus on technology transfer from fundamental to complex systems, and focuses on advanced sampling and chemical analysis diagnostics, laser-based and mass-spectrometric diagnostics in fundamental combustion devices and chemical kinetics experiments, elementary reaction rate measurements, chemical markers for combustion performance characterization, combustion and emission measurements in complex systems (engines, furnaces, household applications, etc).

WG4: Standard definition for data collection and mining toward a virtual chemistry of Smart Energy Carriers that aims towards the identification of the main requirements and tools for the development of databases, software and mathematical tools for data collection and handling as well as chemistry optimization using data mining techniques. Definition of “crucial” experiments and simulations, uncertainty and sensitivity analysis in combustion modelling will be key issues to be considered.

WG5: Integration of fundamental knowledge towards technology application for Smart Energy Carriers exploitation that is to apply/integrate the knowledge tools developed in WG1-WG4. This will provide optimized ready to use tools and techniques for an effective use of SECs on large scale. The research activities of the WG will be driven by the identification of validation test cases, identified in collaboration with the industrial partners to provide scale-bridging information from the laboratory units to the real applications by means of integration of detailed kinetic mechanisms in large scale numerical simulations, and assessment of the uncertainty related to numerical predictions for their use in new design and regulation.

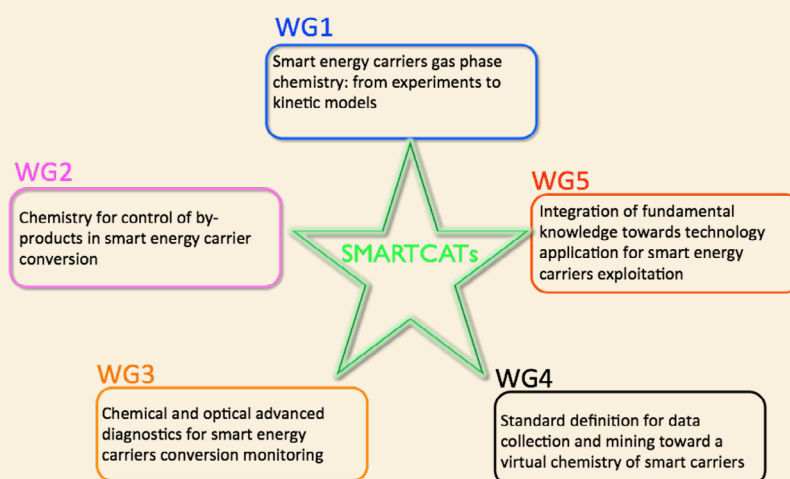


Figure 2. The SMARTCATs workgroups

A total of 75 organizations from 25 countries participate in the SMARTCATs COST Action. There is a strong participation from the industrial sector (more than 20 large companies and SMEs) and particularly from industries strongly related to the aviation sector (gas turbine manufacturers, fuel providers, engineering consulting companies).

CONCLUSIONS

Europe has a highly productive and scientifically visible fuels and combustion community, encompassing several groups with strong expertise in experimental, theoretical, and numerical simulation approaches. The SMARTCATs Action is building an effective network academic/research and industrial players aimed at addressing the “grand challenge” of matching the most promising SECs with the advanced energy conversion technologies for the 21st century. This is of particular importance to the aviation sector where extensive assessment of potential alternative fuels is crucial.

ACKNOWLEDGEMENTS

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QUASI AUTOMATED APPROACH FOR CONSTRUCTION OF REDUCED CHEMICAL KINETIC MECHANISM FOR AUTOXIDATION OF BLEND OF CONVENTIONAL AND ALTERNATIVE FUELS

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Abstract. Quasi-automated approach was used to expand pseudo detailed mechanism for aviation fuel autoxidation. This was achieved by inclusion of a mixture of 5 normal alkanes (C10 to C14) as the initial condition in "Reaction Mechanism Generator (RMG)" instead of solely one normal alkane (C12) as used in manual construction of pseudo detail mechanism. An industrial solvent composed of approximately equal amount of (C10 to C14) known as "Banner Solvent" was thermally stressed in a near isothermal plug flow reaction in order to generate chemical kinetic experimental data for the mixture. The detailed RMG generated mechanism composed of 918 reaction steps involving 61 chemical species originated from 5 hydrocarbon constituents and molecular oxygen was in a good agreement with the experimental results. By the application of species lumping the detailed mechanism was significantly reduced to only 33 reaction steps initiated from two lumped groups of normal alkanes. The reduced mechanism was validated with the experimental results of Banner solvent and neat diesel autoxidation obtained from near isothermal plug flow reactor. Since RMG presents a number of numerical issues in dealing with heteroatomic species, the authors customized the RMG libraries in order to overcome such limitation for hydroperoxide species. Quantum chemistry method, B3LYP/6-311G(d,p)/IEFPCM was used to estimate the rate parameters of antioxidant reactions. This is a work in progress and continues to combine the resultant reduced mechanism with the reduced mechanism for cyclo alkane in order to construct more representative kinetic schemes for blend of conventional and aviation fuel.

Keywords: Fuel thermal stability, Chemical Kinetics, Automated Chemical Kinetic Mechanism Generation

INTRODUCTION

Publicly available kinetic mechanisms for autoxidation of petroleum based jet fuels are constructed based on reactions and species generated from a single surrogate hydrocarbon in the range of aviation fuel cut, for instance normal dodecane. One of these mechanisms, the pseudo detailed mechanism, presents the most sensitive and representative reactions and chemical species amongst thousands of other reaction pathways and species found in thermally degraded aviation fuel spectrum. With a great deal of success in prediction of autoxidation reactions and surface deposition in mild and rigorous aero engine representative conditions, the same mechanism falls short of being consistent with conditions where blends of conventional and alternative fuels are used. This is primarily because of inherent dissimilarity in the autoxidation propensity of major hydrocarbon building blocks shaping the blends. The results of a preliminary experimental work carried out in our lab in small scale thermal oxidation test device, Petroxy, indicates the propensity and type of autoxidation reactions between normal alkanes, cyclo alkanes and iso alkanes is substantially dissimilar. This dissimilarity for n-dodecane (n-C₁₂) and decalin (cyclic hydrocarbon) is shown in Figure 1. These preliminary results indicate that pseudo detailed mechanism which is put together based on only one hydrocarbon presents limitation for the application to condition where blend of conventional and alternative fuels are used. Our approach for construction of more updated liquid phase autoxidation mechanism is to include at least two or three monocomponent hydrocarbons (depending on the in question blend of aviation fuel) as representative of two or three different classes of building blocks (representative of normal, iso and cyclo alkanes) together with dioxygen (dissolved oxygen) corresponding to the amount of oxygen in air saturated fuel in a system composed of as many reactions as possible between chemical species which are stem from hydrocarbon building blocks in the reaction medium. The choice of monocomponent hydrocarbons will be based on the major constituents of jet fuel. Addition of more building blocks results in significant increase of possible chemical reactions and chemical species (intermediate and stable products). Therefore, further attempt is required to reduce the detailed mechanism in order to be significantly less computationally expensive for the application in "Computational Fluid Dynamic (CFD)" and at the same time to maintain the main chemistry of the in question system. The manual generation of chemical kinetic mechanisms in general begins with the selection of important species which usually include reactants and products

as well as significant intermediate species that are necessary to calculate the generation of key products or other key quantities. The type of reactions that can occur between these coupled groups of chemical species must then be specified along with appropriate thermochemistry data. Although, the identity and the reaction patterns for most of the species in the range of aviation fuel are fairly understood, inclusion of all these species and reactions requires expertise in kinetic mechanism generation techniques. However, manual construction of mechanism for a mixture of monocomponent hydrocarbons (the surrogate fuels representative of aviation fuel) is a tedious and error prone process. For this reason the automated reaction generation is required. Therefore "Reaction Mechanism Generator (RMG)" computer code was used as an automated tool for kinetic mechanism generation. RMG is an open source code developed by Prof. W. Green research group at "Massachusetts Institute of Technology (MIT)". RMG was originally developed in Java language by Jing Song in 2004 following approaches pioneered by NetGen at and ExxonMobil Mechanism Generator(XMG)ⁱⁱ however, a better readability, better error handling and broader access to variety of existing chem-informatics libraries is achieved by Python version of RMG known as RMG-Py. Over the years, several detailed kinetic mechanisms generated by RMG have been published in open literature, including models for butanolⁱⁱⁱ, ketone biofuels^{iv}, JP-10^v jet fuel all in high temperature oxidation and combustion regime.

RMG-Py was used^{vi} in our research group for construction a detailed mechanism for diesel autoxidation process. The detailed mechanism was reduced through an algorithmic approach based on chemical species. Comparison between the detailed and reduced kinetic mechanisms is shown in Figure 2. The reduced mechanism was numerically integrated and compared with the result of neat diesel autoxidation which proved a good agreement for the first phase autoxidation process as shown in Figure 3. The rate parameters for the competing reaction of antioxidant with normal alkanes substrates in H-abstraction by peroxy radicals was calculated using quantum chemistry method B3LYP/6-311G(d,p)/IEFPCM as shown in Figure 4 and Figure 5.

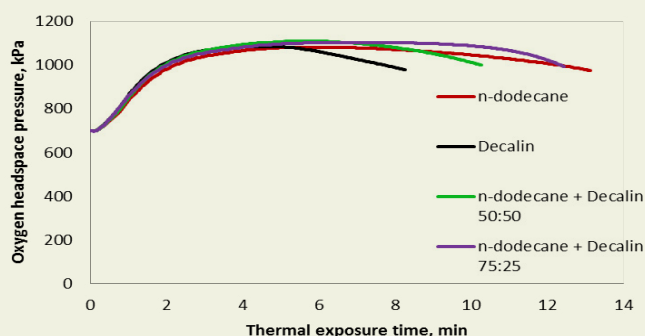


Figure 1: Dissimilar autoxidation propensity between normal alkane and cyclic hydrocarbon obtained in a small scale thermal oxidative test device (Petroxy)

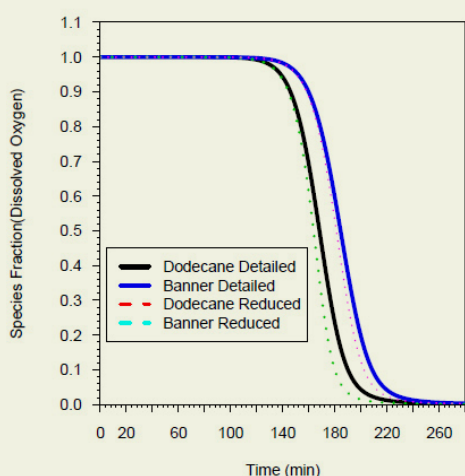


Figure 2: Comparison between calculated rate of autoxidation using reduced and mechanisms for normal dodecane and mixture of 5 hydrocarbons resembling banner solvent

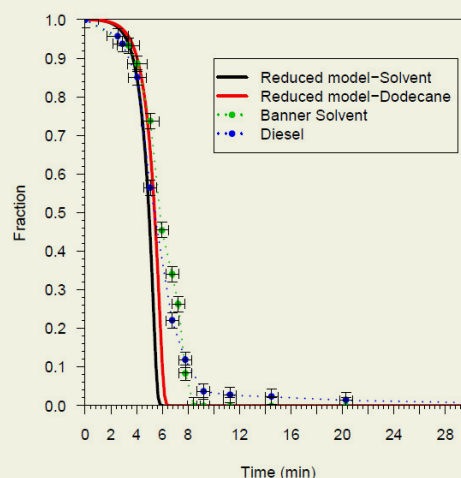


Figure 3: Validation of reduced with the experimental results of autoxidation of neat diesel and Banner solvent

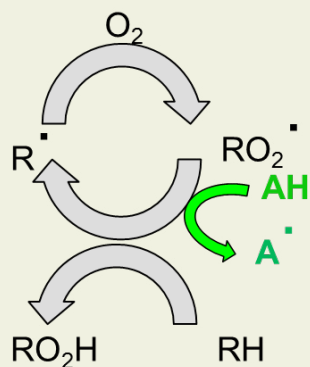


Figure 4: Competing reactions between Antioxidant(AH) and hydrocarbon substrates(RH) in H-abstraction reaction by RO_2

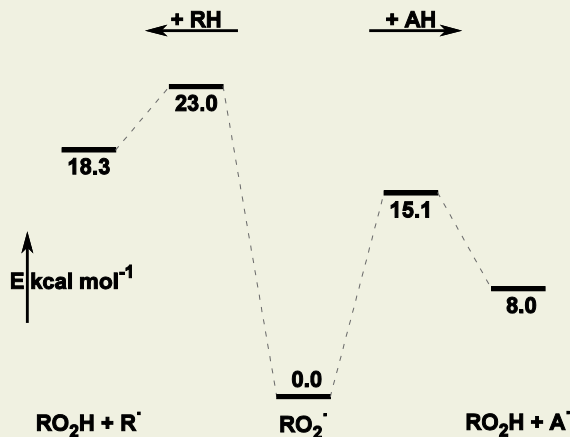


Figure 5: Calculated activation energy of the reaction of antioxidant with RO_2 radicals

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A STUDY ON THE EMISSIONS OF ALTERNATIVE AVIATION FUELS

Marina Braun-Unkhoff

DLR

Abstract. Since the last decade, the aviation sector is seeking for alternatives to kerosene from crude oil, as part of the efforts combating climate change by reduction of greenhouse gas (GHG) emissions, in particular carbon dioxide (CO₂) and ensuring security of supply at affordable prices. These efforts were also triggered by commitments and policy packages, e.g. the 'Flightpath 2050' initiative released by the European Commission.

The technical feasibility as well as the compatibility of alternative jet fuels with today's planes has been proven, with advanced biofuels as the only low-CO₂ option for substituting kerosene, for blends at up to 50%. Within the European Advanced Biofuels Flight Path launched 2011 by the EU, a roadmap was defined with clear milestones to speed up the commercialization of aviation biofuel deployment in Europe.

The use of sustainable kerosene offers several advantages, going beyond reduced CO₂ emissions. When burning a jet fuel, the exhaust gases are a mixture of many species, with unburned hydrocarbons, aromates and further precursors of particles and soot among them. These gases are released in the atmosphere, and may affect the growth and lifetime of contrails, depending on several parameters, e.g. pressure, temperature, turbulence, and relative humidity. Especially contrails are known to be of influence on the climate due to their radiative forcing.

These issues will be addressed by focusing on the emissions of alternative fuels taken into account their individual composition, including two types of crude-oil based kerosenes for reference. Plug flow calculations will be performed by using a detailed chemical-kinetic model for relevant temperatures, pressures, residence times, and fuel-air ratios. Results will be shown for emissions of NO_x, CO, benzene and acetylene as major soot precursors. In addition, an overview of what is known on the emission pattern from measurements will be given.

Climate Impact and Mitigation Concepts

FUTURE AVIATION CO₂ EMISSIONS IMPACT ON CLIMATE

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Abstract. A compact Earth system model (OSCAR v2.1) is used to assess the global climate impact of aviation carbon dioxide (CO₂) emissions. The impact has been quantified over the 1940–2100 period according to two aviation emissions scenarios based on the Advisory Council for Aeronautics Research in Europe (ACARE) 2050 objectives and the Quantifying the Climate Impact of Global and European Transport Systems (QUANTIFY) A1 reference scenario developed according to the Intergovernmental Panel on Climate Change (IPCC) Special Report on Emissions Scenarios (SRES) storyline. The new calculated change in radiative forcing (RF) due to CO₂ aviation emissions for 2005 is equal to 20 mW/m² for ACARE 2050 and 22 mW/m² for QUANTIFY A1. It is lower than the previously published figure (28 mW/m²). The revised lower CO₂ emission level used for this study and the different simple climate models used are the main reasons for the differences. In 2050, the RF increase is lower for ACARE 2050 (52 mW/m²) than in the other study (>70 mW/m² for all scenarios). Conversely, the QUANTIFY A1 scenario 2050 value for RF (80 mW/m²) is slightly above the Lee et al. values. Compared to the 2010 values, in 2050, the relative contribution of the CO₂ aviation emissions to the temperature increase (ΔT) is expected to increase by 60% (0.95%, 0.89%–1.0% 68% uncertainty range to 1.53%, 1.41%–1.62% 68% uncertainty range) in the case of the ACARE 2050 scenario and more than double (from 1.0%, 0.98%–1.1% 68% uncertainty range to 2.30%, 2.09%–2.46% 68% uncertainty range) in the QUANTIFY A1 one.

Keywords: CO₂, aviation emissions scenario, climate change, OSCAR model, compact Earth system model

INTRODUCTION

It has previously been shown that subsonic aircraft emissions perturb the radiative budget of the Earth in various ways (Sausen et al., 2005; Lee et al., 2009). Aviation emissions are estimated to contribute to 5% (2–14%, 90% likelihood range) to the anthropogenic climate forcing with a nearly threefold uncertainty due to non-CO₂ effects (Lee et al., 2010). In light of the 1.5–2°C COP21 objective, this paper aims to quantify the impact of aviation CO₂ emissions on climate from 1940 to 2050 and up to 2100 using a compact climate model with updated aviation emission scenarios and using appropriate emissions for all other sectors that will respect the Paris agreement.

DESCRIPTION OF THE MODEL

In this study, we use the OSCAR v2.1 compact Earth System model described in Gasser et al., 2016. OSCAR v2.1 is a compact coupled carbon cycle and climate model that calculates the global concentration of CO₂, CH₄, N₂O and halogenated compounds by balancing their historical anthropogenic emissions against the removal processes that define the lifetime of each gas species. As it is done in simplified climate models (Raupach, 2013), the global air surface temperature change (ΔT_{AS}) is calculate using a climate response function according to the following convolution:

$$\Delta T_{AS} = \lambda_T RF(t') \frac{dr_T}{dt} (t - t') dt' \quad (1)$$

with t being the time (year), λ_T the climate sensibility (K/W.m⁻²) of the model used and r_T the response function (year). Those two last parameters have been calibrated against the fifth phase of the Coupled Model Intercomparison Project (CMIP5) results (Taylor et al., 2013).

The various parameterization options offered by OSCAR (i.e., 12 for the oceanic cycle, 13 for the biospheric cycle, 7 for land use and 28 for the climate model) allow 3×10^4 different possible setups that can be used to calculate uncertainties using Monte Carlo methods.

AVIATION EMISSION SCENARIOS

In the frame of the "IMPACT *de l'aviation sur le climat présent et future*" French project funded by the Direction Générale de l'Aviation Civile (DGAC), two emission scenario named ACARE 2050 and QUANTIFY A1 have been used to model the global radiative forcing and temperature increase triggered by CO₂ aviation emissions. Fig. 1 shows the temporal evolution of the aviation CO₂ emissions for five different scenarios over the 1940 -2050 period: three QUANTIFY scenarios (A1, B1 B1-ACARE), an ACARE 2050 scenario and neutral grow one. QUANTIFY A1 is linked to a world of rapid economic growth while ACARE 2050 is more representative of a "green" scenario such as the B1 scenario (2050 values rather close). Hence, for this paper, the QUANTIFY A1 (business as usual) and the ACARE 2050 (optimistic) scenario are used in order to show the rather large range of possible future impacts.

ACARE 2050 is a future emission scenario developed in agreement with the ACARE 2050 CO₂ emission reduction objective (ACARE, 2011). The objective is to reach a 75% CO₂ reduction per kg fuel/km/passenger in 2050 in reference to the 2000 value. From 1940 to 1999, the emission data are taken from Sausen and Schumann, 2000. A linear interpolation is used to calculate the value between 1995 and 2005 using the 2005 value from the System for Assessing Aviation's Global Emission (SAGE) (Kim et al., 2007). Then, according to the EU-ACARE 2050 objectives, the 2005 base value is extended using a traffic growth coefficient of 4.6% yr⁻¹ associated with an efficiency gain of 2.7% yr⁻¹ until 2050. The ACARE 2050 scenario is an optimistic scenario with CO₂ emissions increasing at a slow rate between 2010 (653 Mt) and 2020 (777 Mt) up to 1280 Mt in 2050. The QUANTIFY A1 scenario is taken as described in Owen et al., 2010. For this scenario, the CO₂ emissions from planes are higher than in the ACARE 2050 case and increase from 870 Mt in 2010 to 1063 Mt in 2020 to reach a maximum of 2418 Mt in 2050.

The historical non-aviation CO₂ emissions for the 1940 - 2010 period come from the Carbon Dioxide Information Analysis Center (CDIAC) (Boden et al., 2013). As the main objective of the study is to quantify the impact of the aviation sector on future climate in a 1.5 -2 °C temperature increase projection (i.e. COP21 Paris agreement), RCP2.6 is used for emissions from other sectors (i.e. energy, industry, agriculture). Indeed, among the four RCPs assessed by the IPCC, RCP2.6 is the one that aims to limit global warming to less than 2 °C above preindustrial levels (Van Vuuren., 2011).

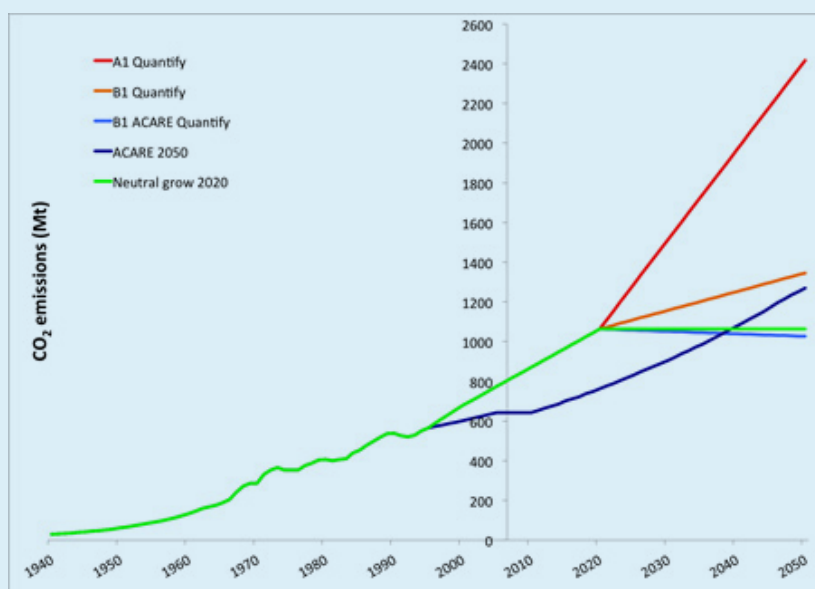


Figure 1. Past and future CO₂ aviation emissions (Mt) using the QUANTIFY A1, ACARE 2050 and other scenarios over the 1940 - 2050 period.

RESULTS

OSCAR v2.1 was used to model the temporal evolution of different global climate change indicators such as the CO₂ atmospheric concentration, the global radiative forcing (RF) and the air surface temperature (T) under the influence of two CO₂ aviation emissions scenarios. RF and T are relative to their preindustrial level and are denoted ΔRF and ΔT , respectively. The results with (red lines) and without (blue lines) airplane emissions are shown on Fig. 2 for ΔRF and ΔT using the QUANTIFY A1 (top) and the ACARE 2050 scenarios (down). The relative contribution (%) is shown in green.

When using the QUANTIFY A1 scenario, the RF absolute contribution of aviation increases from 22 mW/m² (20–23 mW/m², 68% uncertainty range) in 2005 to a maximum of 80 mW/m² (73–85 mW/m², 68% uncertainty range) in 2050. Due to the fact that non-aviation emissions decrease massively from 2020 (RCP2.6), the relative contribution of the aviation sector to the RF increase is doubled between 2020 (1.30% 1.23–1.36%, 68% uncertainty range) and 2050 (2.77 %, 2.52–2.94%, 68% uncertainty range). OSCAR modelled a temperature increase of 11 mK (8–13 mK, 68% uncertainty range) in 2005 up to 42 mK (33–46 mK, 68% uncertainty range) in 2050. The relative contribution to the temperature increase shows a maximum of 2.3% (2.09–2.46 %, 68% uncertainty range) in 2050.

The ACARE 2050 scenario shows the benefit of decreasing the CO₂ emissions from planes in term of RF and temperature. Indeed, in 2050, the RF from planes is reduced to 52 mW/m² (47–57 mW/m², 68% uncertainty range) while the temperature increase is maximal in 2050 with 28 mK (22–33 mK, 68% uncertainty range) of increase. Such as for the QUANTIFY A1 scenario, the aviation transport sector contributes to slightly more than 1% of the global RF and T increase in 2020. Although, an increase of RF and T due to the CO₂ aviation emissions is encountered after 2020, the relative contributions of CO₂ airplane emissions stay, however, lower by about 1% for RF and 0.77 % for T in 2050 (1.77%, 1.63–1.86%, 68% uncertainty range for RF and 1.53%, 1.41–1.62%, 68% uncertainty range for T) compared to the values calculated using the QUANTIFY A1 scenario.

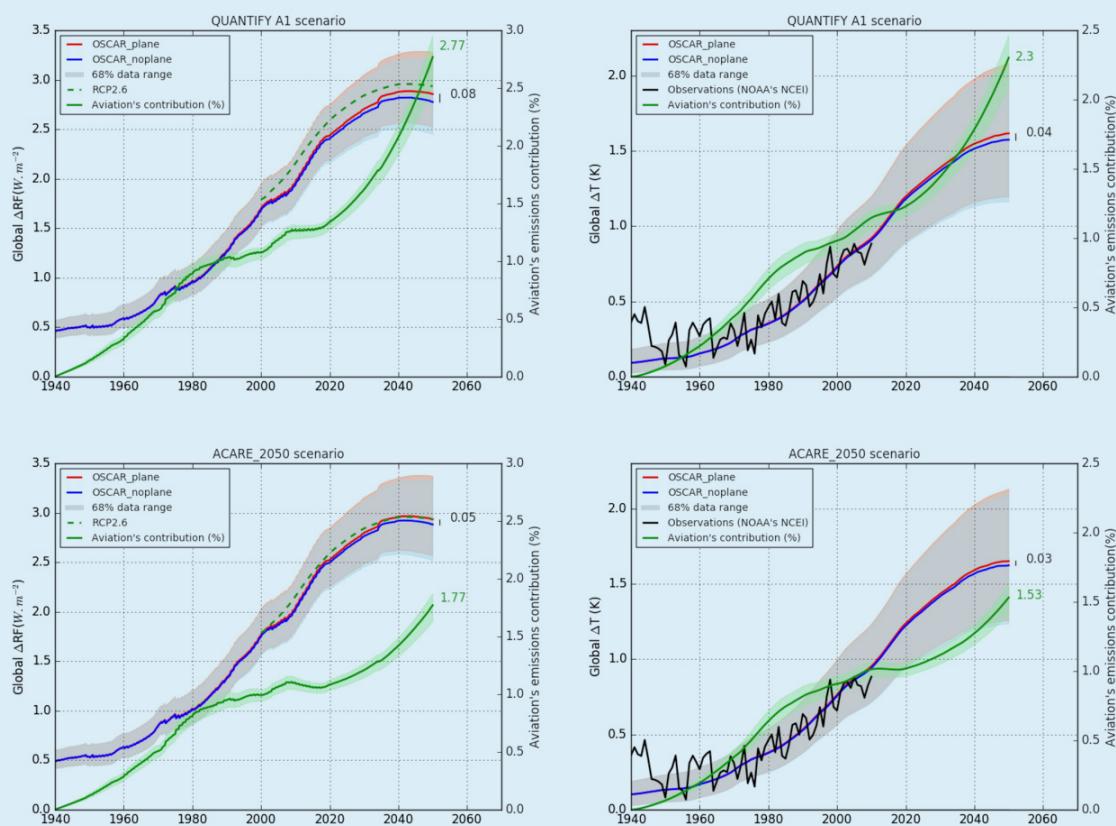


Figure 2. Temporal evolution (1940 - 2050) of the Δ RF (W/m²) and Δ T (K) for the QUANTIFY A1 (top) and ACARE 2050 scenarios (down).

CONCLUSIONS AND DISCUSSION

A long-term simulation of the CO₂ aviation impact on climate was done using the compact coupled carbon cycle and climate model OSCAR v2.1 over the 1940 - 2050 period in the 1.5–2°C context (e.g. RCP2.6) using two emission scenarios. The emissions are based on referenced historical data (1940–1999) and on the QUANTIFY A1 CO₂ aviation emissions scenario and ACARE 2050 objectives (2000–2050) for the future. The calculated RF value for 2005 (20 mW/m² for ACARE 2050 and 22 mW/m² for QUANTIFY A1) is lower than the reference value from Lee et al., 2009 (28 mW/m²). The revised lower CO₂ emission level used for this study and the different simple climate models used are the main reasons for the differences. In 2050, the RF increase is lower for ACARE 2050 (52 mW/m²) than in the other study (>70 mW/m² according to the scenario). However, the QUANTIFY A1 scenario value for RF due to aviation (80 mW/m²) is slightly above the Lee et al.

values. In 2050, the two RF values calculated using the ACARE 2050 and QUANTIFY A1 emission scenarios span a range of possible values in the future (2050). Compared to the 2010 values, in 2050, the relative contribution of the CO₂ aviation emissions to the temperature increase (ΔT) is expected to increase by 60% (0.95%, 0.89%–1.0% 68% uncertainty range to 1.53%, 1.41%–1.62% 68% uncertainty range) in the case of the ACARE 2050 scenario and more than double (from 1.0%, 0.98%–1.1% 68% uncertainty range to 2.30%, 2.09%–2.46% 68% uncertainty range) in the QUANTIFY A1 one. Therefore, in the context of limiting global warming to below 2°C, the aviation is projected to have a stronger impact on climate in the near future, especially, if no significant effort is done to mitigate the emission from this sector (e.g. QUANTIFY A1 scenario).

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SEASONAL ANALYSIS OF CONTRAIL AND CONTRAIL CIRRUS

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Abstract. The evaluation of the radiative forcing of contrails is one of the main properties required when quantifying the climate impact of aviation. The use of geostationary satellite sensors, such as the SEVIRI instrument on board of the second generation of Meteosat satellites, constitutes the perfect tool to study the life cycle of contrails. It provides the necessary high spatial and temporal resolution. The inherent difficulty in distinguishing aged contrail cirrus from natural cirrus clouds presents a limitation that leads to the fact that most studies based on satellite imagery limit the quantification of contrail impact on climate to linear contrails.

The ACTA algorithm enables the possibility of tracking contrails until their dissipation, regardless of their form in later stages. Using ACTA, a dataset comprising 12 months' worth of contrails and contrail cirrus has been created. Using ACTA on its own or combined with algorithms developed for the Meteosat SEVIRI sensor, following properties have been derived: optical depth, radiative forcing, energy forcing, coverage and lifetime.

Here we present a seasonal analysis of these properties based on over 25000 contrails.

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CLIMATE IMPACT OF CONTRAIL AND CONTRAIL CIRRUS

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Abstract. The representation of contrail cirrus in climate models has advanced in the last years tremendously. Nevertheless, uncertainties in particular regarding the representation of contrail microphysics still remain. We extend a contrail cirrus scheme within a climate model by implementing a microphysical two-moment scheme to improve the simulation of microphysical properties of contrail cirrus. The global radiative forcing of contrail cirrus estimated for the year 2002 is close to the results of Burkhardt and Kärcher (2011). Although a higher fraction of optical visible contrails are simulated, the larger compensation of longwave and shortwave radiative forcing due to differences in the vertical overlap with natural clouds and a new radiation scheme prevent larger values of radiative forcing. The global radiative forcing of contrail cirrus for the year 2006 is estimated to be 56mW/m^2 . We also estimate the radiative forcing due to contrail cirrus for several aviation scenarios for the year 2050, considering the increase of air traffic volume, the shift of flight level, the climate change and the reduction of soot emissions.

Keywords: contrail cirrus, contrails in climate model, radiative forcing of contrail cirrus

INTRODUCTION

Aviation contributes around 5% to anthropogenic radiative forcing (Lee et al., 2009). Since the aviation sector increases every year by about 5% (ICAO, 2007), this effect is growing in importance. Of the aviation effects, contrail cirrus is the largest known radiative forcing component (Burkhardt and Kärcher, 2011). Contrails form in the wake of air planes if the air is cold and moist enough. Contrail cirrus comprise those line-shaped contrails and the irregularly shaped cirrus clouds arising from them. Their ice crystals scatter shortwave radiation leading to a reduction in solar radiation at the surface (shortwave cooling). On the other hand, absorption and emission of longwave radiation reduce the outgoing terrestrial radiation, because absorbed infrared radiation is emitted from the cloud tops at significantly lower temperatures than from the Earth surface (longwave warming). For contrail cirrus the warming effect dominates on average.

CONTRAIL CIRRUS IN A GLOBAL MODEL

We use a contrail cirrus parameterization developed for the ECHAM5 model (Bock and Burkhardt, 2016a), which is based on the work of Burkhardt and Kärcher (2009). In these parameterizations contrail cirrus is introduced as a new cloud class in the model. Their persistence, advection, spreading, and deposition/sublimation can be estimated independently from the processes of the natural clouds. Hence, the whole life cycle of contrail cirrus is simulated. Contrail cirrus form according to the Schmidt-Appleman criterion (Schumann, 1996) and persist in ice supersaturated regions which are parameterized in the model (Burkhardt et al., 2008). The water and heat budget in the model are closed. Contrail cirrus and natural cirrus compete for available water vapor and contrails feedback on natural cirrus cloudiness due to contrail-induced changes in the temperature and moisture fields in the upper troposphere (Burkhardt and Kärcher, 2011).

For the extension of the contrail cirrus parameterization to a microphysical two-moment scheme (Bock and Burkhardt, 2016a), several processes important for the properties and life cycle of the contrails had to be introduced or improved. Besides the ice crystal number concentration, contrail cirrus volume (air volume in which contrail ice crystals are homogeneously distributed) was introduced as a new prognostic variable with turbulent diffusion and sedimentation leading to its growth. The growth of the contrail volume turned out to be a crucial process for the initial development of young contrails, limiting water vapor deposition. The latter controls the increase in contrail ice water content and ice crystal size and has therefore a strong impact on microphysical processes during the early part of the contrails' life cycle.

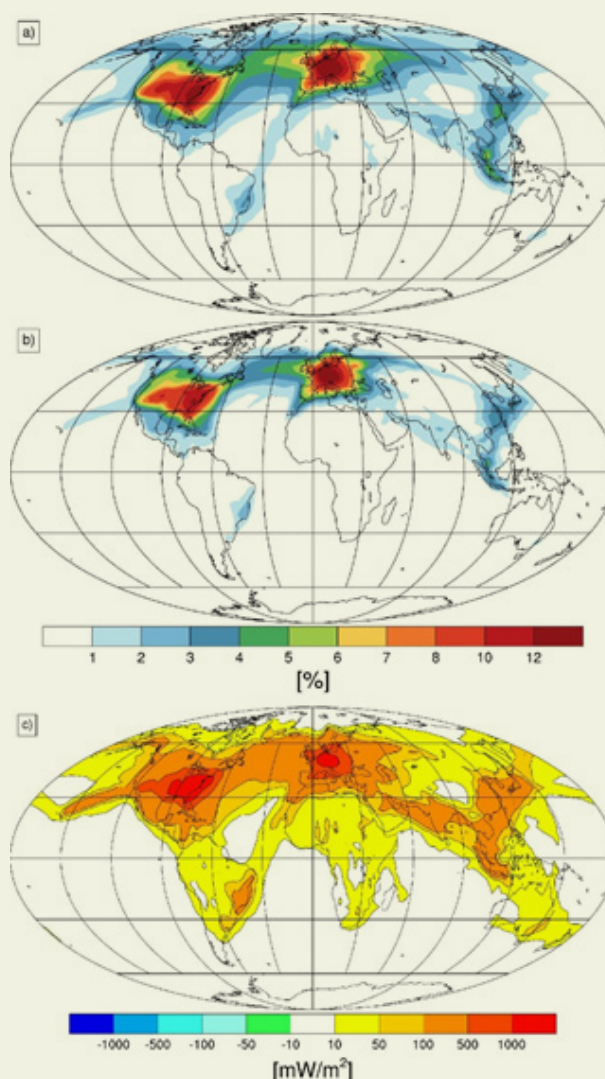
Second, the representation of water deposition was improved as compared to the earlier one-moment

microphysical scheme (Burkhardt and Kärcher, 2009), limiting the amount of deposited water to an estimate of the diffusional growth of ice crystals dependent on the ice crystal number concentration and ice crystal size. This is, in particular, important in the later stages of the contrail cirrus life cycle but also in areas below the flight level which are dominated by sedimentation. Due to the improved representation of microphysical processes, the temporal evolution of contrail cirrus optical depth, τ , can be resolved more realistically.

RADIATIVE FORCING OF CONTRAIL CIRRUS

Prescribing different air traffic inventories for specific basis years, we simulate contrail cirrus coverage, microphysical properties, and radiative forcing (Bock and Burkhardt, 2016b). We use the simulation for the year 2002 using the AERO2k inventory for a comparison with the results from Burkhardt and Kärcher (2011). The coverage of contrail cirrus with solar optical depth > 0.02 amounts to 0.61%, considerably higher than that estimated by Burkhardt and Kärcher (2011). Such optically thick contrail cirrus contribute 84% to the total contrail cirrus coverage. The main reason for this discrepancy is the fact that contrail cirrus optical depth is large due to the large number of small ice crystals. This could not be resolved with the old contrail cirrus scheme comprising the microphysical one-moment scheme. Our estimate of global radiative forcing due to contrail cirrus is 35mW/m^2 , for the year 2002, similar to the 39mW/m^2 of Burkhardt and Kärcher (2011). This is surprising given that coverage due to contrail cirrus with optical depth larger 0.02 is increased by a factor of about 2.7 in the new model, suggesting a larger radiative forcing. The decrease in radiative forcing relative to the contrail cirrus coverage can be explained by a decrease in the vertical overlap of contrail cirrus with natural clouds and by the larger compensation of longwave and shortwave radiative forcing, associated with the new radiation scheme.

The simulated radiative forcing for 2006 using the AEDT inventory is 56mW/m^2 (Fig. 1). This strong increase by a factor of about 1.6 relative to the estimate for 2002, using the AERO2k inventory, corresponds to the strong increase of flight distance by a factor of 1.8 from the AERO2k inventory for the year 2002 to the AEDT inventory for the year 2006. It should be noted that the increase in flight distance is attributable not only to the increase in air traffic but also to the use of slant flight distance instead of track flight distance and to differences in the data and methods used in producing the inventory. Estimating radiative forcing for 2006 prescribing track distance, we find that about one third of the increase in contrail cirrus radiative forcing may be attributable to the fact that we now use slant distance. The other two thirds could be explained by the increase of flight distance, especially at main air traffic altitudes, and the better representations of flight distance in the newer AEDT inventory. We found that in an area where the representation of flight distance is strongly changed due to the superior data and methods used in the new inventory, that is, in the northern Pacific flight track, contrail cirrus radiative forcing changed only slightly.

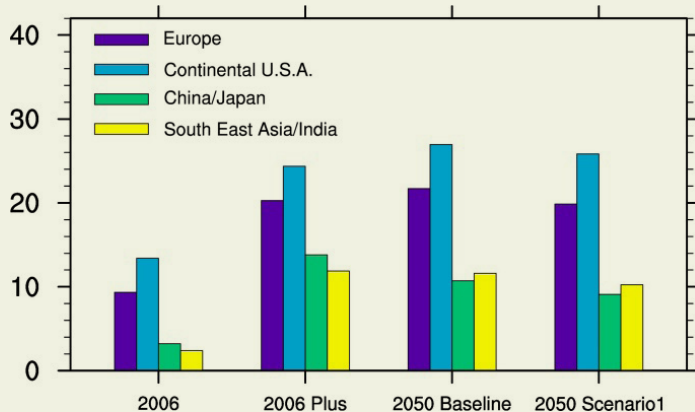


FUTURE SCENARIOS FOR 2050

We estimate the effect of a change in air traffic for the year 2050 with our contrail cirrus parameterization (microphysical 2-moment scheme) within ECHAM5. We perform simulations for four scenarios developed

at the Volpe National Transportation Centre using the U.S. Federal Aviation Administration (FAA) Aviation Environmental Design Tool (AEDT) (Roof et al., 2007; Barret et al., 2010). This contains a base case for the year 2006 and three future 2050 scenarios. The 2050 baseline scenario describes the increase in air traffic volume, whereas the second 2050 scenario additionally considers the improvement in fuel efficiency. The complete usage of renewable alternative fuel is included in the third 2050 scenario. Therefore, the separate impacts of increases in air traffic volume, the climate change, the improved fuel efficiency and soot reductions when using alternative fuels are investigated. Also regional aspects are shown.

We estimate a strong increase of radiative forcing from 2006 to 2050 due to the larger air traffic volume and the shift of air traffic towards higher altitudes, even though climate change and a reduction in soot emissions act to reduce the climate impact. The relative increase in air traffic is strongest in the tropics and has therefore a particularly large impact on the global contrail cirrus radiative forcing. The shift of future air traffic into higher altitudes intensifies this trend in the tropics. Nevertheless, the Continental U.S.A. and Europe contribute most to the global radiative forcing due to contrail cirrus also for the 2050 scenarios (Fig. 2). We consider in our simulations the climate change until 2050 following the RCP 6.0., which leads to a warming of the upper troposphere and therefore a lower frequency of ice supersaturation. Climate change



appears to limit contrail cirrus radiative forcing in the tropics and leads to a slight increase in the USA and Europe. An improvement in fuel efficiency leads to a higher critical temperature for contrail formation, as a result of which the region where contrail could form increases. Nevertheless this has a negligible effect on the global radiative forcing of contrail cirrus. The reduction of soot emissions changes the microphysical properties of contrail cirrus and leads to a decrease in optical thickness and climate impact of contrail cirrus.

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ALTERNATIVE ROUTING: CLIMATE IMPACT MITIGATION STUDIES

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Abstract. The EU FP7 project REACT4C explored the feasibility of operational measures such as flight altitude and route changes to reduce the climate impact from aviation. For this purpose a feasibility study on climate-optimized flight planning was performed for the North Atlantic flight corridor (NAFC). In this paper we present results from an evaluation of climate impact of such climate-optimized trajectories with a set of chemistry-transport models.

Such climate-optimized flight routing is performed by taking into account prevailing synoptical weather pattern. For winter five distinct patterns were identified, hence accordingly five emission inventories were generated for the NAFC region. Subsequently an experiment design was developed, in order to evaluate climate impact of these optimized routings for a specific winter season. The weather-dependent optimized inventories were integrated in the chemistry-climate models by respecting corresponding prevailing pattern. Specifically, two study periods were selected, one, for the winter periods in 2004/2005 and, a second one, 2006/2007. On a daily basis prevailing weather patterns were analysed as defined in 5 distinct patterns, and the corresponding optimized traffic inventory was integrated in the time series of aviation emissions. Simulations were performed by a set of chemistry-climate models which are OSLO CTM2/3, ULAQ-CTM, EMAC and MOZART-3, producing a multi-model estimate. Each model simulated two numerical simulations, one using economically optimized inventories and another using climate-optimized inventories. The comparison of atmospheric concentrations between both simulations determines the impact of climate-optimal routing. Results will be shown of changes in atmospheric concentrations of reactive species, focusing in particular on NO_x , NO_y , O_3 and HO_x , of these weather-dependent climate-optimized inventories.

FLAME STABILIZATION AERODYNAMICS AND EMISSIONS PERFORMANCE AT STRATIFIED OR FULLY PREMIXED INLET MIXTURE CONDITIONS

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Abstract. The work presents a comparative study of the performance between fully-premixed and stratified propane flames stabilized in a disk burner configuration operating with a swirl coflow over a range of stoichiometric to ultra-lean conditions. Radial equivalence ratio gradients are regulated by staged premixing of propane and air within a double cavity formed along three concentric disks. Measurements of temperatures, OH* and CH* chemiluminescence, FTIR and gas analysis provided information on the impact of the variable inlet fuel-air profile and its interaction with the swirling coflow on flame structure and burner emissions performance.

Keywords: partially premixed, stratified, full premixed, flame stabilization, burner performance, emissions

INTRODUCTION

To extend the environmentally friendly scope of gas turbine operation and their capability to adapt to a wider range of commercial alternative fuel types, investigations into the flame stabilization performance over a range of relevant inlet conditions (e.g. equivalence ratio gradients, preheat) are warranted. The control and extension of the stability margin without compromising emission levels and safety requirements is a key technology issue in the (re-) design and optimization of current combustors along these lines.

Lean premixed conditions have so far become widely exploited to benefit from their potential for an improved trade-off in soot/CO/NO_x emissions (Dunn-Rankin et al. 2008). In more recent years controlled partial premixing of the fuel-air mixture has emerged as a promising methodology to mitigate some of the complications that arise in the effort to expand the usefulness of the lean fully premixed concept (Lieuwen and Yang 2005; Stohr et al. 2011; Chaudhuri and Cetegen 2008; Kuenne et al. 2012). In large-scale lean premixed pre-vaporized systems, combustion often takes place under spatially non-uniform stoichiometry (mixture stratification), either by design or due to undesirable limiting operation.

The effects of local equivalence ratio gradients on the turbulent flame structure and propagation under various mixture placements has been studied for both premixed (e.g. Lieuwen and Yang, 2005; Andrews et al. 2009; Stohr et al. 2011) and stratified (e.g. Kuenne et al. 2012; Kamal et al. 2015; Xiouris and Koutmos 2012; Karagiannaki et al. 2014) model flame configurations. These works have highlighted the impact of effectively controlling inlet compositional stratification and its interaction with the main combustion zone on heat release, ignitability limits and emissions performance (e.g. Kamal et al. 2015; Kuenne et al. 2012; Karagiannaki et al. 2014).

Such information is also useful when there are constraints in the use of the fully premixed concept or when existing systems are upgraded, modernized or retrofitted (e.g. Contino et al. 2013; Carrera et al. 2011). Therefore comparative examinations of the structure and performance of the premixed versus the stratified stabilization in practical baffles are required over a variety of flame configurations.

The present work compares the performance characteristics of fully-premixed and stratified propane flames stabilized in an axisymmetric disk burner configuration under the effect of swirl. The inlet mixture conditions can be regulated by staged premixing of propane and air within an upstream double cavity premixer. Measurements of temperatures, OH* and CH* chemiluminescence, FTIR and gas analysis assisted in the interpretation of the variations in flame structure, topology and performance. The present data, complemented by further detailed information could be exploited in the computational modelling of these flames.

FLAME CONFIGURATIONS STUDIED

The premixer/burner and the combustion facility are shown in Figure 1 (Xiouris and Koutmos (2012) and Karagiannaki et al. (2014)). The premixer/burner geometry was made up of three disks connected along their axis with a hollow tube. Under fully premixed operation a mixture of propane and air was supplied through the central tube ($D_c=0.052$ m) and the flames were stabilized at the afterbody disk recirculation. The stratified flames were obtained by separately feeding the fuel into the hollow connecting tube ($D_p=0.01$ m, Figure 1c) and then injecting it through an annular 1mm slot into the primary fuel-air mixing cavity (Figure 1d). The second cavity promoted partial-premixing with the central air and prevented flashback by balancing mixing and autoignition times.

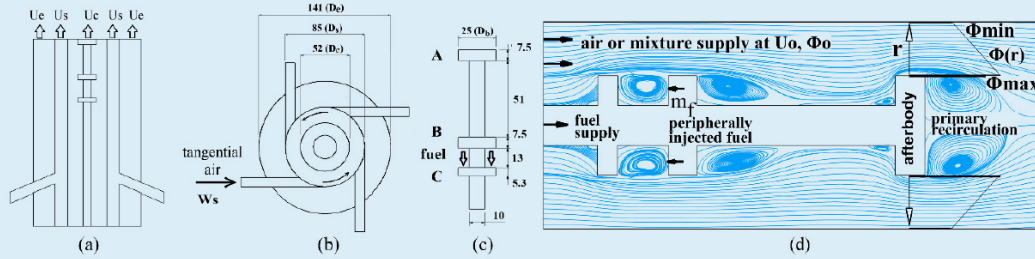


Figure 1. (a and b) Tunnel; (c) burner; (d) fuel placement arrangement

Under each operating condition the afterbody stabilization region can be fuelled, either with a radial equivalence ratio gradient (Figure 1d) regulated via the central air and the primary cavity injected fuel, or with a uniform mixture supplied through the central pipe. The flow topology within the premixer can be better visualized with the help of simulations (Xiouris and Koutmos, 2012) depicted in Figure 1d together with the possible placement of the fuel supply.

Fuel flows were regulated by Bronkhorst MV-304/306 *High-Tech* MFCs with accuracy 1.25% FSD. The burner was surrounded by an annular swirl co-flow ($D_s=0.085$ m, Figures 1a, b) aerodynamically introduced upstream of the premixing plane. The swirl-burner system was shielded by a smooth annulus air co-flow ($D_e=141$ mm, Figure 1a). The Reynolds number, based on the afterbody diameter and the central air velocity (U_c), was maintained at 7985 while the blockage ratio ($BR=(D_b/D_c)^2$) was 0.23. The investigated conditions and parameters are given in Table 1. The stratification at the afterbody exit, could be varied between $\Phi_{min} \approx 0.07/0.03$ and $\Phi_{max} \approx 0.90/0.67$ (Figure 1d). Swirl intensity levels ($S=W_s/U_s$) were varied from 0 to 1.0. The premixed flames are compared against their stratified counterparts on the basis of their proximity to LBO through the parameter, $\delta = (m_{Fuel} - m_{Fuel, LBO})/m_{Fuel, LBO}$ (%). The relevant range of the operating equivalence ratios that directly correspond to these δ values is given in Table 1.

Table 1. Operating conditions							
Case	δ (%)	L_R/D_b		Φ Global		P (kW)	
Swirl		0.00	0.65	0.00	0.65	0.00	0.65
Stratified Conditions							
LS	51	1.06	1.13	0.285	0.31	9.28	10.11
US	24	1.32	1.4	0.234	0.25	7.62	8.31
BS	7	1.56	1.68	0.20	0.22	6.57	7.17
Fully Premixed Conditions							
PLS	51	1.78	2.72	1.04	1.03	35.48	34.93
PUS	24	1.71	2.28	0.86	0.84	29.13	28.68
PBS	7	1.70	2.0	0.74	0.73	25.14	24.75

- δ (%): percent deviation from Lean Blow Off,
 - in stratified cases, $\delta = (m_{\text{Fuel}} - m_{\text{Fuel, LBO}}) / m_{\text{Fuel, LBO}}$ (%), ($m_{\text{Fuel, LBO}}$, Fuel flow at Blow-Off), $U_{\text{Fuel, LBO, S=0}} = 0.9$ m/s, $U_{\text{Fuel, LBO, S=0.65}} = 0.97$ m/s.
 - or equivalently in premixed cases, $\delta = (\Phi - \Phi_{\text{LBO}}) / \Phi_{\text{LBO}}$ (%) (Φ_{LBO} , equivalence ratio at Blow-Off), $\Phi_{\text{LBO, S=0}} = 0.69$, $\Phi_{\text{LBO, S=0.65}} = 0.68$.
- LR/ Db: Measured afterbody recirculation length. ($D_b = 0.025$ m)
- Central air supply velocity, $U_c = 4.87$ m/s and $Re_{db} = 7980$ for all cases, mean coflow velocity in annular swirl stream, $U_s = 9$ m/s (Swirl = W_s / U_s , W_s mean tangential velocity at exit from swirl stream), external annular stream velocity, $U_e = 10$ m/s.
- Φ_{Global} : global equivalence ratio, either based on mass flows of injected fuel and central pipe air supply (stratified cases) or on the premixture composition (premixed).

EXPERIMENTAL METHODS

Mean temperatures, OH*/CH* chemiluminescence (CL) images (Figure 2), species concentrations and exhaust major pollutants (Figure 3), were obtained using thin digitally-compensated, high temperature thermocouples, a LaVision® FlameMaster imaging system and a combination of Fourier Transform Infrared Spectroscopy (FTIR, Spectrum TwoTM spectroscopy analyzer, PerkinElmer®) and Kane-May KM9106 Quintox flue gas analyzer (Xiouris and Koutmos, 2012; Karagiannaki et al. 2014).

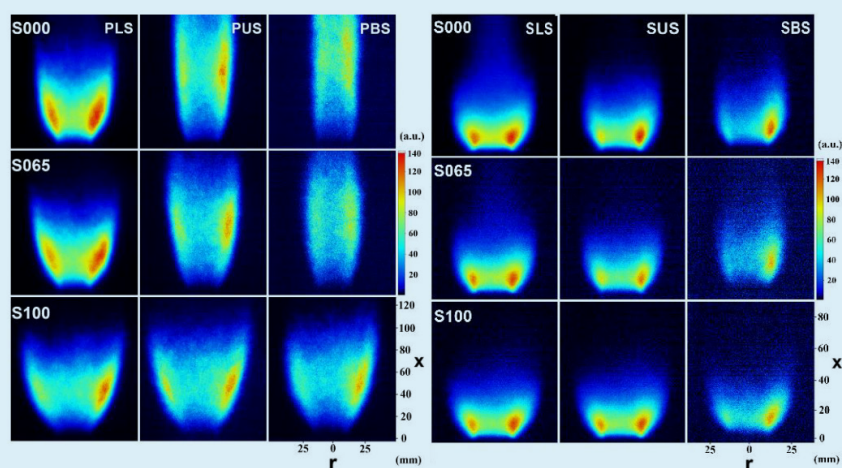


Figure 2. OH* chemiluminescence images for (a) premixed; (b) stratified flames at three fuel levels and swirl intensities

SUMMARY AND DISCUSSION

The study examined some of the differences and similarities that develop in axisymmetric disk flame stabilization due to variations in the inlet fuel-air mixture profile. A range of topologies of flames sustained under fully premixed or stratified inlet conditions were compared for plane and swirling wake development across the stoichiometric and lean regime. The inlet radial equivalence ratio stratification promoted a wider LBO margin across the range of swirl intensities with respect to the fully premixed configuration. In the present set up fully premixed conditions augmented the primary recirculation by up to 50%, with respect to the stratified conditions, and almost doubled the cold wake vortex lengths, with the larger values pertaining to the higher swirls. For comparable proximities to LBO premixing results in more uniformly distributed temperature regions spread over a greater wake extent. The chemiluminescence images (Figure 2) suggested that stratification produces an overall more compact, frustrum shaped flame that remains well attached to the burner face and is less sensitive to swirl variations or fuel reductions. Close to ultra-lean operation premixed flames detached from the burner face, attained a cylindrical shape and reached lengths of up to seven bluff-body diameters, up to three times the lengths of the stratified cases. Over the full operational range the stratified set up maintained higher efficiency levels (Figure 3). In the present

burner configuration the adjustment of the swirling field and the CRZ together with the regulation of the inlet mixture profile seem to allow convenient management of its operating parameters and emission levels.

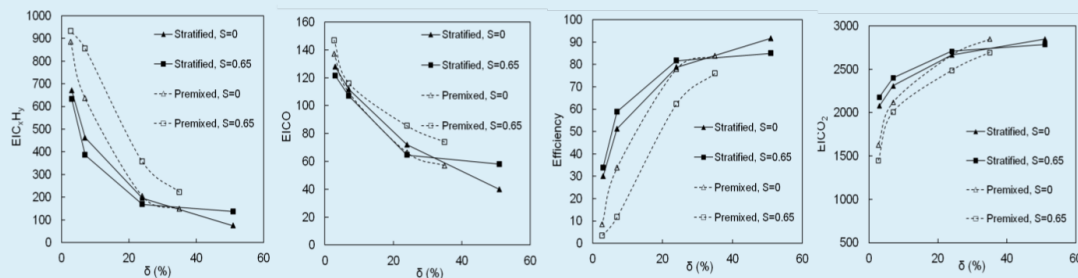


Figure 3. Distributions of the emission indices of, (a) unburned hydrocarbons, (b) CO, (c) CO₂ and, (d) the respective combustion efficiencies for the reported cases.

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INTERCOOLED RECUPERATED AERO ENGINE: DEVELOPMENT AND OPTIMIZATION OF INNOVATIVE HEAT EXCHANGER CONCEPTS

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Abstract. At the present paper the main activities, performed in the LEMCOTEC research project focused on the further optimization of the recuperation system of the Intercooled Recuperated Aero engine (IRA-engine) concept are presented. This concept, developed by MTU Aero Engines AG is based on the use of an advanced thermodynamic cycle combining both intercooling and recuperation through a system of heat exchangers mounted inside the hot-gas exhaust nozzle, providing fuel economy and reduced pollutant emissions. The investigation and the optimization efforts of the recuperation system were performed with the use of 2D/3D CFD computations, experimental measurements and thermodynamic cycle analysis for a wide range of engine operating conditions. The optimization activities were based on the development of a customizable numerical tool which was based on an advanced porosity model approach in which the heat exchangers were modeled as porous media of predefined heat transfer and pressure loss behaviour and could also incorporate major and critical heat exchanger design decisions in the CFD computations. The optimization efforts resulted in two completely new innovative heat exchanger concepts, named as CORN (COncal Recuperative Nozzle) and STARTREC (STraight AnnulaR Thermal RECuperator). These concepts were following an annular tubes design inside the hot-gas exhaust nozzle leading to the elimination of swirl effects and to homogeneous flow distribution. Additionally, the two new concepts provided significant benefits in terms of fuel consumption, pollutants emission and weight in relation to more conventional heat exchanger designs proving that further optimization potential for this technology exists.

Keywords: Heat exchangers, Porosity model, Recuperation, Aero engine optimization

INTRODUCTION

The present paper is focused on a large part of the main activities, performed in the E.U. funded LEMCOTEC Collaborative Project, which its key-objective is to reduce air-traffic emissions by improving the thermal efficiency of aero-engines, (<http://www.lemcotec.eu/>). The enhancement of aero engine performance and the reduction of fuel consumption and pollutant emissions have always been on the focal point of intense engineering optimization efforts for both environmental and economic reasons. A large number of these efforts has been focused on the development of alternative technologies and their incorporation in innovative aero engine concepts. Such a technology concept is implemented in the Intercooled Recuperative Aero-engine (IRA engine) configuration, which is presented in Figure 1a, which combines both intercooling and recuperation.

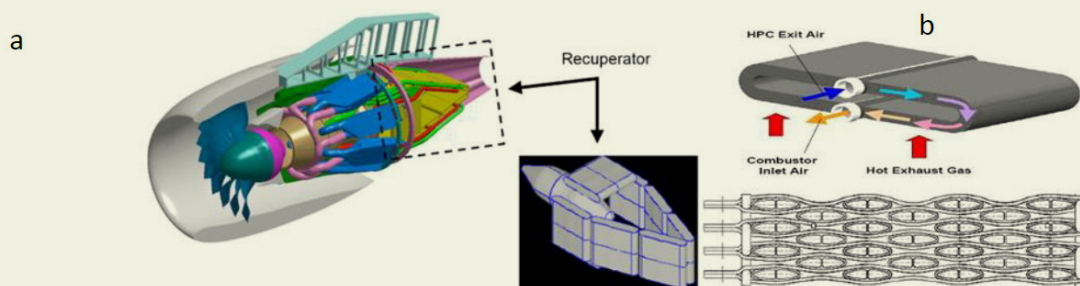


Figure 1a. The IRA - Intercooled Recuperative Aero-engine.
1b. The MTU-heat exchanger.

This concept is based on a system of heat exchangers mounted inside the hot-gas exhaust nozzle and an intercooler placed between the compressor stages. The hot-gas exhaust heat, downstream the low pressure turbine exit is driven back to the combustion chamber and thus, the preheated ambient air enters the combustion chamber with increased enthalpy, providing fuel economy and reduced pollutant emissions. In addition, the use of intercooling, a technology which performs at its best for thermodynamic cycle conditions which facilitate recuperation, contributes to a reduction of high pressure compressor work leading to a further improvement of aero engine efficiency. Both intercooling and recuperation are performed through the use of specially designed and integrated heat exchangers.

OPTIMIZATION OF HEAT EXCHANGER CONCEPTS

The present work is focused on the optimization of the heat exchangers geometries and installation in order to maximize the recuperation benefits, specifically targeted for IRA engine. More details about the IRA engine concept can be found in [Boggia & Rüd, 2004], [Wilfert et al., 1999]. The implementation of recuperation in IRA engine is performed through the mounting of a number of heat exchangers inside the hot-gas exhaust nozzle, downstream the low pressure turbine. The basic heat exchanger (HEX) of the IRA engine, which was invented and developed by MTU Aero Engines AG and was used for the initial HEX performance studies, is presented in Figure 1b. It consists of elliptically profiled tubes placed in a 4/3/4 staggered arrangement targeting high heat transfer rates and reduced pressure losses. Additional information of the HEX operation can be found in [Schonenborn et al., 2004]. The HEX tubes geometry and arrangement can significantly affect the turbine expansion and thus, degrade the produced turbine work, due to the imposed pressure losses. The overall heat exchanger design plays a critical role in this direction since the pressure losses are directly linked to the available heat exchange surface and its geometry, which in its turn strongly affects the HEX effectiveness and the exhaust gas waste heat exploitation. As a result, a compromise is necessary to be taken into account between the HEX design parameters in order to achieve the maximization of recuperation benefits. Towards this direction, the development of accurate and validated numerical tools is of particular importance since they can provide time- and cost-efficient design solutions which can lead to the a-priori estimation of the HEX major operational characteristics (i.e. pressure losses and effectiveness). These operational characteristics can then be integrated in a thermodynamic cycle analysis of the aero engine in order to assess the recuperation effects on aero engine efficiency and fuel consumption. Thus, these tools can significantly contribute to the development, assessment and optimization of various innovative heat exchanger concepts which otherwise could not be affordable in laboratory (due to time and cost limitations).

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho U \\ \rho V \\ \rho W \\ \rho E \end{bmatrix} + \frac{\partial}{\partial x_i} \begin{bmatrix} \rho U_i \\ \rho U_i U + P \delta_{ij} \\ \rho U_i V + P \delta_{ij} \\ \rho U_i W + P \delta_{ij} \\ \rho E U_i + P V_i \end{bmatrix} = \frac{\partial}{\partial x_i} \begin{bmatrix} 0 \\ \mu \left(\frac{\partial U}{\partial x_i} + \frac{\partial U_i}{\partial x} \right) - \frac{2}{3} \mu \frac{\partial U_k}{\partial x_k} \delta_{ij} \\ \mu \left(\frac{\partial V}{\partial x_i} + \frac{\partial U_i}{\partial y} \right) - \frac{2}{3} \mu \frac{\partial U_k}{\partial x_k} \delta_{ij} \\ \mu \left(\frac{\partial W}{\partial x_i} + \frac{\partial U_i}{\partial z} \right) - \frac{2}{3} \mu \frac{\partial U_k}{\partial x_k} \delta_{ij} \\ \left(\mu \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) - \frac{2}{3} \mu \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) U_j - k \frac{\partial T}{\partial x_i} \end{bmatrix} + \frac{\partial}{\partial x_i} \begin{bmatrix} 0 \\ \overline{\rho u u_i} \\ \overline{\rho v u_i} \\ \overline{\rho w u_i} \\ \overline{\rho u_i u_i} + \rho T u_i \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{(a_0 + a_1 v)}{L} \mu U + \frac{(b_0 + b_1 v + b_2 v^2)}{L} \rho U |U| \\ \frac{(a_0 + a_1 v)}{L} \mu V + \frac{(b_0 + b_1 v + b_2 v^2)}{L} \rho V |U| \\ \frac{(a_0 + a_1 v)}{L} \mu W + \frac{(b_0 + b_1 v + b_2 v^2)}{L} \rho W |U| \\ U_{overall} (T - T_{inner}) S_{exchange} \end{bmatrix}$$

Figure 2. Implementation of pressure loss and heat transfer source terms in the porosity model.

At the present work the development and optimization of innovative heat exchanger concepts, focused on the Intercooled Recuperated Aero Engine, are presented which are an evolution of the original MTU HEX design. The investigation and the optimization efforts of the present work were performed with the use of 2D/3D CFD computations, experimental measurements and thermodynamic cycle analysis for a wide range of engine operating conditions. The optimization activities were mainly based on the use of an innovative customizable 3D numerical tool which could efficiently model the heat transfer and pressure loss performance of the heat exchangers of the IRA-engine installation. The developed numerical tool was based on an advanced porosity model approach in which the heat exchangers were modelled as porous media of predefined heat transfer and pressure loss correlations which have been previously derived through detailed CFD computations and experimental measurements and are numerically incorporated in

the CFD computations by the addition of appropriate source terms in the momentum and energy equations, as presented in Figure 2. The innovative customizable 3D numerical tool could also incorporate major and critical heat exchanger design decisions in the CFD computations by supporting the numerical integration of heat exchanger geometrical characteristics (e.g. tubes collectors number, streams flow splitting and mixing, tubes core arrangement). Additional details about the customizable numerical tool can be found in (Yakinthos et al., 2015). At the first stage of the present investigation, the NEWAC nozzle configuration, related to the NEW Aero engine Core concepts/NEWAC research project, was investigated with the use of CFD computations (following also a porous media approach for the heat exchangers), presented in detail in Figure 3a. This nozzle configuration corresponds to a quarter of the overall nozzle installation due to the heat exchangers symmetric arrangement. The NEWAC nozzle configuration consists of 4 heat exchangers (HEXs) per quarter of the exhaust nozzle. The HEXs 1-2-3-4 are placed at angles 17-20-13-17 degrees in relation to the axial flow direction. As it can be seen in Figure 3b, strong swirl effects are formed inside the NEWAC nozzle which increase pressure losses and deteriorate the HEXs performance and the recuperation benefits in the aero engine cycle. The CFD computations were performed using the SST (Shear Stress Transport) turbulence model of Menter (Menter, 1994), for a wide range of HEX conditions as presented in (Schonenborn et al., 2004). Additional details can be found in (http://ec.europa.eu/research/transport/projects/items/newac_en.htm), (Yakinthos et al., 2010), (Missirlis et al. 2010).



Figure 3a. NEWAC nozzle configuration, 3b. Swirl effects in NEWAC nozzle.

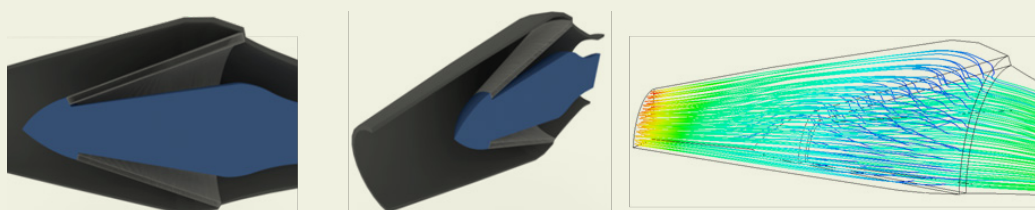


Figure 4. CORN (COncal Recuperative Nozzle) geometry and velocity streamlines.

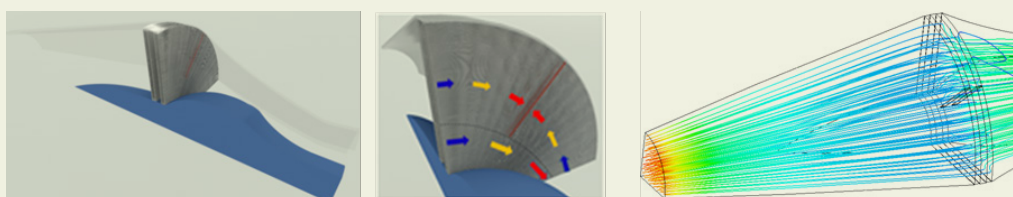


Figure 5. STARTREC (STraight AnnulaR Thermal RECuperator) geometry and velocity streamlines.

At the next steps, additional investigations targeting the optimization of the HEXs installation inside the hot-gas exhaust nozzle were performed through additional similar CFD computations and the use of the customizable numerical tool. The optimization efforts resulted in two completely new innovative HEX concepts, named as CORN (COncal Recuperative Nozzle) and STARTREC (STraight AnnulaR Thermal RECuperator), presented in Figures 4 and 5 respectively. Both concepts were based on the MTU HEX original tubes. These concepts were based on the use of innovative heat exchanger designs, following an annular tubes arrangement inside the exhaust nozzle, leading to the reduction (for the STARTREC concept) or complete elimination (for the CORN concept) of swirl effects and a more homogeneous flow distribution with reduced secondary flow losses in relation to the NEWAC nozzle configuration.

At the final stage, the major characteristics of the heat exchangers installation of both concepts were incorporated in GasTurb 11, (Kurzke, 2011) and their effect on the thermodynamic cycle of the IRA, was quantified and compared in relation to a conventional non-intercooled and non-recuperated aero-engine

of similar technology level with the IRA engine. The results, summarized in Table 1, showed that the two new concepts provided significant benefits in terms of specific fuel consumption (corresponding to a direct fuel burn and pollutant emissions reduction) and weight, proving the strong optimization potential of this technology. As it can be seen, the CORN concept provided the best performance in terms of specific fuel consumption reduction and a small decrease in weight, while the STARTREC concept, even though it provided a smaller specific fuel consumption reduction, led to a HEX setup of significant weight reduction.

Table 1. Comparative results of recuperation concepts

Case	SFC reduction (in relation to a conventional aero-engine)	Heat exchangers weight reduction (in relation to NEWAC)
NEWAC nozzle	12.3%	0
CORN	13.1%	~5%
STARTREC	9.1%	~50%

ACKNOWLEDGEMENTS

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THE EXPECTED IMPACT FROM THE INTRODUCTION OF A NEW STRUT-BRACED WING AIRCRAFT CONFIGURATION ON GLOBAL AIR TRAFFIC EMISSIONS AND CLIMATE – RESULTS FROM THE WECARE PROJECT

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Abstract. Aviation is expected to contribute significantly to the anthropogenic climate change and hence climate impact reduction measures are required as soon as possible. Therefore, the DLR project WeCare deals with the investigation of potential strategic and tactical options for the reduction of aviation's climate impact. Here, we present the results of an analysis of the global emission distribution and a climate impact assessment for the introduction of a Strut-Braced Wing (SBW) aircraft into the air transportation system, which was carried out within WeCare. A model chain consisting of an air traffic demand and aircraft movement forecasting model, an aircraft fleet aging and renewal simulation, an advanced methodology to generate air traffic emission inventories and a climate impact assessment tool has been applied to study how new aircraft configurations might contribute to a reduction of aviation's climate impact in the future. We found that the SBW aircraft has the potential to reduce fuel consumption of the aircraft fleet of the seat category 100-150 seats by nearly 26% in 2050 due to its reduced drag and a higher propulsion efficiency of the Counter-Rotating Open Rotor (CROR) engine it is equipped with. NO_x emissions can even be reduced further by 45% due to a new lean combustion technology. The climate impact assessment indicates that this large reduction potential – in combination with a slightly lower cruise altitude of the SBW aircraft compared to today's reference aircraft – may reduce the warming caused by aircraft of that size (including the projected growth in the future) by nearly 17%.

Keywords: strut-braced wing, new aircraft configuration, technological measures, environmental impact, global air traffic emissions, emission inventory, climate impact

INTRODUCTION

Air travel is a key part of our society and the gradual increase in air traffic demand is expected to result in a multiplication of aircraft movements in the coming decades (AIRBUS, 2014). Emissions from aircraft engines on the other hand cause significant changes of concentrations of radiative forcing agents at usual cruising altitudes, making aviation's climate impact an exceptional challenge which is subject of various research activities (Lee et al., 2010). One of these projects, called WeCare (Utilizing Weather information for Climate efficient and eco efficient future aviation) is currently being carried out internally by the German Aerospace Center. Based on previous findings (e.g. Koch, 2013) the project aims at evaluating different ways how the climate impact of aviation can be mitigated both strategically, e.g. through the introduction of new aircraft types or systematic changes of flight operations, and tactically, e.g. by using daily-based meteorology to circumnavigate certain "climate-sensitive" regions (Niklaß et al., 2014). For instance, recently the project team analysed to what extent the introduction of stopovers during long-haul flights could contribute to a reduction in fuel consumption and global emissions as well as to a change of the corresponding climate impact. For this purpose, a modelling system has been developed that is capable of simulating global air traffic scenarios and performing respective emission and climate impact assessments based on the introduction of such new operational concepts (Linke et al., 2016). This simulation environment also includes models that allow for a projection of regionally distinguished air travel demand (Terekhov et al., 2015) and a derivation of expected future flight movements on a route and aircraft category basis (Ghosh et al., 2015). On the technological side, the project is investigating a new aircraft configuration known as Strut-Braced Wing aircraft (SBW). The aircraft itself is designed in a different DLR project, but preliminary design characteristics have already been provided by the design team. SBW aircraft are characterized by supporting struts connecting the wings to the fuselage and reduce wing loads accordingly. Such a design which is actually widely used for General Aviation aircraft, like e.g. Cessna 172, allows for the construction of thinner wings and thus – assuming a constant wing mass – an increase of the wing span and aspect ratio. The latter goes along with a higher aerodynamic efficiency due to the reduced induced drag which in turn

leads to a reduced weight compared to a conventional cantilever wing design. In combination, this allows for the use of smaller engines with reduced fuel consumption and less emissions while providing a similar transport capacity as a conventional narrow-body aircraft (Sanchez Barreda, 2013). The purpose of this study is to apply the above mentioned methodology to assess the expected impact resulting from the introduction of the SBW aircraft configuration on global air traffic emissions and climate. In the following section, the methodology is described before preliminary results are presented in section 3. Section 4 completes the paper with conclusions and an outlook.

METHODOLOGY AND APPLICATION

Here, we assess the SBW aircraft with respect to its environmental impact. The focus is laid on the global distribution of gaseous emissions as well as on the corresponding changes of the Average Temperature Response over a period of 100 years (ATR100), which has been proven to be an adequate climate metric for such assessments (Grewe and Dahlmann, 2015). Due to the global character of the study, local effects at airports, such as implications on noise and local air quality issues are not considered here.

For the assessment, a modeling suite is used which is described below; furthermore, simulating the insertion of a complete new aircraft type into the air transportation system requires certain assumptions concerning the future air traffic network, which it is introduced into, depending on the envisaged Entry-Into-Service (EIS). As the environmental impact mainly depends on the aircraft characteristics in terms of aircraft and engine performance, also some details of the SBW design are outlined below.

MODELING SYSTEM

For the study presented here, DLR's *Global Air Traffic Emissions Distribution Laboratory* (GRIDLAB) was applied. GRIDLAB combines modules for the calculation of flight missions based on aircraft performance data with flight planning and optimization capabilities as well as with emission models to compute emission distributions along aircraft trajectories. Thus, not only changes of cumulated amounts of gaseous emission provoked by new technologies or altered flight operations can be captured, but also their variation in altitude and geographic location. Details of the modelling system can be found in (Linke, 2016). The inputs to the model chain constitute air traffic scenarios that have been derived using an air travel demand and flight movement forecasting system (AIRCAST; Terekhov et al., 2015; Ghosh et al., 2015; Kölker et al., 2016). Based on these scenarios and further assumptions regarding the introduction of new technological or operational measures, like e.g. the introduction of a SBW aircraft, GRIDLAB produces emission inventories which are eventually transferred into the climate impact assessment tool AirClim developed by DLR (Grewe and Stenke, 2008). In order to increase computational efficiency, the modelling system makes use of a database of precalculated 'reduced' emission profiles that has been generated by a detailed trajectory and emission calculation for the respective SBW aircraft (see technical specifications below) as well as the reference aircraft which is used to model the business-as-usual scenario. For simulating the flight missions it is generally assumed that the aircraft tends to fly as close as possible to its respective optimum altitude (i.e. the altitude in which the aircraft is most fuel efficient).

ASSUMED AIR TRAFFIC SCENARIO

For the ecological assessment of the introduction of a SBW aircraft configuration, assumptions regarding its EIS as well as the duration of the introduction phase ("ramp-up") have to be made. Here, we assume that the SBW is supposed to substitute an existing aircraft category of 100-150 seats (e.g. Airbus A320, Boeing 737) and that introduction starts in 2015. Using AIRCAST, aircraft movements of the respective aircraft category are projected into the future from 2015 to 2050, resulting in datasets containing departure and destination cities as well as annual flight frequencies for the connections using a time step of 5 years. Baseline for the development of regional demand properties are economic parameters obtained from the so-called *Randers* scenario (Randers, 2012). Previous studies have shown that the seat category 100-150 seats contributes to about 18-19% of the Available Seat Kilometres offered by the global world fleet; for the sake of simplicity an Airbus A320 aircraft performance model obtained from EUROCONTROL's Base of Aircraft Data (BADA, Version 4.1; Mouillet, 2013) is used to model all flights of that seat category as it is the most frequently operated

aircraft type in that category. In this “business-as-usual” scenario we assume, that today’s technology levels will be maintained throughout the projection until 2050. In contrast, in the SBW scenario we substitute the A320 class gradually by the SBW aircraft according to a substitution plan calculated with DLR’s Fast Forward FFWD (Apffelstaedt et al., 2008) module that models aircraft fleet aging, disposal and renewal.

SBW AIRCRAFT AND ENGINE CHARACTERISTICS

The SBW aircraft design is conducted within the DLR project FrEACs, preliminary design data, including aircraft performance data is provided for this study. The main aircraft characteristics are listed in Fig.1, which also shows a visual impression of the current design state. The aircraft is equipped with a Counter-Rotating Open Rotor (CROR) engine, which is one of the new engine concepts currently under investigation by engine and propulsion scientists. The CROR engine provides a high propulsion efficiency due to a large rotor diameter and respective ultra-high bypass ratios without losing specific thrust due to additional weight and drag caused by large nacelles as with turbofan engines of a similar size (Plohr, 2015). The CROR engine designed by DLR (DLR-CROR) is assumed to contain a so called Twin Annular Premixing Swirler (TAPS) as first used in the GENx engine. It applies a two-stage lean combustion technique that allows for a significant reduction of NO_x emissions under cruise conditions. Due to a completely different combustion behavior compared to conventional engines usual fuel flow correlation methods for the determination of emission indices (EI) are not applicable here. Instead, an EI estimation is used which is based on a thermodynamic process model developed by DLR for the GENx-1B70 as the CROR is expected to have similar process characteristics.

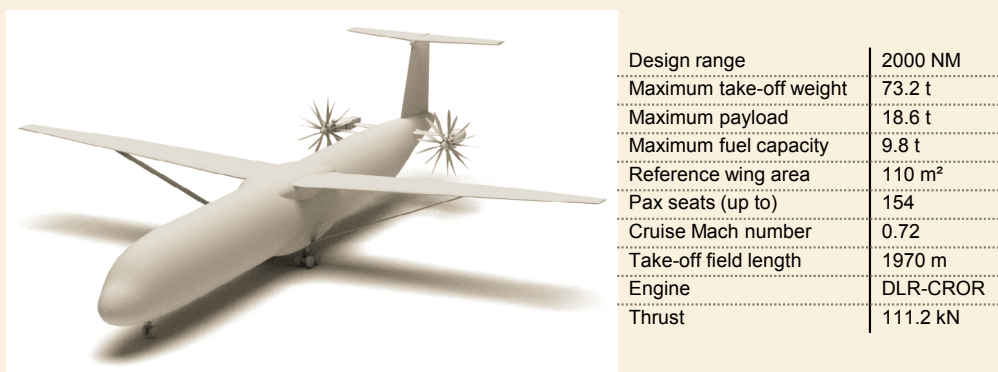


Figure 1. Strut-Braced Wing aircraft design and main characteristics

One of the key challenges in integrating the TAPS into a CROR engine with a significantly smaller mass flow and thus a smaller combustor size is the miniaturization. Here, we assume that in the future a downscaling of the TAPS combustor will be possible while maintaining the same emission level as with the GENx TAPS today. Based on that assumption, the SBW-CROR emission behavior is modeled by applying the EIs of the GENx-1B70 obtained from the ICAO engine emission databank for take-off, climb and approach phases. For cruise an average EI simulated with the above mentioned GENx model for the same mission conditions is used (Plohr, 2016). It should be noted that the combination of the aerodynamic advantages of a Strut-Braced Wing with the CROR engine technology (higher propulsion efficiency) and the TAPS combustor concept leads to a significant reduction of fuel consumption as well as NO_x emissions compared to the technology levels used in today’s aircraft.

RESULTS

In order to estimate the climate impact from the introduction of a SBW aircraft into the global air transportation system, first emission inventories were calculated for both, the business-as-usual scenario and the SBW scenario, for the years 2015 to 2050. The relative share of the SBW fleet from the entire aircraft fleet under consideration is depicted in Fig. 2.

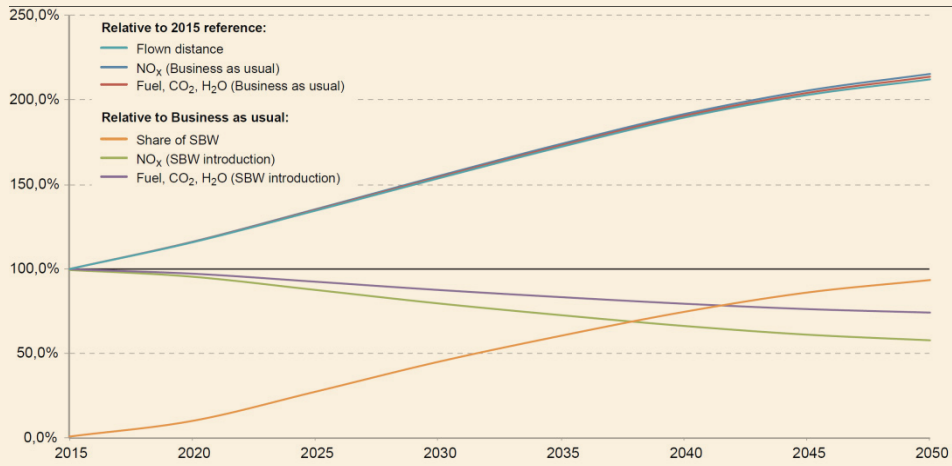


Figure 2. Relative development of fuel consumption and emissions in the scenarios

It can be seen that – according to this substitution plan – there is a 50% share reached in 2032, whereas in 2050 the share amounts to 93%. Over the entire period the flown distance more than duplicates. The fuel consumption and the overall NO_x emission amount in the business-as-usual scenario increases by approximately 110% compared to the 2015 level. With the SBW introduction, the fuel consumption can be decreased by nearly 26% by the year 2050 relative to the reference scenario (today’s technology level). Due to the special low-NO_x CROR engine the NO_x emission level can even be reduced by 45% in 2050. The fuel consumption reduction that can be achieved through the introduction of a SBW aircraft is shown in the differential inventory in Fig. 3. From the figure, the global route structure, which aircraft of the seat category 100-150 seats will be operated on in the future, is obvious. Regions of dark red color mark areas where the SBW aircraft introduction would lead to large fuel savings. The more flights are operated on those routes, the more fuel can be saved through the utilization of an SBW aircraft instead of a conventional short-haul aircraft. Especially the Chinese airspace is characterized by large potential savings as in 2050 there is a huge amount of air traffic projected in the respective seat category.

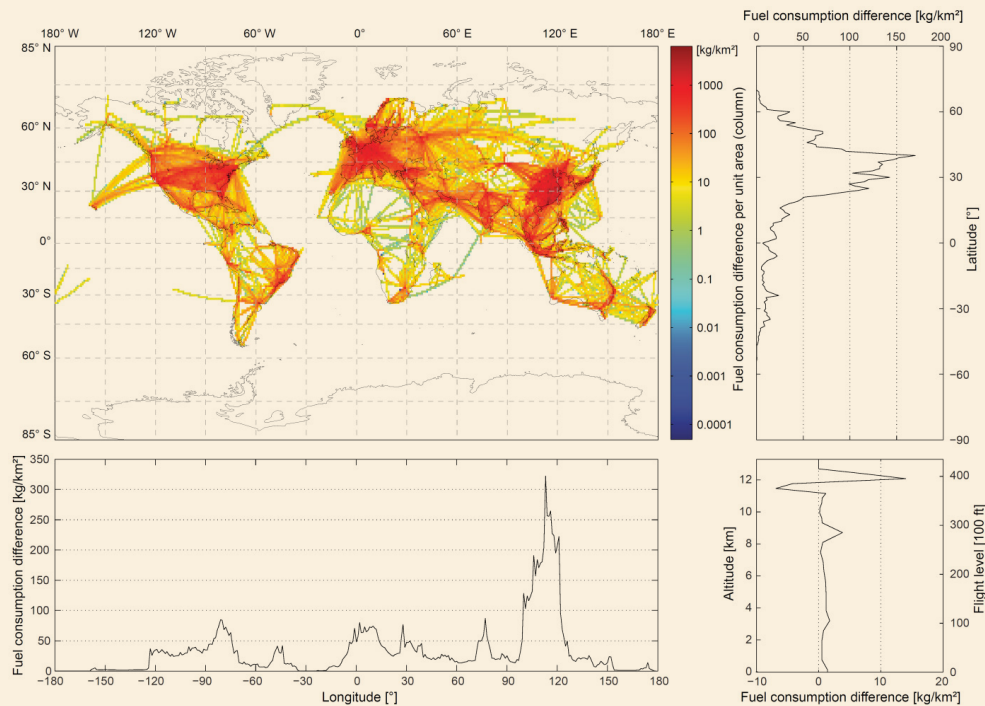


Figure 3. Fuel consumption changes in 2050 due to a SBW aircraft introduction (positive values depict reductions with respect to business-as-usual scenario)

The altitude profile (Fig. 3, bottom right) shows that there is obviously a slight shift of fuel burn in cruise from 39000 ft altitude to lower flight levels. This phenomenon can be attributed to the slightly lower optimum

altitude curves of the SBW aircraft compared to the A320. This effect will be of importance for the climate assessment presented below. The geographic distribution of the absolute NO_x emissions amounts is shown in Fig. 4. NO_x emissions primarily develop in flight phases with a high engine load, like e.g. during take-off and climb. Hence, high NO_x concentrations can be found in the vicinity of airports. Here, due to the logarithmic scale red dots could indicate future megacity locations.

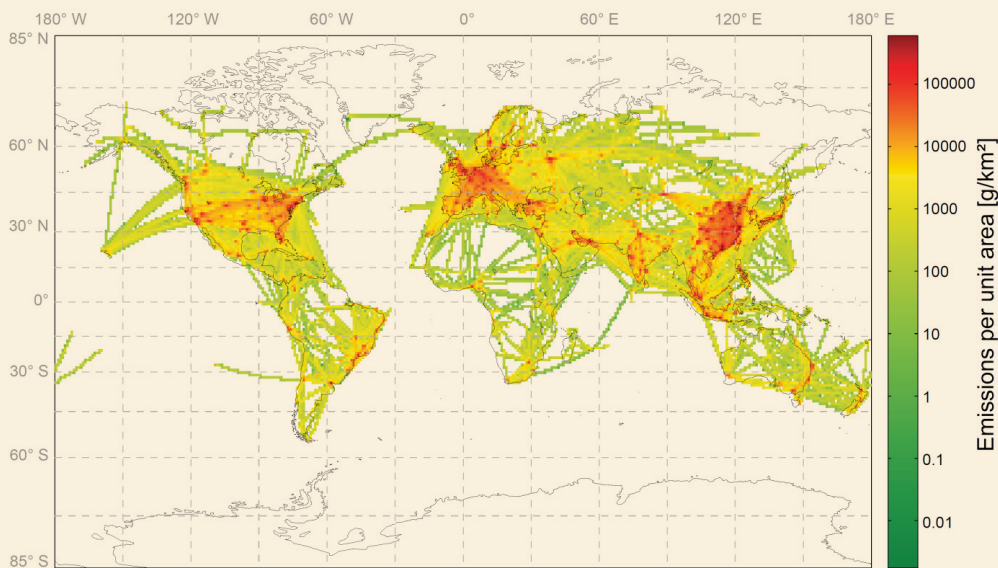


Figure 4. Absolute NO_x emission inventory of the year 2050 for a SBW scenario with a share of 93%

Using AirClim, the calculated emission inventories were finally evaluated with respect to their ATR over 100 years starting in 2015 and the SBW scenario was compared to the reference case (business as usual with today's technology level). It was found (see also Fig. 5), that the introduction of a SBW aircraft might reduce the warming associated with the air traffic growth in the seat category 100-150 seats by nearly 17%. The main driver for this is the massive reduction of NO_x emissions in combination with a slightly lower average cruising altitude (see above) leading to a reduced ozone (O₃) production. O₃ acts as greenhouse gas at those altitudes, contributing to atmospheric warming (e.g. Lee et al., 2010). Also reduced CO₂ and water vapour concentrations decrease the warming effect. As NO_x also causes methane (CH₄) depletion and methane is a greenhouse gas as well, there is also a net warming effect due to a higher methane concentration. Similarly, the primary mode ozone (PMO) contributes to an increased warming. Finally, due to the decreased average cruising altitude with more humid air, the probability of contrail formation increases which results in an additional warming. These findings are generally consistent with previous research, e.g. by Frömming et al. (2012).

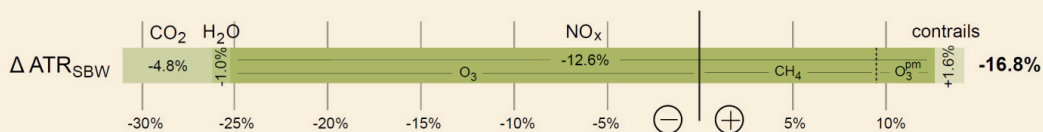


Figure 5. Relative changes in ATR due to a SBW introduction distinguished by contributing radiative forcing agents (compared to business-as-usual)

CONCLUSIONS

The results of an analysis of the global emission distribution and a climate impact assessment for the introduction of a SBW aircraft into the air transportation system have been presented. Several models developed by DLR have been applied sequentially for the study which gives an idea to what extent new aircraft configurations might contribute to a reduction of aviation's climate impact in the future. In particular, we found that the SBW aircraft has the potential to reduce the fuel consumption of the aircraft fleet of the seat category 100-150 seats by ~26% in 2050 and to decrease NO_x emissions even more by 45%. The climate impact assessment indicates, that this large reduction potential in combination with a slightly lower cruise

altitude of the SBW aircraft compared to today's reference aircraft may reduce the warming caused by aircraft of that size (including the projected growth in the future) by nearly 17%. It should be noted, that the SBW design process in the FrEACs project is not yet fully accomplished and only preliminary performance data was available. The study shall be redone and results shall be adjusted as soon as a final aircraft model is ready. However, in general the obtained achievable reductions are within a plausible range and well reflect expert's expectations. Furthermore, it is important to note, that the CROR NO_x emission indices were estimated based on simplifying assumptions. A more detailed NO_x profile could be used in the future to increase accuracy. Moreover, the substitution plan that was generated by FFWD is based on the assumption that the SBW aircraft is directly used to substitute today's short-haul aircraft, which is not realistic as there is already the next generation of short-haul aircraft being introduced (i.e. A320neo, B737MAX). It would be more realistic to assume an introduction of the SBW aircraft as their successor, probably not before 2030. Future research could spend more effort in modeling also intermediate technology-levels to capture these effects.

ACKNOWLEDGEMENTS

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DRAG REDUCTION IN AIRCRAFT WINGS USING DIELECTRIC BARRIER DISCHARGE (DBD) PLASMA FLOW CONTROL ACTUATORS

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Abstract. The year 2050 flightpath set by the Advisory Council for Aeronautics Research in Europe (ACARE), has established ambitious goals regarding the reduction of pollutant emissions produced by the aircraft aeroengines. In order to achieve these environmental targets for aviation, a reduction of CO₂ and NO_x emissions is obligatory, which is directly related to the reduction of the specific fuel consumption (SFC) of aeroengines. Low SFC values can be partially achieved by low demands on thrust and by consequence by low aircraft aerodynamic drag. The aerodynamic drag can be reduced by various active and passive flow control techniques. An innovative and promising active flow control technique towards the aerodynamic drag reduction is the use of plasma actuators. In the current study, the positive effect of a particular plasma actuator (which is referred in the literature as the dielectric barrier discharge (DBD) actuator) on controlling the flow on wings and hence, reducing the aerodynamic drag, is numerically investigated. The results of the study show that, at low speed conditions, such as during the approach and landing flight segments, the aircraft's total drag can be reduced up to 5%. It is concluded that the use of DBD plasma actuators for flow control on the lifting surfaces of an aircraft has a potential to reducing the total aerodynamic drag of an aircraft. As a consequence, this has a direct impact on the aeroengine SFC which in turn can lead to a 5% pollutants emissions reduction.

Keywords: Drag reduction, Plasma actuators, Dielectric Barrier Discharge, Active flow control, Pollutants emissions reduction

INTRODUCTION

The goals that have been set by the Advisory Council for Aeronautics Research in Europe (ACARE) regarding to the NO_x and CO₂ pollutant emissions, lead to a demand for more aerodynamic efficient aircraft, with lower specific fuel consumption (SFC) values. These goals can be achieved by reducing the required thrust, and consequently, by reducing aircraft aerodynamic drag (Caruana 2010). Drag reduction can be managed by using more efficient wing and fuselage configurations (Abbas et al. 2013) or by means of active and passive flow control techniques (Bushnell 2003).

Such an active flow control mechanism is the Dielectric Barrier Discharge (DBD) plasma actuator. The DBD plasma actuator consists of two electrodes that are separated by a dielectric material. High voltage is applied on the electrodes, resulting in a non-thermal plasma sheet as shown in fig.1. This causes an ionic wind, similar to a wall jet into the boundary layer, thus it is able to modify its properties.

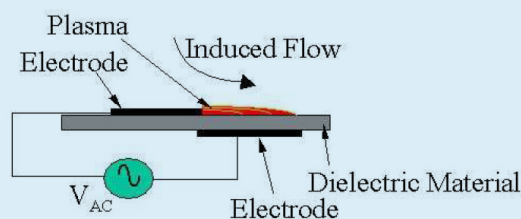


Figure 1. DBD plasma actuator configuration, figure from (Suzen et al. 2005).

The current work focuses on the effect of the DBD plasma actuator on a NACA 0012 lift and drag coefficients. A 2D Computational Fluid Dynamic analysis was carried out using the ANSYS FLUENT commercial computational fluid dynamics (CFD) software (ANSYS, Release 15) with the use of user defined functions (UDFs).

METHODOLOGY

The modelling of the DBD plasma actuator and the coupling of the plasma force with the momentum equations is carried-out using the mathematical model of (Suzen et al. 2005). This model introduces two new transport equations in order to model the resulting jet-like body force that acts on the fluid. These equations are solved in combination with the Reynolds Averaged Navier-Stokes (RANS). The resulting plasma body force interacts with the momentum equations as an additional body force source term in the RANS equations. Finally, for modelling turbulence the SST k- ω model (Menter 1994) was implemented. The corresponding equations are briefly presented below. Namely, the induced plasma body-force (eq.1), the transport equation of the net charge density ρ_c (eq.2), the transport equation of the external electric field φ (eq.3) and the momentum transport equations (eq.4). Details regarding the implementation of the adopted DBD model can be found in (Suzen et al. 2005).

The

$$\vec{f}_B = \rho_c (-\nabla\varphi) \quad (1)$$

$$\frac{\partial}{\partial x_j} \left(\varepsilon_r \frac{\partial \rho_c}{\partial x_j} \right) = \frac{\rho_c}{\lambda_d^2} \quad (2)$$

$$\frac{\partial}{\partial x_j} \left(\varepsilon_r \frac{\partial \varphi}{\partial x_j} \right) = 0 \quad (3)$$

$$\frac{\partial \rho \bar{U}_i}{\partial t} + \bar{U}_j \frac{\partial \rho \bar{U}_i}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) \right] - \frac{\partial}{\partial x_j} (\rho \overline{u'_i u'_j}) - \rho_c \frac{\partial \varphi}{\partial x_i} \quad (4)$$

The computational domain which was used for the computations is a structured like C-type mesh with 4×10^5 number of cells, as shown in fig.2 and is divided in two domains. The main fluid domain that refers to the whole region around the NACA 0012 airfoil, and the plasma actuator solid domain that is the region where the DBD plasma actuator is placed. In the fluid domain the momentum, the turbulence model, the net charge density and the voltage transport equations were solved, while in the solid domain only the voltage transport equation was solved.

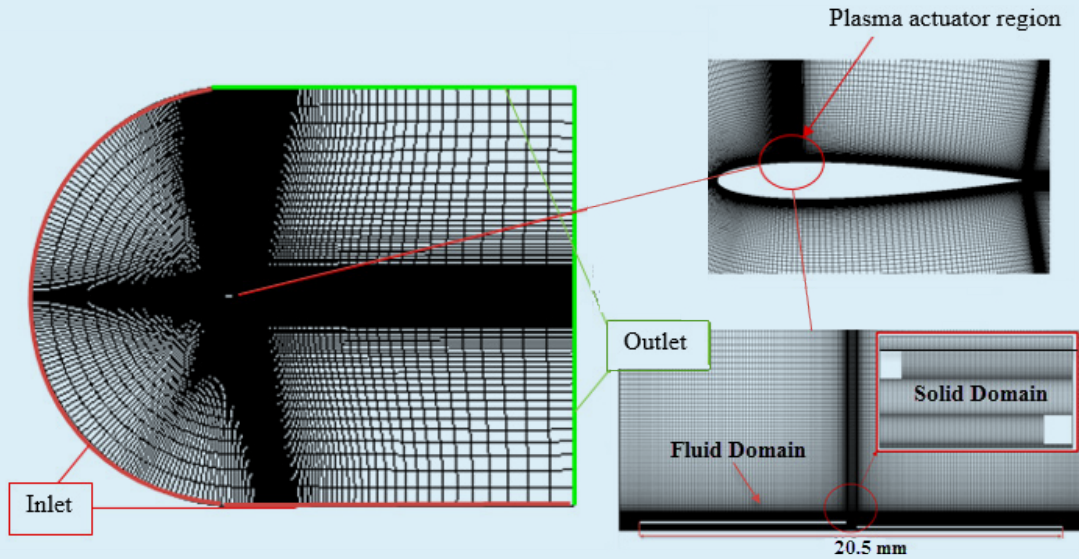


Figure 2. C-type like computational domain and fluid boundary conditions.

RESULTS

The NACA 0012 airfoil has a chord length of 0.5m, and the DBD plasma actuator is placed on the quarter chord of the airfoil where the separation of the flow initiates. Regarding the boundary conditions, the freestream velocity is 20 m/s and the freestream turbulence intensity is about 1%. The applied voltage values on the DBD plasma actuator implemented in the current study are 10 kV and 30 kV.

Figure 3 presents indicative streamlines around the NACA 0012 at 15° angle of attack with and without actuation at 30kV. When the DBD actuator is on, a reduction of the wake thickness is observed, which leads to a drag reduction and lift increase.

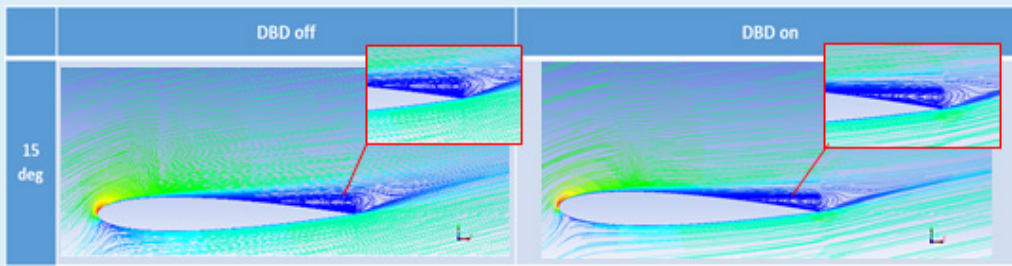


Figure 3. Streamlines around NACA 0012. Left: DBD off. Right: DBD on (30kV).

The results regarding the lift (C_l) and drag (C_d) coefficients distributions as a function of angle of attack (AOA), with DBD actuator on at 10kV and 30kV and DBD off, in comparison to the results of the Xfoil free software (Drela M. 1989) are shown in fig.4. The effect of the DBD actuation for the different voltages at 15° AOA on the lift and drag coefficients are summarized in table 1. It is shown that when the airfoil AOA takes high values, such as 15-16 degrees, where the flow separation and stall occurs, a 10% reduction in C_d and a 4% increase in C_l is observed. The same percentage difference for the aerodynamic coefficients percentage improvement can be also applied in a wing (Raymer 1992).

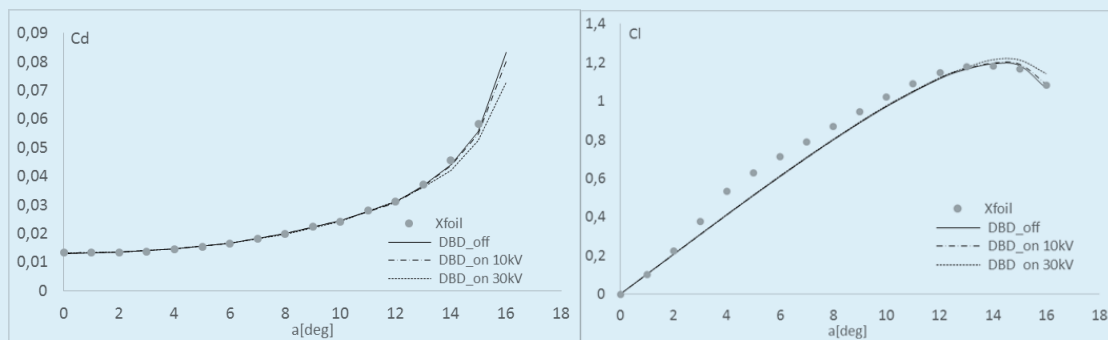


Figure 4. Left: C_d versus angle of attack. Right: C_l versus angle of attack.

Table 1. Lift and drag coefficient values at AOA=15° in different DBD actuator modes

Actuator mode	Applied voltage kV	$C_{l_{max}}$ @ 15°	C_d @ $C_{l_{max}}$
Off	-	1.184	0.57
On	10	1.192	0.55
On	30	1.23	0.52

The Thrust Specific Fuel Consumption (TSFC) is defined in equation (5) (Saravanamuttoo et al. 2001).

It is evident that for an aeroengine with constant TSFC in a specific mission segment where the DBD can have an effect, a reduction in drag and consequently in thrust leads to a proportional reduction in the required fuel mass.

$$TSFC = \frac{\dot{m}_f}{T} \quad (5)$$

Based on (Raymer. 1992) the percentage of the wing drag in the landing and take-off segments of flight is about 45 - 50% of the overall aircraft drag during these segments. So a 10% drag reduction, which has the potential to be achieved by the DBD plasma actuators, leads to a 5% reduction of the total aircraft drag during take-off and landing.

For a typical aeroengine the NO_x and CO₂ pollutant emissions reduction is proportional to aerodynamic drag reduction, (Kyprianidis et al. 2015) and (Ashok et al. 2014). As a result, a 5% NO_x (based on NO_x Emissions Index (g NO_x /kg fuel) and 5% CO₂ reduction is expected when an equivalent percentage of drag reduction is achieved.

Furthermore, the DBD plasma actuators can be used in order to reduce the skin friction drag of the other aircraft components apart from wings, such as the fuselage and the empennage, in the cruise segment of flight. Additionally, DBDs can be used to reduce other forms of drag during cruise (i.e. interference drag, induced drag) and even change the boundary layer characteristics over the wings (transition control) in favour of reducing fuel consumption and pollutant emissions. Finally, the DBD active flow control system can also contribute in the versatility of the aircraft, by providing the option of modifying the aerodynamic characteristics and the aircraft manoeuvrability during flight. Based on the low power and low weight requirements (Kriegseis et al. 2011), the low construction complexity, and the lack of mechanical parts (Moreau 2007), this innovative active flow control technique is a promising candidate for future aircraft active flow control basically in the low speed segments of the aircraft flight.

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AIRCRAFT LEVEL ASSESSMENT OF CONTRAIL MITIGATION

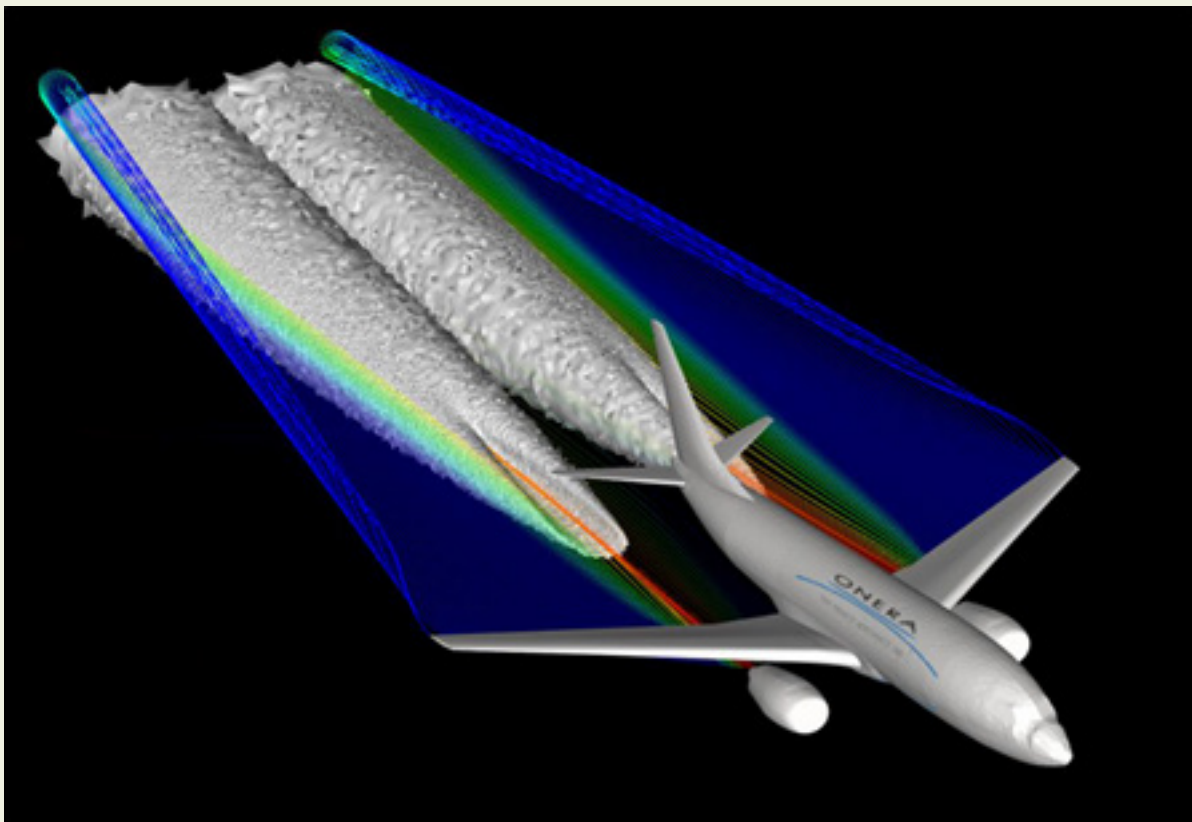
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Abstract. Contrails may contribute to a large-share of the radiative forcing due to aviation. In this context, understanding of contrails formation mechanisms in the near field of an aircraft may be helpful to provide strategies aiming at reducing their impact.

Three-dimensional RANS simulations of contrails formation produced by a commercial aircraft in cruise conditions are performed. A realistic geometry (here a Boeing 737) is taken into account including engine core and bypass flows which allows several possible parametrical studies and avoids using parameterizations for the description of the plume's dilution. The near field's plume thermodynamic properties are obtained by spatial simulation of the dynamical flow around the aircraft. A coupling is carried out with a microphysics model implemented in the CFD code CEDRE to simulate particle growth using an Eulerian approach. The implemented microphysics model is capable of simulating water condensation onto soot particles, taking into account their activation by adsorption of sulfuric species. The concentrations of which are obtained by forecasting the species chemical evolution within the bulk plume, with the addition of a detailed kinetic model to the simulation.

In this study, we investigate the potential role of soot particles concentration onto contrails properties by comparing results obtained with two different soot emission indices. Results suggest that a sensitive drop of emitted soot particles at the engine core exit would induce lower ice particle concentration, leading to both less visible and less spread contrails.



Green Flights
Climate Optimal Flight Trajectory

A NOTE ON HOW TO INTERNALIZE AVIATION'S CLIMATE IMPACT OF NON-CO₂ EFFECTS

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Abstract. In the Paris Agreement 2015 (COP21, CMP11), the world's leaders have confirmed that there is a need for fundamental changes of existing patterns of production and consumption to mitigate global warming, which affects the livelihood of an increasing amount of people worldwide. Changes of these patterns involve significant economic costs, but polluters can refuse to pay their pollution costs adequately due to the absence of market prices for environmental public goods. In order to create financial incentives for pollution reduction, policy makers are paying closer attention to instruments of environmental economics.

Within this study, the lack of incentivizing airlines to internalize their climate costs is tried to be closed by the introduction of climate-charged airspaces, as non-CO₂ emissions have location- and time-dependent effects upon the climate. In order to create an incentive for airlines to minimize flight time and emissions in highly climate-sensitive regions, a climate charge should be imposed for operators of aircraft when flying through them. Cost-minimizing airlines are expected to re-route their flights to reduce their climate charges and hence cash operating costs. Accordingly, this leads to the desired outcome of incentivizing reduction of global warming and even driving technological innovation towards cleaner technologies.

The evaluation of the climate impact mitigation potential of climate-charged airspaces is performed based on optimal control techniques. Climate sensitivities are expressed by climate change functions characterizing the climate impact caused by an emission at a certain location and time. The cost-benefit potential (climate impact mitigation vs. rise in operating costs) is investigated for an US-route and benchmarked against climate-optimized trajectories.

Keywords: climate mitigation concept, internalization, cost-benefit assessment, air transportation modeling, optimal control

INTRODUCTION

The degradation of the environment affects the livelihood of a growing number of people and all living beings. But polluters have little incentives to voluntarily internalize their pollution costs, as they can take the position of a free rider: they benefit of the *non-excludability* and partially of the *non-rivalry* character of environmental goods, even if they are not willing to contribute to the costs to prevent environmental degradation adequately. If they are invited to share these costs, they may give an incorrect answer and understate their preference for the public good – including a zero willingness to pay as an extreme case – due to expectations that the availability of the good will be ensured by those with a higher willingness to pay. This might lead to under-provision of the good and cause market failure. For the competing demands on the environment a zero price cannot bring about an optimal allocation. Scarcity and degradation of public goods call for the introduction of prices. Internalization can be pursued through a variety of instruments of environmental policy like government regulation, tradeable permits (cap-and-trade systems), taxes or charges (Siebert, 2008).

Anthropogenic global warming has a special difficulty from an environmental economics point of view, since it is highly susceptible to the free-riding problem: consequences of climate change are long-lasting and widely spread around the globe. Inter-dependencies between aviation and climate change are complex and non-linear, and the amount of emissions is not equal to its climate impact. Approximately two-thirds of aviation-induced global warming is expected to be caused by non-CO₂ effects like the emission of nitrogen oxides (NO_x) and the formation of contrail induced cloudiness (CiC), which are highly sensitive on chemical and meteorological background conditions. Consequently, their climate response largely depends on

emission location and time. NO_x emissions, for example, have a larger impact on climate when released at higher flight levels as more ozone can be produced during a longer time period due to an increase of atmospheric residence time [Schumann, 2012]. Therefore, environmental policy making should change the focus on climate impact mitigation instead of emission reduction only.

The crucial questions are then (i) how to include aviation's climate impact of non-CO₂ effects adequately into an environmental policy measure and (ii) what is a reasonable 'shadow price' for global warming. The study at hand focuses on the first question.

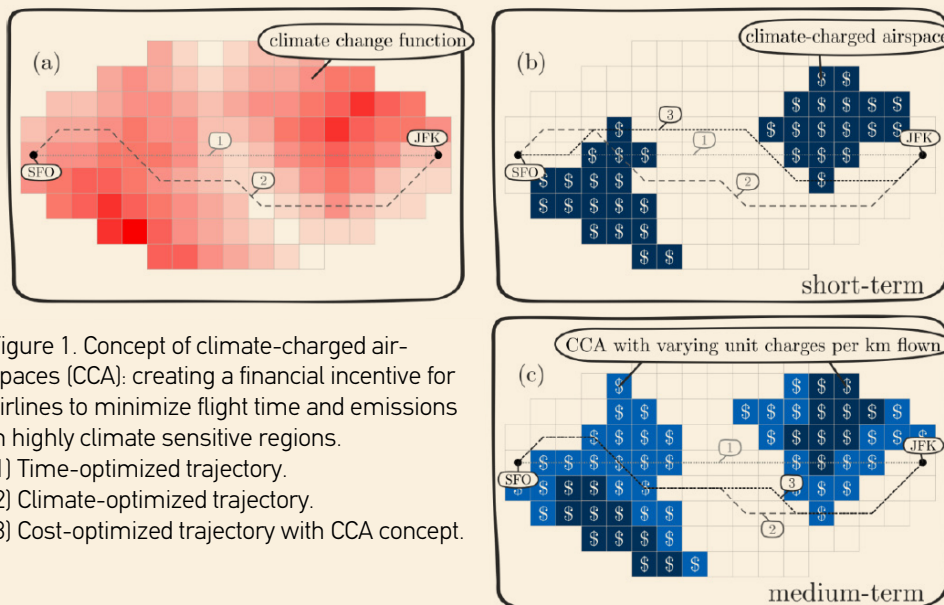


Figure 1. Concept of climate-charged airspaces (CCA): creating a financial incentive for airlines to minimize flight time and emissions in highly climate sensitive regions.
 (1) Time-optimized trajectory.
 (2) Climate-optimized trajectory.
 (3) Cost-optimized trajectory with CCA concept.

CONCEPT OF CLIMATE-CHARGED AIRSPACES (CCA)

In order to create an incentive for airlines to minimize flight time and emissions in highly climate sensitive regions, we suggest to impose a climate charge for operators of aircraft that fly in these areas (see figure 1); contrary to approaches that propose an environmental charge for CO₂ and/or NO_x emissions. An airspace *j* should be levied with an environmental unit charge U_{cj} per kilometre flown, d_j , if its climate sensitivity with respect to aircraft emissions¹ exceeds a specific threshold value C_{thr} :

$$CCA_j(\mathbf{x}) = \begin{cases} U_{cj}, & \text{if } CCF_{tot}(\mathbf{x}) \geq c_{thr} \\ 0, & \text{if } CCF_{tot}(\mathbf{x}) < c_{thr} \end{cases} \quad (1)$$

Thus, cost-minimizing airlines will re-route their flights to reduce the climate charges and hence their cash operating costs². In this manner, climate impact mitigation coincides with the cutting of costs. The operator of an aircraft can decide individually for each flight according to individual needs whether to minimize flight time and to pay compensation for higher climate damage (trajectory 1 in fig. 1) or to minimize costs and, concurrently, reducing the climate impact by total or partial avoidance of CCA (trajectory 3 in fig. 1). Consequently, dealing with complex climate-change functions do not need to be integrated into the responsibility of an airline and their planning processes to mitigate non-CO₂ effects on climate. CCA could be defined and monitored by air traffic control instead.

The certainty of the climate benefit of optimized trajectories is highly dependent on the quality of CCF and their correctness. Thus, existing uncertainties in climate impact modelling could lead to optimized trajectories – according to prevailing CCF_i of different agents *i* – that might turn out to be either over- or underestimated with respect to their climate mitigation potential. In order to be environmental effective a resilient handling of these uncertainties is necessary. Therefore, the implementation of the CCA concept focuses in a first step only on those areas that are likely highly sensitive to climate (short-term, see fig. 1b). But its implementation can be adapted to current level of scientific understanding (LOSU) at any time (medium-term, see fig. 1c) by introducing varying unit charges U_{cj} for different levels of climate sensitivities.

Ideally, the total shadow price of a single flight ($\sum_i U_{cj} d_j$) should equal all its external costs associated with climate change. This means compensating actual economic, environmental and health damage. But by estimating socio-economic costs, concurrently, also the level of uncertainties rises,

¹The climate sensitivity of an area is expressed here by total climate change functions (CCF_{tot}) characterizing the environmental impact caused by non-CO₂ effects of aircraft's emissions at a certain location and time.

²According to Eurocontrol (2016), many airlines choose to fly longer – at times when fuel costs are relatively low – and re-route their flights over Europe away from more expensive airspace areas to minimize costs.

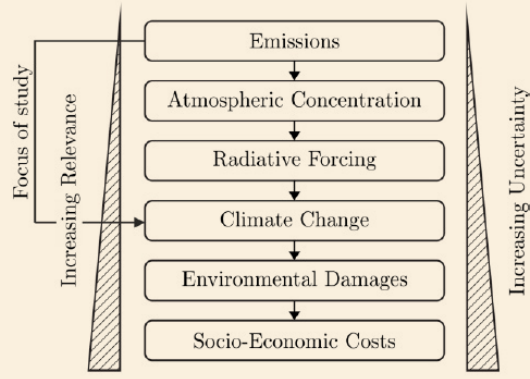


Fig. 2. Cause-effect chain from emissions to socio-economic costs according to Fuglestvedt et al. (2010)

due to the currently low state of understanding and the simplifications made during modelling, see fig. 2. The main object of this work is, however, to evaluate the concept of CCA, not to estimate the exact value of the charge in terms of money. Thus, in order to reduce uncertainties, the shadow price calculation is limited to climate change in terms of average temperature change (ATR).

MODELING APPROACH

Within this study, the cost-benefit potential of the CCA concept is evaluated and benchmarked against the mitigation potential of climate-optimized trajectories (COT). Therefore, optimized aircraft trajectories are determined by employing optimal control techniques within the *Trajectory Optimization Module (TOM)*. *TOM* minimizes a cost functional J while satisfying dynamic constraints as well as state (i.e. maximum speed), control (e.g. thrust limit) and path limitations (e.g. maximum pressure altitude). A comprehensive description of *TOM* is given by Lühns et al. (2016) and Niklaß et al. (2015).

A. Calculation of optimized trajectories with respect to climate and economy

For benchmark purposes, a multi-objective optimization with regard to climate and monetary costs is performed within this study. Therefore, monetary costs (COC) and climate change functions (CCF) are integrated into *TOM*'s cost functional J_{COT} . The Pareto optimal set is found by varying the weights of monetary (c_v) and climate (c_ψ) 'costs' with $c_v + c_\psi = 1$ and $c_v, c_\psi \in [0, 1]$. A trajectory is optimal with regard to monetary costs, if $c_v = 1$, and optimal with regard to climate, if $c_\psi = 1$.

Climate Change Functions: $CCF(x, t)$ are computed by Niklaß et al. (2016) with the climate response model AirClim and expressed as average temperature response integrated over a time period of 100 years (ATR₁₀₀) per unit emission. $CCF_i(x, t)$ are calculated individually for CO₂, H₂O, NO_x (ATR₁₀₀ per unit emission), and CiC (ATR₁₀₀ per flown unit distance).

Monetary Cost Functions: The economic impact of a flight trajectory is described by the share of cash operating costs (COC) calculated as function of mission time ($t_f - t_0$) and mission fuel ($m_0 - m_f$). COC are derived from Liebeck et al. (1995) and scaled to 2012 US dollars with the average US inflation rate of average consumer prices (IMF, 2014).

B. Implementation of climate-charged airspaces (CCA)

Climate charges, C_{cj} , are expressed for a flight through an climate-charged airspace j in analogy to en-route and terminal charges:

$$C_{cj} = U_{cj} \cdot \left(\frac{MTOW}{k_1} \right)^{k_2} \cdot I_{AC} \cdot d_j \quad (2)$$

where d_j is defined as the distance traveled in CCA _{j} , MTOW as maximum take-off weight of an aircraft and $I_{AC} \in [0, 1]$ as incentive factor for climate-friendly technologies. It is conceivable to link I_{AC} with prospective CO₂ and NO_x certification standards for cruise as are currently being discussed for CO₂ by ICAO (2016). Cost-optimized trajectories are obtained by minimizing the cost functional $J_{CCA} = f(COC, C_{cj})$.

EXPECTED RESULTS

The feasibility of the CCA concept is evaluated for an U.S. route from San Francisco (SFO) to New York (JFK). Therefore, optimized trajectories (minimization of J_{COT} and J_{CCA} with varying climate charges U_{cj}) are identified with TOM and benchmarked against each other from a cost (increase of cash operating cost) and environmental (reduction of average temperature response) point of view.

Similar computations have been already performed by Niklaß et al. (2016) for climate-restricted airspaces (CRA, $U_{cj} \rightarrow \infty$) with varying threshold values. As shown in figure 3, the introductions of CRAs allow climate impact mitigation efficiencies in the same order of magnitude as COT. But, however, a large volume fraction of the airspace has to be closed to achieve high climate impact reductions (see figure 4). ATR can be reduced, for instance, by 10% on the route from Lisbon, Portugal (LIS) to Miami, USA (MIA) for a cost increase of less than 1% by closing 26.6% of the North-Atlantic airspace in-between 8,500 and 12,500m of altitude. Similarly high efficiencies are expected also for climate charged areas, but with the advantage of being more operationally feasible.

ACKNOWLEDGMENT

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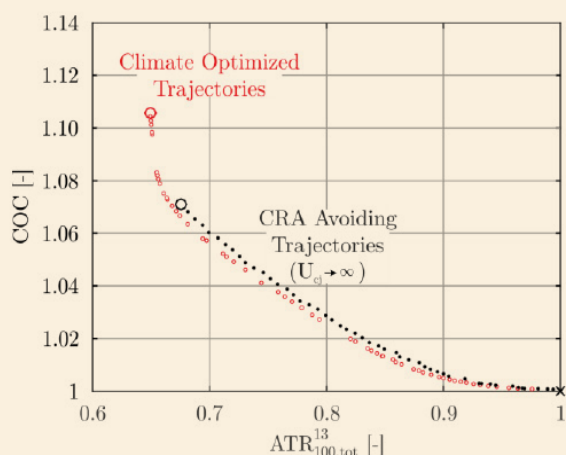


Fig. 3. Average temperature response (ATR) and cash operating costs (COC) for climate-optimized trajectories (COT, red) and CRA avoiding trajectories ($U_{cj} \rightarrow \infty$, black, solid) (Niklaß et al. 2016).

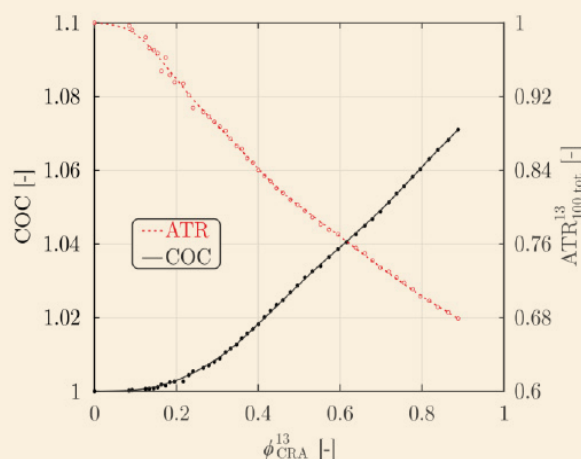


Fig. 4. Average temperature response (ATR, red) and cash operating costs (COC, black, solid) as function of the restricted volume fraction of upper airspace (ϕ_{CRA}^{13} , $U_{cj} \rightarrow \infty$) (Niklaß et al. 2016).

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FEASIBILITY OF CLIMATE-OPTIMIZED AIR TRAFFIC ROUTING FOR TRANS-ATLANTIC FLIGHTS

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Abstract. Current air traffic routing is motivated by minimizing economic costs. Fuel use is a major part of those costs. In addition to the climate effect of CO₂ emissions from this fuel use, aviation contributes to climate change through non-CO₂ effects, such as changes in atmospheric ozone and methane concentrations and formation of contrail-cirrus. These non-CO₂ effects depend significantly on where and when the aviation emissions occur. For example, persistent contrail-cirrus only forms in atmospheric regions which are ice supersaturated. Similarly, depending where they are emitted, nitrogen oxides might be rapidly rained-out or transported over long distances and hence leading to either little or substantial ozone production, respectively. The climate impact of aviation could potentially be reduced if flights were re-routed to avoid regions where emissions have the largest impact. We present the first results where such a strategy is simulated for all frequently occurring winter and summer weather patterns in the North Atlantic. We find that even small changes in routing, which increase the operating costs (mainly fuel) by 1% lead to considerable reductions in climate impact of 10%. The cost increase could be compensated by market based measures, if costs for non-CO₂ effects were included. Our methodology is a starting point for climate-friendly flight planning, which could also be applied globally. Although there are challenges to implementing such a system, we present a road map with the steps to overcome these.

SIMULATION OF AIR TRAFFIC USING WEATHER-BASED CLIMATE COST FUNCTIONS – FEASIBILITY ANALYSIS

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Abstract. The aviation-related climate impact share today is estimated at about 5%. Lately, very often this has provoked discussions on how to reduce the climate impact of the aviation industry especially in the area of non-CO₂ components like ozone, methane and cirrus contrails. DLR has joined the global effort for environmentally sustainable aviation by exploiting an eco-efficient flying in the internal project WeCare (Utilizing **W**eather information for **C**limate efficient and eco efficient **f**uture aviation). The project focuses on three different areas: climate optimal routings, cost benefit analysis of mitigation options and demonstrable effects of air traffic. The operational and technical measures are considered to be the two classes of measures that can make the air traffic more climate friendly. In this paper, we aim to assess the operational measures by exploiting the effect that the climate optimized trajectories has on the existing air traffic management (ATM) by means of fast-time simulation.

The main data source for the traffic samples is Eurocontrol's SO₆ flight information data. In addition, the compatible airspace structure for each simulated day is used. Airspace data is gathered and consolidated from EUROCONTROL's Demand Data Repository (DDR2). There are several fast-time simulations performed, which will analyse the feasibility of the climate optimized trajectories as well as the impact they have on the ATM system.

Scenario one, or the reference scenario, is based on the air traffic scenario for the chosen day representing the current ATM system. Scenario two and three include air traffic scenario with an optimized flights for the prototype data and all weather data climate cost functions.

The methodology for this feasibility study is as follows: In the first step evaluation methodology for the final assessment is defined. The evaluation methodology focuses on parameters such as number of flights, sector capacities, controller workload and number of affected flights with both horizontal or vertical change, and flight duration. In the second step the simulations of all the three scenarios are performed and evaluated based on the predefined assessment methodology. In order to evaluate the influence of the optimized trajectories on the system's overall performance, the results of each scenario are compared.

The assumption is that the expected results will both cover qualitative and quantitative aspects. First ones can be obtained by an increased understanding of the (complex) aviation system's behaviour due to changes such as trajectory optimization. This understanding will deepen by offering quantitative results on the change on the above mentioned parameters. The quantitative values will depend on the number of optimized flights as well as on the airspace size. The more aircraft are affected, the more the number of flights in the neighbouring sectors will be increased. As a consequence, capacity will drop and controller workload will be increased.

The preliminary results however slightly differ from the original assumption. Though the traffic demand in the analysed airspaces does not increase dramatically, meaning that the sector capacity does not change, the controller workload drastically increases and the main reason is the increased number of vertical movements by the optimized flights.

Interdependency and aviation environmental Modelling

ASSESSING TRENDS IN AVIATION NOISE AND EMISSIONS IN EUROPE USING ADVANCED MODELLING CAPABILITIES

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Abstract. In 2013, IMPACT and the Aircraft Assignment Tool (AAT) were introduced at 1st ECATS Conference as two new major tools of the European aviation environmental modelling tool suite. Both tools are based on the experience gained during more than 15 years of environmental modelling development in support of European and ICAO Committee on Aviation Environmental Protection (CAEP) environmental assessments.

IMPACT is a web-based modelling platform which constitutes a significant improvement towards achieving robust trade-off assessments between noise and fuel burn and/or gaseous emissions. IMPACT combines the Advanced Emissions Model (AEM) and the multi-airport noise model STAPES into a common modelling platform, with a goal to provide these environmental models with common input data in terms of aircraft trajectories (along with other flight parameters of relevance for environmental modelling purposes). A key component of IMPACT is a new aircraft trajectory calculator, which computes complete aircraft trajectories from the departure airport to the arrival airport, along with engine thrust and fuel flow information.

AAT is a generic tool that takes as input an existing demand and fleet forecast and converts it into a forecast of movements by particular aircraft type on specific airport pairs. The geographical scope is dependent on the forecast, and can range from a single airport pair to full global operations. The output of AAT can be used as input to environmental models such as IMPACT and to assess the evolution of the aircraft fleet for future planning and policy purposes.

AAT combined with IMPACT made it possible to assess trends in noise and emissions in Europe until 2035, under various traffic forecasts and aircraft technology scenarios, for the European Aviation Environmental Report 2016.

Keywords: noise, fuel burn, emissions, aircraft performance, forecast.

INTRODUCTION

In 2013, IMPACT and the Aircraft Assignment Tool (AAT) were presented at 1st ECATS Conference as two new major tools of the European aviation environmental modelling tool suite. Both tools are based on the experience gained during more than 15 years of environmental modelling development in support of European and ICAO Committee on Aviation Environmental Protection (CAEP) environmental assessments.

IMPACT

The IMPACT modelling tool was first introduced at the 2013 CAEP Steering Group meeting as a successor to two models already approved by CAEP: the Advanced Emissions Model (AEM) and the SysTEM for AirPort noise Exposure Studies (STAPES).

AEM is a EUROCONTROL model that can determine the amount of fuel burned by a specific aircraft type equipped with a specific type of engine, flying a specific 4D trajectory. It can also determine the precise by-products of burning that fuel such as: carbon dioxide (CO₂), water vapour (H₂O), oxides of sulphur (SO_x), oxides of nitrogen (NO_x), unburnt hydrocarbons (HC), carbon monoxide (CO), particulate matter (PM), and some volatile organic compounds (VOCs) such as benzene and acetaldehyde. The core emission calculation engine of AEM implements the Boeing Fuel Flow Method 2 (BFFM2), which is described in the Aerospace Information Report 5715 (SAE International, 2009).

STAPES is a multi-airport noise model that is the result of successful collaboration by the European Commission (EC), the European Aviation Safety Agency (EASA) and EUROCONTROL. STAPES consists of a noise modelling software, hosted and maintained by EUROCONTROL, which is compliant with the calculation method recommended in the ICAO Doc 9911 (ICAO, 2008) and ECAC Doc. 29 (ECAC, 2005)

guidance documents, combined with an airport database that provides information on runway and route layouts, along with statistics on their usage (i.e. distribution of aircraft operations). The STAPES airport database, jointly maintained by EASA and EUROCONTROL, currently covers 45 European airports that are representative in terms of their noise impact on the surrounding population (i.e. number of people within the L_{den} 55 dB noise contours). Population estimates are based on the population database supplied by the European Environment Agency (EEA), complemented with local census data when available. STAPES is a CAEP-approved noise model that has contributed to CAEP's noise trends assessment and future stringency analyses since 2009.

The introduction of IMPACT constitutes a significant improvement towards achieving robust trade-off assessments between noise and fuel burn and/or gaseous emissions. IMPACT integrates the core emission calculation engine of AEM and a reengineered and enhanced version of the core noise calculation module of STAPES into a common modelling platform, with a goal to provide these environmental models with common input data in terms of aircraft trajectories (along with other flight parameters of relevance for environmental modelling purposes).

A key component of IMPACT is a new aircraft trajectory calculator, which computes complete aircraft trajectories from the departing airport to the destination point, along with engine thrust and fuel flow information. This common trajectory data is then exported to the core engine of AEM and the core noise calculation module of STAPES to calculate emissions and noise. With this modelling approach, consistent assessments of trade-offs between noise and fuel burn and/or gaseous emissions are enabled over the portion of the trajectories within the Terminal Manoeuvring Area (TMA). The IMPACT trajectory calculator relies on the Aircraft Noise and Performance (ANP) database and the latest release of EUROCONTROL's Base of Aircraft Data (BADA 4). The ANP database provides the noise and performance characteristics of a wide range of civil aircraft types, which are required to compute noise contours around civil airports using the calculation method described in ICAO Doc 9911 (ICAO, 2008) and ECAC Doc. 29 (ECAC, 2005). BADA (Base of Aircraft Data) is an aircraft performance model developed and maintained by EUROCONTROL, in cooperation with aircraft manufacturers and operating airlines. BADA is based on a kinetic approach to aircraft performance modelling, which enables the accurate prediction of aircraft trajectories and the associated fuel consumption (EUROCONTROL, 2010). The latest BADA 4 family constitutes a major improvement in terms of aircraft performance modelling accuracy (Gallo *et al.*, 2006).

The complete trajectory computed by the IMPACT aircraft trajectory calculator is illustrated in Figure 1.

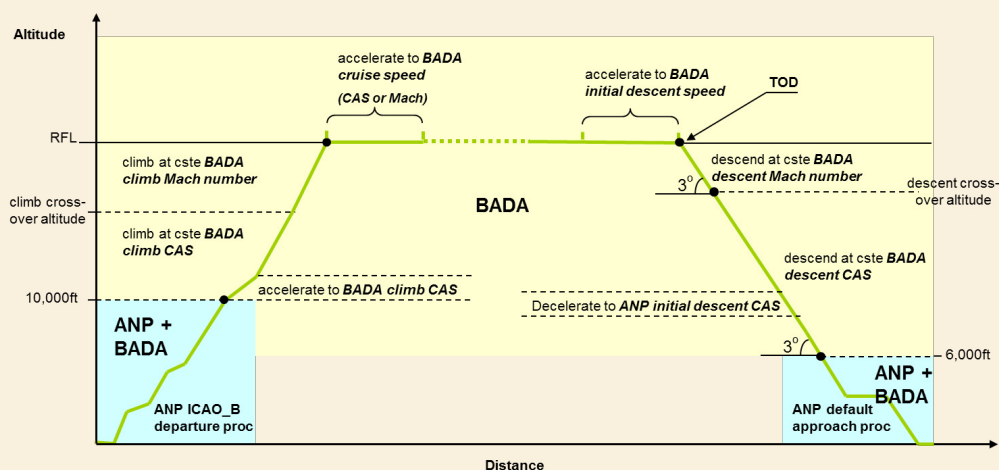


Figure 1. IMPACT full flight procedure.

Another key characteristic of IMPACT is that it is a web-based modelling platform remotely accessible by the users, via a dedicated and secured portal (Figure 2). All calculations are performed on dedicated servers hosted by EUROCONTROL. In particular, users do not need to install any specific software on their machines; they only need a web browser to connect to the IMPACT web portal, upload their input data, launch calculations, visualise, and download the results. This web-based approach enables easy update of the different databases used by IMPACT, without the need to redistribute a new software package, and provides the flexibility to select the database versions to be used in a study. Another major advantage is that

it secures sensitive aircraft reference data such as the BADA data.

IMPACT supports different types of input data, which can be retrieved from various sources (i.e. real-time and arithmetic model-based simulations, real data, or more theoretical definitions of flight procedures). The main results produced by IMPACT include noise contour shapefiles, surface and population count using the European Environment Agency (EEA) population database, fuel burn and emissions of a wide range of pollutants, gridded (i.e. geo-referenced) emission inventories within the LTO portion; as an introduction to further – more detailed – Local Air Quality (LAQ) assessments.

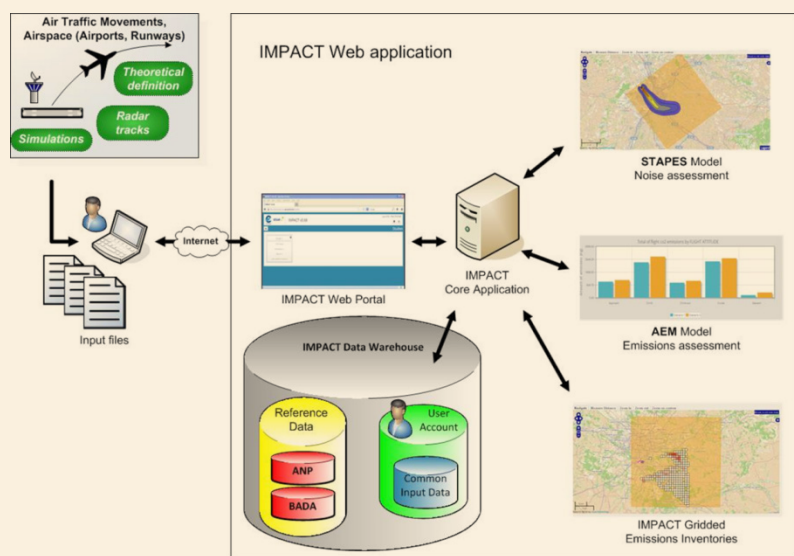


Figure 2. IMPACT Web-based Modelling Platform.

During the CAEP/10 work programme, IMPACT was thoroughly reviewed against other CAEP-approved models and contributed to the CO₂ Standard analysis as well as the greenhouse gas and LAQ trends assessment. While meeting CAEP assessment needs, IMPACT was also developed to comply with the Single European Sky ATM Research (SESAR) environmental assessment requirements and is the recommended assessment tool for this European ATM research programme.

THE AIRCRAFT ASSIGNMENT TOOL (AAT)

To meet European needs and as part of their support of CAEP, the European Commission, EASA and EUROCONTROL have developed a fleet and operations forecasting capability called the Aircraft Assignment Tool (AAT). The AAT is a generic tool that takes as input an existing demand and fleet forecast, such as that from CAEP's Forecasting and Economic Analysis Support Group (FESG), and converts it into a forecast of movements by particular aircraft types on specific airport pairs. The geographical scope is dependent on the forecast, and can range from a single airport pair to full global operations. The output of the AAT can be used as input to environmental models such as IMPACT. Such information can also be used to assess the evolution of the aircraft fleet for future planning and policy purposes.

The typical AAT input data consists of: a demand forecast; a set of base year operations (e.g. the Common Operations Database for CAEP applications); aircraft retirement curves; a set of in-production aircraft over the forecast period (future fleet) along with their respective transport capability (seats/tonnes), maximum range and their market shares in the group they belong to (shares may vary in time). The AAT can also handle user-defined phase-out functions for specific aircraft types.

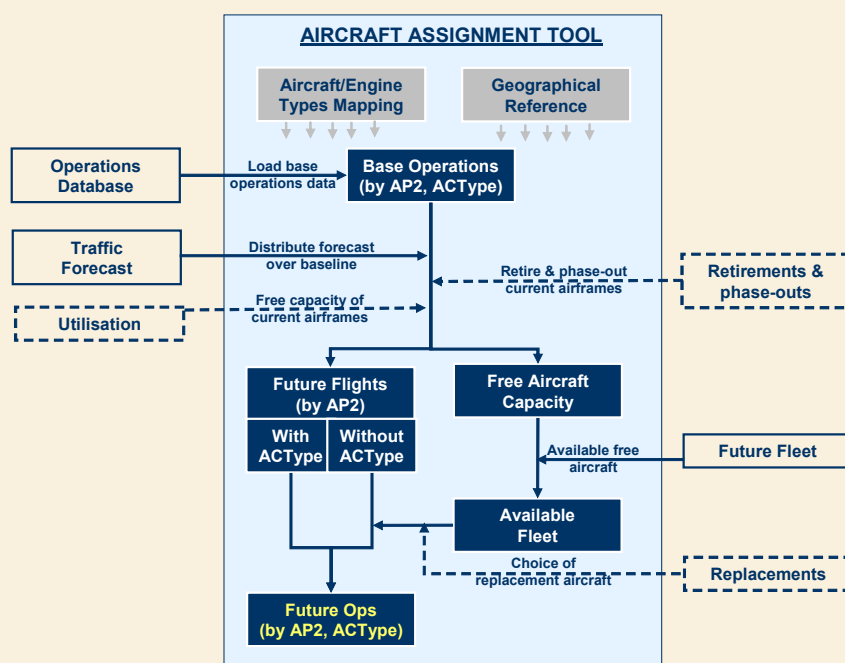
Aircraft types in AAT are typically grouped by user-defined categories based on their transport and range capability.

Within a particular category, each aircraft type is assigned a specific market share. Market shares are specified by the user, which allows the application of various calculation methods including: equal market shares (all aircraft in a bin have the same share); market-driven market shares (shares are derived from the relative operating costs of each aircraft, e.g. using a multinomial logit); and historical market shares (shares

are derived from past aircraft deliveries). If the demand forecast is expressed in available seat-kilometres (ASK) or available tonne-kilometres (ATK) for freighters, the AAT adjusts the number of movements on a given route to the size of the aircraft assigned to this route and their respective market shares.

The AAT was developed following four key non-functional requirements:

- **Flexibility:** With a variety of possible uses, the AAT is flexible enough to process input data from different sources and deliver output data fit for various modelling tools.
- **Speed:** To allow regular updates within strict deadlines and with limited resources (e.g. EUROCONTROL forecasting process), the AAT architecture allows relatively easy operation and fast run-times.
- **Openness:** In order to be transparent, the AAT does not develop its own assumptions (based on historical data patterns or the like). Instead the assumptions are formulated, and the input data constructed, by the user outside the AAT. This allows the AAT to be used for analysis of scenarios and "what-ifs" following different "stories" as defined and specified in the inputs by the user.
- **Accessibility:** The AAT is accessible via a web portal and therefore only requires a web browser and an internet connection to be run.



(AP2 = Airport pair; ACType = Aircraft type)

Figure 3. Aircraft Assignment Tool (AAT) design.

During the CAEP/10 cycle, the AAT was reviewed by the Forecasting and Economic Analysis Support Group (FESG) and was used in the CO₂ standard's cost-effectiveness analysis.

USING IMPACT AND AAT FOR THE EUROPEAN AVIATION ENVIRONMENTAL REPORT 2016

AAT was integrated into the EUROCONTROL/STATFOR 20-year forecast toolset for the passenger market segment. Combined with IMPACT, it made it possible to assess trends in noise and emissions in Europe until 2035 under various traffic forecasts and aircraft technology scenarios for the European Aviation Environmental Report 2016 (EASA *et al.* [2016]). Figures 4 and 5 present respectively the estimated L_{den} 55 dB population exposure and full-flight CO₂ trends from 2005 to 2035.

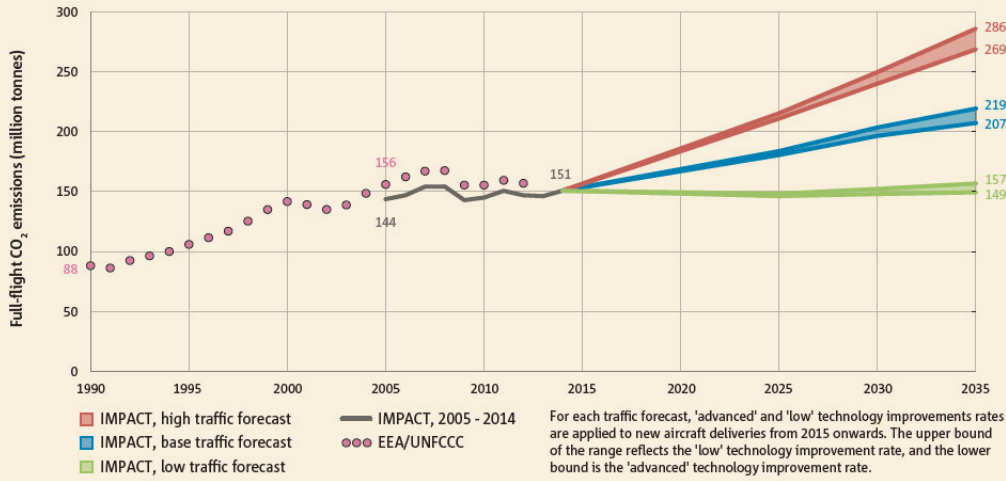


Figure 4. EAer 2016 – L_{den} 55 dB population exposure at 45 STAPES airports

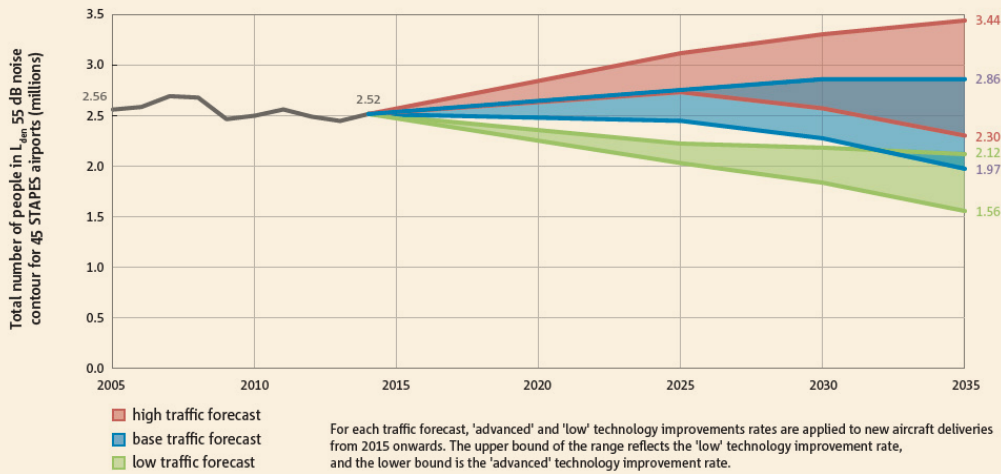


Figure 5. EAer 2016 – Full-flight CO₂ emissions for all departures from EU+EFTA

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MODELLING OF AIRCRAFT EMISSIONS IN THE AIRPORT AREA

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Abstract. Currently the primary subject of concern of airport air quality are the NO_x and PM emissions from aircraft engines, because they are the initiators of photochemical smog and regional haze, which at further steps may impact on human health directly. The analysis of emission inventories at Ukrainian and major European airports has highlighted, that aircraft are the dominant source of air pollution in most of the cases considered. Aircraft are a special source of air pollution due to some features. To assess of aircraft engine emissions contribution in local air quality (LAQ) assessment it is important to take in mind the features, which define emission and dispersion parameters of the source. The aircraft emission inventory is usually calculated on the basis of certificated engine emission indices, which are stored in an ICAO databank. The emission indices rely on well-defined measurement procedures and conditions during aircraft engine certification. Under real real-world operating conditions, however, these conditions may be quite different and deviations from the certificated emission indices may occur. This could lead to significant differences between emissions from actual airport operations and emission inventories used in modeling airport air quality. The measured NO_x and CO₂ concentrations at Boryspol International Airport (Kyiv) were used for the improvement and validation of the complex model PolEmiCa. Comparison of measured and modeled NO_x concentration in the plumes from aircraft engines was significantly improved by taking into account the EINO_x which was determined under real operating conditions.

Keywords: aircraft engine, emission index, airport air pollution, aircraft engine emissions

INTRODUCTION

Aircraft engine emissions have a direct impact on air quality in local, regional and global scales. Today the aviation sector is responsible for example for 12% of the CO₂ emissions from the transport sector, compared to 74% from road transport [ICAO report, 2013]. Several studies exhibited extremely high concentrations of toxic compounds (including nitrogen oxides (NO_x), particulate matter (PM₁₀, PM_{2.5} and UFP), unburned hydrocarbons (UHC) and carbon monoxide (CO)) due to airport-related emissions and a significant impact on the environment [Herndon *et al.*, 2008] and health of the people living near the airport [Peace *et al.*, 2006].

Aircraft are the dominant source of emissions and air pollution at airports in almost all LAQ analyses [Celikel *et al.*, 2005]. ICAO recommends in the Doc 9889 some tools for air quality analysis – to model emission inventory from every character groups of the spatially distributed sources as well as atmospheric concentrations resulting from emission dispersion.

Aircraft emission inventories are usually calculated on the basis of certificated engine emission (EE) indices, which are provided by the engine manufacturers and stored in the ICAO EE database. The emission indices rely on well-defined measurement procedures and conditions during aircraft engine certification. Under real-world operating conditions, however, these conditions may be quite different and deviations from the certificated emission indices may occur because of:

- **the life expectancy** (age) of an aircraft since the emission of an aircraft engine might vary significantly over the years (the average operating period – 30 years). Usually aging aircraft/engine show higher emission indices compared with same younger engine type;
- **the engine type** (or its specific modification, for example with respect to different combustion chambers) installed at an aircraft, which can be different from the same engine type operated in an engine test bed during certification;
- **meteorological conditions** – temperature, humidity and ambient air pressure, which can be different under certification conditions.

Thus, in practice the aircraft engine thrust used in real operations is significantly smaller (close to 85-90%), than what is prescribed by the ICAO (100%) for performance and cost-efficiency reasons [Herndon *et al.*, 2008]. This could lead to significant differences between emissions from actual airport operations and emission inventories used in modeling airport air quality.

Basically, the Gaussian plume model is used for prediction of vertical and horizontal dispersion of air pollution produced by aircraft engine emissions [ICAO Doc 9889, 2011]:

$$C(x; y; z; H) = \frac{Q}{2 \cdot \pi \cdot \sigma_y \cdot \sigma_z \cdot u} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \cdot \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right] \right\} \quad (1)$$

where C – concentration at point with coordinates (x, y, z) , $\mu\text{g}/\text{m}^3$; u – velocity of moving emission source, m/s ; Q – source emission rate, $\mu\text{g}/\text{s}$; σ_y, σ_z – horizontal and vertical dispersion parameters; H – effective height of source, m .

As with any dispersion model, the initial properties of a plume are important to model its rise and location. Such plume or jet parameters, as rise height Δh_A due to buoyancy effect, horizontal σ_y and vertical σ_z dispersion parameters are needed as input to dispersion modeling of aircraft sources.

However, setting of initial plume parameters by default for various types of aircraft fleet in modeling systems recommended by ICAO Doc 9889 is not quite reasonable. Since mentioned parameters depend on aircraft and engine type, engine operation mode and meteorological conditions. To assess of **aircraft engine emissions contribution in LAQ assessment** it is important to take in mind some features, which define emission and dispersion parameters of the source.

The most important feature of the emission source under consideration is the presence of a exhaust gases jet, which can transport contaminants over rather large distances due to the high exhaust velocities and temperatures. The extent of such a distance is defined by the engine power setting and installation parameters, mode of the aircraft movement and the meteorological parameters. The aircraft is moving source with spatially and temporally changing of velocity, acceleration and direction of the aircraft movement within wide limits inside the territory of LAQ assessment. Since the most part of LTO cycle the aircraft is maneuvering on aerodrome surface (engine run-ups, taxiing, accelerating on the runway etc.), the ground significantly impacts on the structure and behavior (Coanda and buoyancy effect) of exhaust gases jet. Corjon A. (1997) found, that the primary vortices approach the ground leading to boundary layer formation (it is a subject to an adverse pressure gradient). The newly formed vorticity separates from the ground and consists a secondary vortex, which wraps around the primary one and induces an upward velocity and causes primary vortices rebound from the ground. During take-off and landing the wings of an aircraft produce lift which in turn generates powerful trailing vortices. The engine jets are entrained into the two counter-rotating wingtip vortices, with further deflection and stretching of the plume towards the vortex centerline [Cure S., 2007].

So, eliminating of fluid dynamic of jet from aircraft engine, the ground influence on the jet structure/ its behaviour and also process of interaction between the jet and wing trailing vortex in modelling systems may overestimate the height of buoyancy exhaust gases jet from aircraft engine, underestimate its length and radius of expansion, dispersion characteristics and contaminants concentration values. The revealed features of aircraft, as special source of air pollution, should be included in emission and dispersion calculations of airport air quality assessment.

COMPLEX MODEL POLEMICA

The complex PolEmiCa model was developed at the Ukrainian National Aviation University for the calculation of the inventory and dispersion parameters of the aircraft engine emissions during the LTO cycle of the aircraft in the airport area. It consists of the following basic components:

1. **engine emission model** – emission factor assessment for aircraft engines, including influence operation factors;

2. **jet transport model** – transportation of the pollutants by the jet from the aircraft engine exhaust;

3. **dispersion model** – dispersion of the pollutants in the atmosphere due to turbulent diffusion and wind transfer.

The basic equation of the PolEmiCa model for the definition of an instantaneous concentration from a moving source (from a single exhaust event) with preliminary transport on a distance X_A and rise on an altitude Δh_A and dilution σ_{0s} of pollutants by the jet is [Zaporozhets, Synylo 2005, 2015]:

$$c(x, y, z, t) = \frac{Q \exp \left[-\frac{(x-x')^2}{2\sigma_{x0}^2 + 4k_x t} - \frac{(y-y')^2}{2\sigma_{y0}^2 + 4k_y t} \right]}{\{8\pi^3 [\sigma_{x0}^2 + 2K_x t][\sigma_{y0}^2 + 2K_y t]\}^{1/2}} \times \left\{ \frac{\exp \left[-\frac{(z-z'-H)^2}{2\sigma_{z0}^2 + 4k_z t} \right] + \exp \left[-\frac{(z+z'+H)^2}{2\sigma_{z0}^2 + 4k_z t} \right]}{[\sigma_{z0}^2 + 2k_z t]^{1/2}} \right\} \quad (2)$$

The aircraft is considered as a moving emission source, thus current co-ordinates (x', y', z') of the emission source in movement during time t' are defined as:

$$x' = x_0 + u_{PL} \cdot t' + 0.5a_{PL} t'^2 + u_w \cdot (t + t') \quad (3) \quad y' = y_0 + v_{PL} t' + 0.5b_{PL} t'^2 \quad (4) \quad z' = z_0 + w_{PL} t' + 0.5c_{PL} t'^2 \quad (5)$$

where (x_0, y_0, z_0) are initial coordinates of the source; (u_{PL}, v_{PL}, w_{PL}) are velocity vector components of the emission source; (a, b, c) are acceleration vector components of the emission source; K_x, K_y, K_z are coefficients of atmospheric turbulence [Zaporozhets, Synylo 2005, 2015].

The **jet transport model** evaluates basic mechanisms of contaminants transportation and dilution by jet of exhausted gases from aircraft engine and provides basic parameters of the jet for further dispersion analysis, namely – height (Δh_A) and longitudinal coordinate (X_A) of buoyancy effect, length of jet penetration and final jet flux three-dimensional spreading $(\sigma_x; \sigma_y; \sigma_z)$, fig.1.

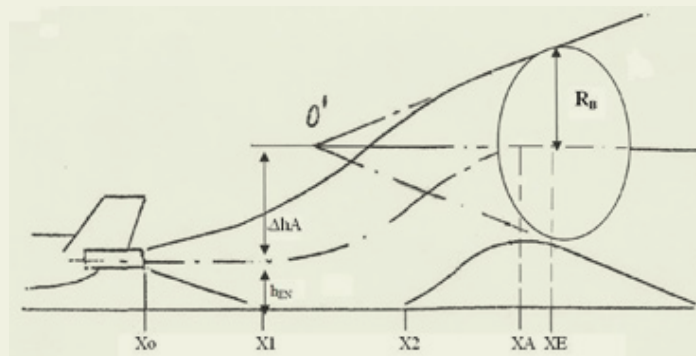


Fig. 1. Jet structure for jet transport model

$\Delta h_A, X_A$ – height and longitudinal coordinate of jet axis rise due to buoyancy effect, m; h_{EN} – height of engine installation, m; R_B – radius of jet expansion, m; X_1 – longitudinal coordinate of first contact point of jet with ground, m; X_2 – longitudinal coordinate of a point of jet lift-off from the ground due to buoyancy effect, m.

The process of contaminant transport by exhaust gases jet is described by the semi-empirical theory of turbulent jets [Abramovich G., 1960]. Buoyancy of a jet is caused by action of Archimedes forces due to excess of temperature of jet gases above air temperature, fig.1. The Archimedes number (δ) is used for the estimation of the plume rise height (7) [Zaporozhets et al., 2005]:

$$Ar_0 = g \cdot D_0 \cdot (Q_T - 1) / U_0^2 \quad (6) \quad \Delta h_A = 0.013 \cdot Ar_0 \cdot \overline{X_A^3} \cdot R_0 \quad (7)$$

where parameter $Q_T = T_0/T_H$ for engines currently in operation changes within the limits of 1.15- 2; $\overline{X_A}$ is the longitudinal coordinate of jet axis in relation to radius of engine exhaust nozzle, $R_0 = D_0/2$.

The complex model PolEmiCa has been sufficiently improved in subject of **jet transport model** by using CFD

package (Fluent 6.3) to investigate the physics and characteristics of ground vortices, which are generated between the ground surface and aircraft engine nozzle, to assess the ground surface impact on the jet flux structure, parameters and basic mechanisms of jet development. A three-dimensional model of a jet was generated in Fluent 6.3 by using Large Eddy Simulation (LES) method to reveal the unsteady ground vortices and turbulence characteristics of fluid flow, investigate transient parameters of hot gases in jet and their dispersion for further concentration evaluation.

The complex model PolEmiCa also has been improved in field of the jet interaction with wing trailing vortices during the take-off stage to assess the impact of wing vortices on the jet parameters (buoyancy height, horizontal and vertical deviation) and the contaminant dilution process. It was found, that wing trailing vortices effect causes the expansion of horizontal dispersions of jet and decrease of buoyancy effect height.

RESULTS AND DISCUSSIONS

Experimental studies at International Boryspol Airport (IBA) were focused on the measurement of NO_x concentrations in aircraft plumes, both the jet- and dispersion-regime of aircraft engines, under real operating conditions (taxi, landing, accelerating on the runway and take-off) [Synylo et al., 2016].

On the basis of the measured NO_x and CO₂ concentrations in the jet from aircraft engines, the EINO_x have been calculated under real operational conditions. The results of the measured NO_x concentrations in the plumes from aircraft engines for take-off conditions at IBA were used for the improvement and validation of the complex model PolEmiCa. Comparison of measured and modeled concentrations of NO_x was significantly improved by taking into account the determined EINO_x, see figure 2. The modeled concentrations included the impact of ground and wing trailing vortices on the jet parameters (buoyancy height, horizontal and vertical deviation).

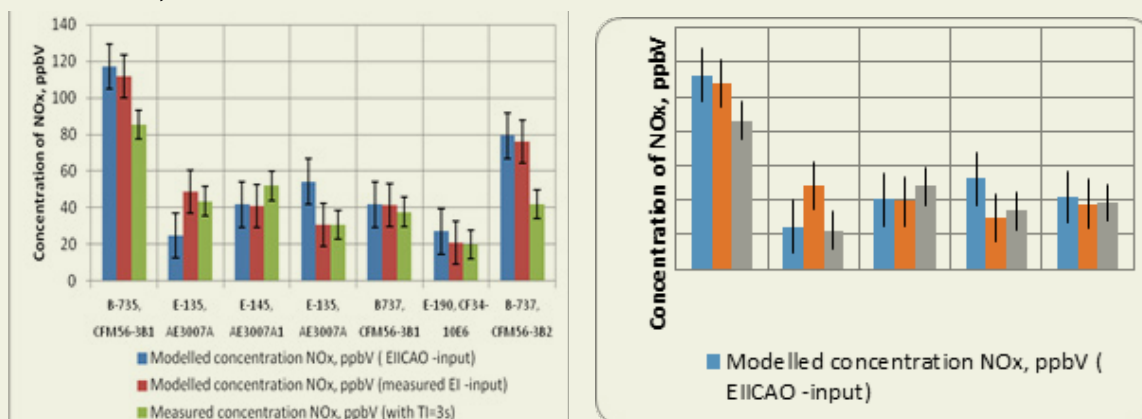


Fig.2. Comparison measured and modeled concentration of NO_x in the jet from aircraft engine at down station B (a – height of sample = 3.6 m) and up station B (b – height of sample = 5.7 m)

The measurement systems applied in the field campaigns allowed the determination of EI, e.g. for NO_x under real operating conditions and to improve the emission inventory of aircraft engines for further modeling tasks. Such an approach has been proven to be successful at Boryspol airport.

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MODELING AIRPORT AIR QUALITY AT HIGH RESOLUTION

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Abstract. In this study, a new approach to study the impact of air traffic on air quality is proposed. The pollutants concentrations are calculated at 10 m resolution using a Large Eddy Simulation (LES) model in order to identify the most affected areas of an airport platform. A day of air traffic on a regional airport is simulated, using real data as aircraft trajectories from radar streams and observed meteorology, NO_x, O₃ and PM₁₀ data. In order to estimate the aircraft emissions the Air Transport Systems Evaluation Infrastructure (IESTA) is used. IESTA is coupled with the non-hydrostatic meso-scale atmospheric model Meso-NH using grid-nesting with 3 domains and LES capabilities. The detailed cartography of the airport distinguishes between grassland, parking and terminals, allowing to compute exchanges of heat, water and momentum between the different types of surfaces and the atmosphere as well as the interactions with the buildings using a drag force. The dynamic parameters like wind, temperature, turbulent kinetic energy and pollutants concentrations are computed at 10 m resolution over the 2 x 4 km airport domain. The pollutants are considered in this preliminary study as passive tracers, without chemical reactions.

Keywords: Airport, air quality, local scale

INTRODUCTION

The airport air quality is a major concern for both neighbourhood and airport users (workers or travellers). This issue is becoming more and more important with the increase of the air traffic and airport activities. These impacts have been studied previously using Chemistry and Transport Models (CTM) by Arunachalam et al. (2011) or Rissman et al. (2013). The aim of these studies was to assess the impact of aviation at the regional scale; they usually concluded that airports are secondary contributors after the other sources of pollutants as road traffic or industries. At the local scale, several tools are used as Gaussian or Lagrangian models (ADMS, EDMS, LASPORT) giving the pollutants concentration as a response to an analytical equation. While those models perform well for mean annual budget and for stable or neutral boundary layers conditions, they don't allow a precise representation of spatiotemporal heterogeneity of the airport concentration. Moreover, most of the time, the emissions of the aircraft are simply simulated as Landing Take-Off (LTO) cycles (Peace et al., 2008; Farias et al., 2006).

A new approach to study the impact of air traffic on air quality at the local scale is proposed here. In fact, a simulation is performed at very high spatiotemporal resolution using an Air Traffic System model (IESTA) coupled with a meteorological model (Meso-NH). This paper describes how the IESTA-Meso-NH coupling enables to calculate the pollutants concentration at 10 m resolution in order to identify the most affected areas of an airport platform during a real day of intense traffic.

MODELS DESCRIPTION

Air Traffic System model: IESTA

In order to estimate the aircraft emissions, the Air Transport Systems Evaluation Infrastructure (IESTA) is used (Aubry et al., 2010, Sarrat et al., 2012). IESTA is a set of numerical models dedicated to the design and modelling of innovative air transport systems and their evaluation, in particular for environmental impacts (noise, fuel consumption, emissions and air quality). From the observed radar aircraft trajectories, the meteorological conditions and the aircraft performances, IESTA simulates the air traffic system, i.e. the aircraft and engines state vectors, allowing to compute thrust, fuel flow and emissions at 10 m resolution and with one second time step. In fact, the Aircraft module of IESTA is able to closely follow the real 4D (spatiotemporal) aircraft trajectories given the aircraft types, using the total energy equations of flight mechanics. It generates a complete state vector for each of the simulation time steps, including the engines required thrust. In this study, the Engine module is not used with the full thermodynamic modelling for each engine, because of a too large number of aircraft to simulate (824 engines a day). Instead, taking the thrust, aircraft speed and weather parameters as input, several methods are used to compute pollutants emissions

indices: for turbofans, ICAO Engine Emissions Databank interpolations; for turboprops, FOI database. Thus, fuel consumption and emission indices are computed for different species (NO_x, SO₂, VOC, CO, CO₂) at every point of each engine trajectory.

Meteorological model: Meso-NH

IESTA is coupled off-line with the non-hydrostatic meso-scale atmospheric model Meso-NH using grid nesting with 3 domains and Large Eddy Simulation (LES) capabilities. The detailed cartography of the airport distinguishes between grassland, parking and building, allowing to compute exchanges of heat, water and momentum between the different types of surfaces and the atmosphere as well as the interactions with the building using a drag force (Aumond et al., 2013). The dynamic parameters like wind, temperature, turbulent kinetic energy and pollutants concentrations are computed at 10 m resolution over the 2 x 4 km airport domain. The pollutants are considered in this preliminary study as passive tracers, without chemical reactions.

MODELS SET-UP

Building the emissions database

In order to compute the emissions database based on real observed data, the aircraft radar streams recorded on September 10th, 2010 are analyzed in order to correct and complete the trajectories.

About 400 aircraft trajectories and 824 engines state vectors are computed from the radar data. Another methodology is applied for few exceptions such as the piston engines aircraft, which are not yet implemented in IESTA; some engines used in the traffic are not ICAO-certified or listed in the FOI tables. For that kind of engines, the corresponding trajectories are, for the most part, allocated to equivalent aircraft, or simply ignored if their contribution is deemed negligible.

Aircraft emissions of these 824 engines are computed using the interpolation in the ICAO tables rather than using the IESTA thermodynamic model because of a large variety of engines types. The emissions of NO_x, CO, CO₂, SO₂ and smoke number are computed at a one second time step. As the available data don't include aircraft APU emissions, the ICAO/CAEP Airport Air Quality Manual (ICAO, 2011) is used to allocate APU emissions to realistic areas and periods. This manual states that an accepted modelling for short-haul aircraft is an APU operating during 45 min and emitting a total of 700 g NO_x, 30 g UHCs, 310 g CO and 25 g PM₁₀.

As expected, the NO_x emissions are the highest near the runway, where the aircraft take off, but also near the parking at the gates as shown in Figure 1.

The emissions from other sources than aircraft are provided by a 1 km resolution database, used in the two largest domains.

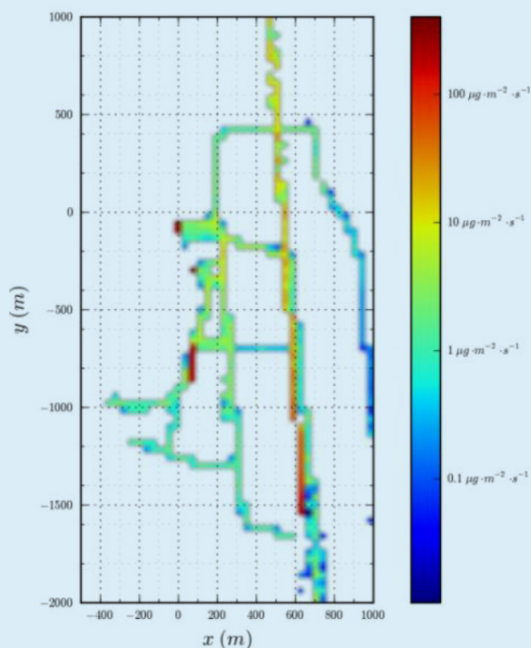


Figure 1: Surface flux of NO_x emissions ($\mu\text{g}/\text{m}^2/\text{s}$) on September 10th, 2010

Initialization and land surface data of Meso-NH

The meteorological variables are initialised by the French weather forecast model analysis AROME at 2 km resolution, at 6:00 UTC. They are also forced by AROME at the large scale boundaries every three hours. In fact, AROME provides the initialisation and forcing for the dynamic variables (wind, potential temperature, humidity, etc.) as well as for the land surface variables (ground water content, surface temperature...).

For the passive tracers, like NO_x, the initial conditions are given by the observations made at a station a few kilometres upstream the airport. A zero gradient condition is applied at the large scale boundaries.

Three domains of simulation (Figure 2) are built, in nesting two ways, allowing the downscaling from the large scale boundaries conditions to a Large Eddy Simulation (LES) model at 10 m resolution.

The land surface parameters are key data for high resolution modelling of the Atmospheric Boundary Layer (ABL). Meso-NH computes surface fluxes for each type of cover according to the characteristics of each tile (albedo, roughness, texture, urbanization, nature, etc). The land surface covers of both larger domains are given by the Ecoclimap database derived from the CORINE Land Cover 2000 data (Faroux et al., 2013). The smallest domain represents the airport area itself, with a 10 m resolution and 3×4.5 km width. The surface occupation data come from the OpenStreetMap (OSM) database, which have been converted to the Meso-NH types of land cover. The three main covers as shown on Figure 2c are the parking and roads, the nature (grassland and crops) and the buildings (terminals, train station, hangars...) where a drag force is applied according to Aumond et al., 2013 and Bergot et al., 2016.

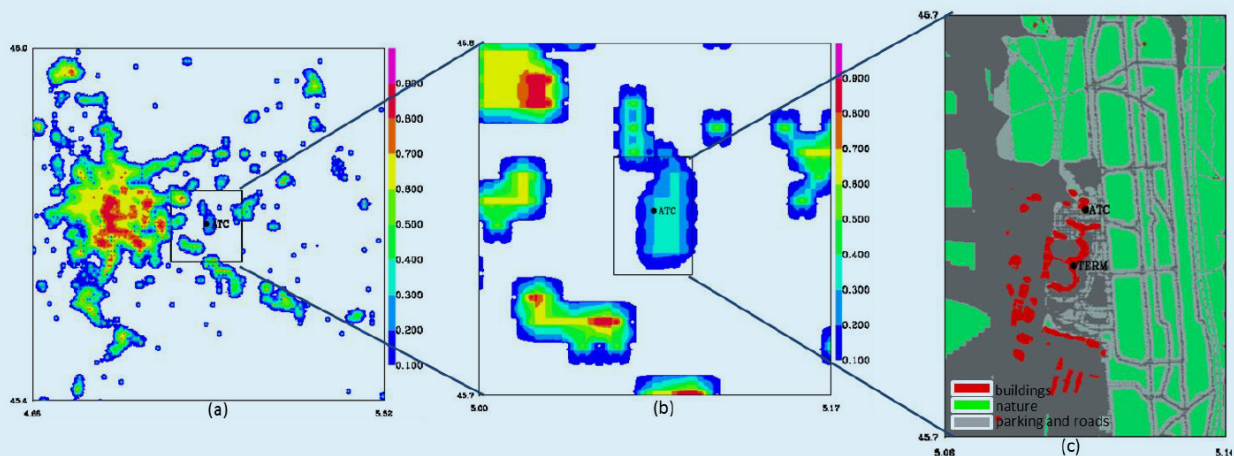


Figure 2: 3 domains of simulation in grid-nesting two ways: (a) 250 m resolution, width=67.5×67.5 km; (b) 50 m resolution, width=13.5×13.5 km; (c) 10 m resolution, width=3×4.5 km

RESULTS

Dynamic situation

The simulation starts at 6:00 UTC on September 10th and runs for 1000 seconds only, because of a very high CPU consumption. In fact, the simulation is run on a supercomputer using 240 multi-core processors. This period represents the maximum of aircraft traffic.

For this day, the weather conditions are good, with high radiation, and increasing temperatures. The wind is low less than 2 m/s from north-west, as shown in Figure 3, in good agreement with the observations (not shown here).

The Turbulent Kinetic Energy (TKE) as well as temperature and wind are impacted by the surface land cover. In fact, buildings have a strong impact: they increase TKE and temperature, the decrease upstream wind, thanks to the drag force applied. The local boundary layer and the vertical mixing are consequently enhanced near the buildings.

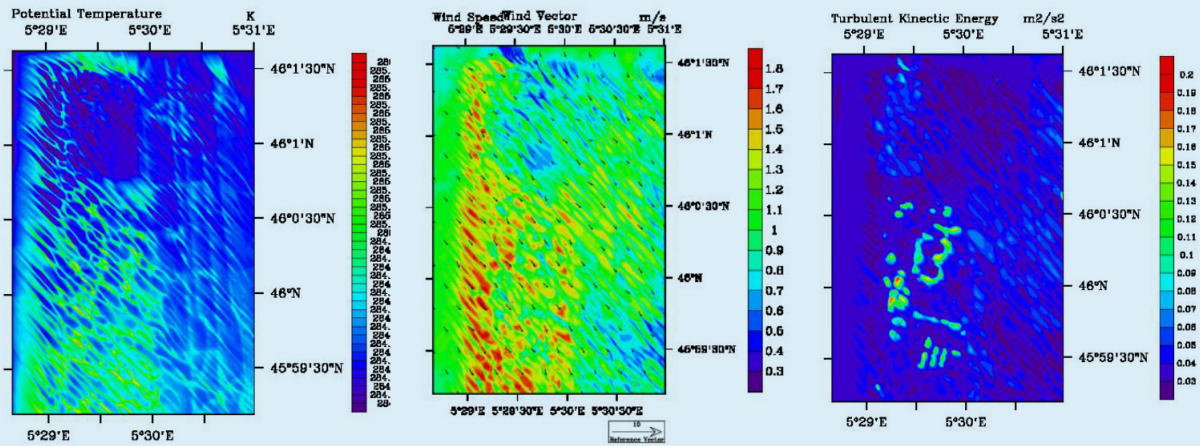


Figure 3: Dynamic situation of the day: (a) Potential Temperature near the ground; (b) Wind module and direction; (c) Turbulent Kinetic Energy

NOx dispersion

As shown in Figure 4, NOx concentrations over the small domain of simulation (10 m resolution) are quite high next to the northern boundary, due to the advection of pollutants from the larger domain and to the road traffic emissions. In fact, the wind from North-North-West, even low, brings a plume with high level of NOx (Figure 4a). The airport itself seems affected by NOx concentration around 50 ppbv, right next to the terminals and parking, where aircraft's engines and APU are operated longer (Figure 4b shows the fraction of buildings, parking or roads together with NOx concentrations)

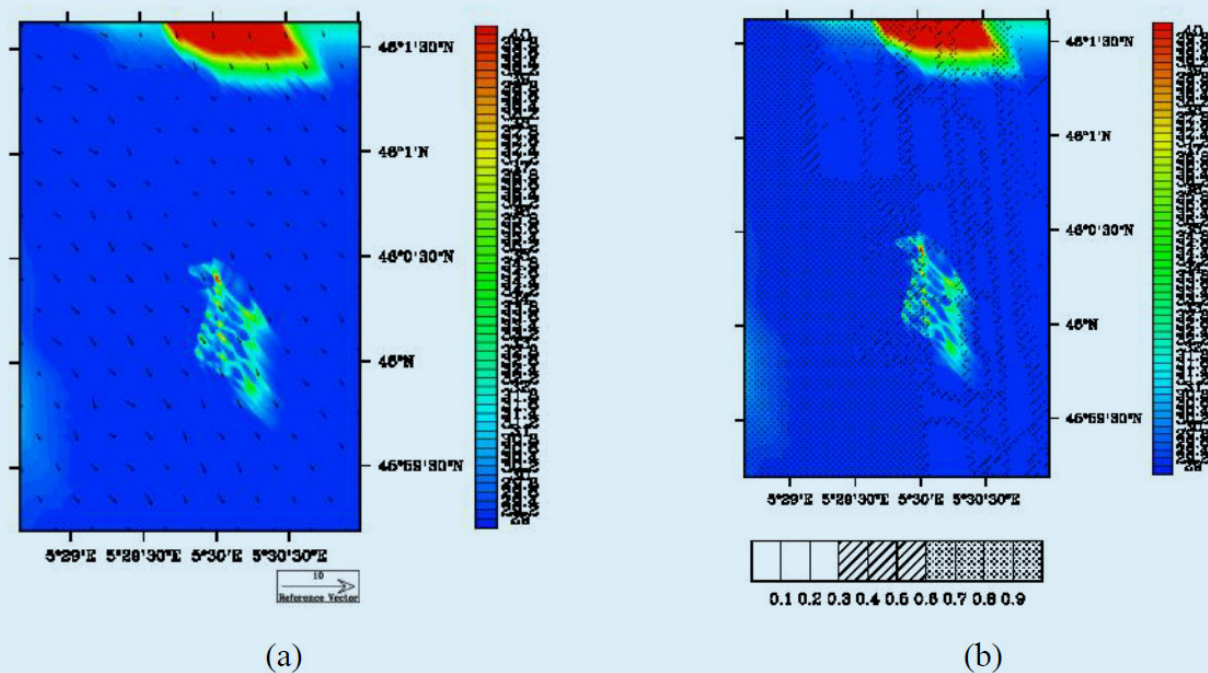


Figure 4: NOx concentration (ppbv) at the first level of the model, i.e. 2m height above ground with (a) wind direction and (b) urban fraction cover

CONCLUSION

A real day of air traffic over a regional airport is simulated using the coupling of two state-of-the-art models: IESTA, modeling the aircraft trajectories and engines emissions and Meso-NH, modeling the atmospheric dispersion at 10 m horizontal resolution. In this preliminary study, the NOx are

considered as passive tracers and the simulation lasts only 1000 s. The coupling of the two models demonstrates the ability to satisfactorily represent not only the emissions (engines, APU), but also the NOx peaks due to northern advection and emissions from both terminals' parking and taxiing area. Moreover, the meteorological dynamic (low winds and buildings interactions) provides innovative approach to airport

air quality studies at high spatio-temporal resolution..

The next step for this study is first to continue the simulation along the day, in order to determine the evolution of the concentrations in and around the airport. Secondly, the reactive chemistry with photochemistry and ozone-VOC interaction should be added to simulate more realistic behavior. These improvements need a lot of computing time with supercomputers but will be done in the coming few months.

ACKNOWLEDGEMENTS

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THE AIRCRAFT EMISSIONS MODEL: FUTURE AVIATION SCENARIO TOOL (FAST)

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Abstract. Investigations into the environmental impacts from aircraft emissions on global climate generally involve research communities (engineers, experimentalists and scientists), policy makers (government and regulatory bodies), aircraft and engine manufacturers and stakeholders (air navigation service providers, airports, and airlines). These communities work collaboratively, seeking solutions for an environmentally sustainable aviation industry. Software infrastructure plays a core and fundamental role in environmental impact studies, since global assessments cannot be directly measured but rather need to be modelled from empirical data. Models are needed to assess the impacts, inform policy makers and evaluate mitigation strategies. The software tool central to these activities are the aircraft emissions models. In this paper, we present the aircraft emissions model, FAST (the Future Aviation Scenario Tool). FAST, is one of only three emissions models that have been approved by the International Civil Aviation Organization (ICAO) Committee on Aviation Environmental Protection (CAEP) for aircraft greenhouse gas modelling. It is a modular software system that can be used to produce 3D gridded emissions of carbon dioxide (CO₂), nitrogen oxides (NO_x), non-volatile particulates (nvPM) and distances, over various temporal resolutions. FAST uses aircraft-engine specific fuel flow data calculated by the aircraft performance software, PIANO; coupled with emissions indices to generate an emissions profile for a specific aircraft payload, cruise altitude and mission distance. These profiles are applied to route specific information (frequency and distance) to determine the global emissions. Finally, we will present case studies on how these emissions have been used in impact models to estimate their climate burden.

Keywords: aircraft emissions models, CO₂, NO_x, nvPM

INTRODUCTION

Aircraft engines emit a variety of chemical species, which includes carbon dioxide (CO₂), nitrogen oxides (NO_x), water vapour and particulates. These emissions can directly affect climate, or indirectly by altering atmospheric concentrations (e.g. ozone) and trigger cloud formation (contrails, contrail-cirrus and soot-cirrus). In this paper, we present the aircraft emissions model, FAST (the Future Aviation Scenario Tool). We will present case studies on how these emissions have been used in different applications.

AIRCRAFT EMISSIONS MODEL: FAST

FAST, is one of only three emissions models that have been approved by the International Civil Aviation Organization (ICAO) Committee on Aviation Environmental Protection (CAEP) for aircraft greenhouse gas modelling. It is a modular software system that can be used to produce 3D gridded emissions of CO₂, NO_x, nvPM and distances, over various temporal resolutions. The basic structure of the FAST aircraft emissions model is illustrated in Figure 1 (left panel). FAST uses aircraft-engine specific fuel flow data calculated by the aircraft performance software, PIANO; coupled with emissions indices to generate an emissions profile for a specific aircraft payload, cruise altitude and mission distance. The emissions indices, including the various speciation could be derived from ground measurements or when possible, in-service tests. The emission profiles are applied to route specific information (frequency and distance) to determine the 3D global emissions, across temporal resolutions. Atmospheric and climate scientists then use the FAST emissions in impact models to estimate their environmental burden. The linkages between FAST and other climate impact models are illustrated in Figure 1 (right panel).

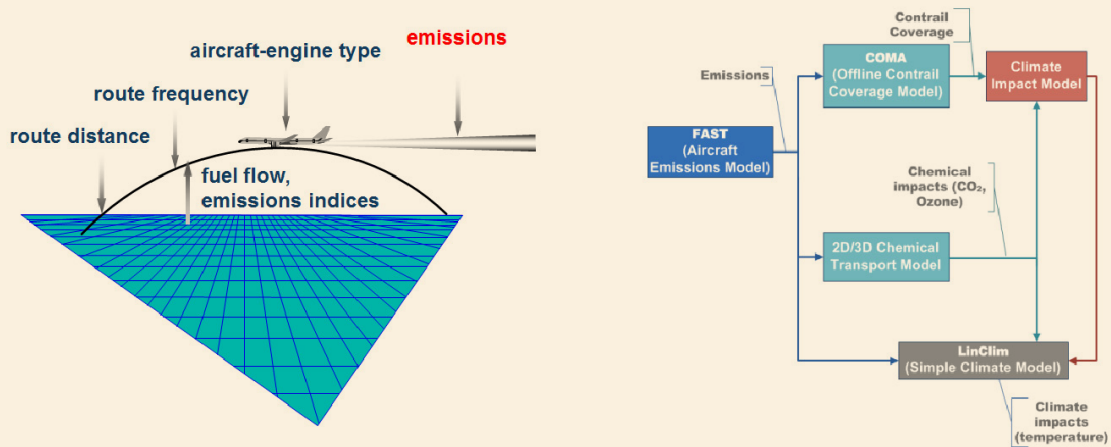


Figure 1. Basic structure of the aircraft emissions model, FAST (left panel) and linkages between FAST and other climate impacts model (right panel).

CASE STUDIES

Over the years, the FAST model has been used in ICAO-CAEP activities such as CAEP trends analysis, CO₂ Standard Stringency assessment and Market-Based Measures (MBMs). It has also been applied in several research projects and these provided an outlook on the spatial and vertical distributions of present day and future aviation emissions, including aviation contribution to total anthropogenic emissions. Example outputs from past projects are presented in Figure 2 (EU FP6 Integrated Project QUANTIFY), Figure 3 (EU Framework 7 Project REACT4C) and Figure 4 (EU Framework 7 Project TEAM_Play).

EU FP6 INTEGRATED PROJECT QUANTIFY

QUANTIFY (Quantifying the Climate Impact of Global and European Transport Systems) is the EU FP6 Integrated Project with the objective of quantifying the impact of air, sea and land transport on global climate. The 4D global aircraft emissions (CO₂, NO_x, particulates and distance travelled) were estimated for the year 2000 by FAST. The base year movements and emissions were used as baseline for projections to the year 2020, 2050 and 2100. A selection of these results are illustrated in Figure 2.

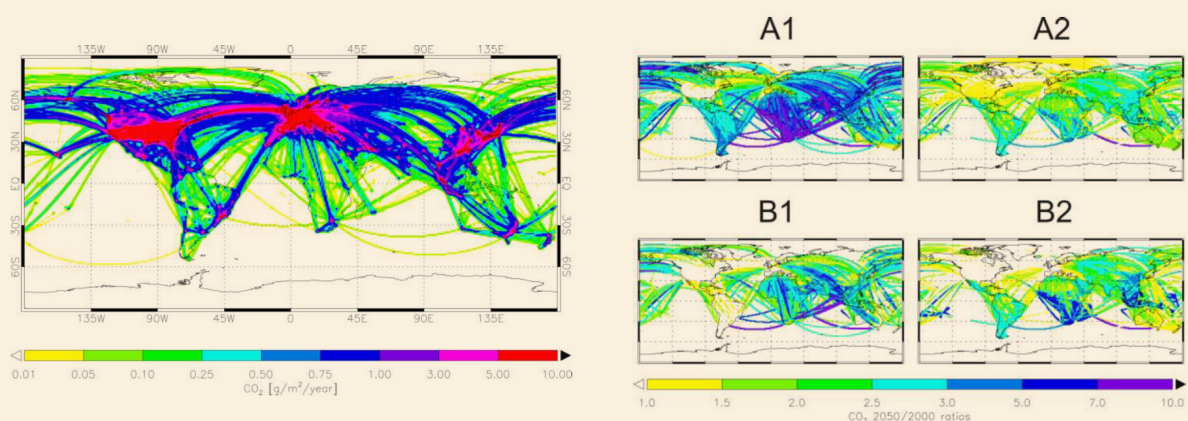


Figure 2. CO₂ aviation emissions in 2000 (left panel) and CO₂ 2050/2000 ratios in IPCC SRES A1, A2, B1 and B2 emission storylines (right panel) from EU FP6 QUANTIFY (Owen et al., 2010).

EU FP7 PROJECT REACT4C

REACT4C (Reducing emissions from aviation by changing trajectories for the benefit of climate) is the EU FP7 Project with the objective of investigating the potential of climate-optimised flight routing as a strategy to reduce the aviation sector's impact on the atmosphere. In this project, FAST was used to generate a 4D global aircraft emissions similar to QUANTIFY, but for the year 2006 and with more representative aircraft types. The 2006 movements and emissions were then used as baseline for a sensitivity analysis, whereby the cruise altitudes were shifted higher and lower by 2,000 ft or one flight level. A sample of the baseline results is illustrated in Figure 3.

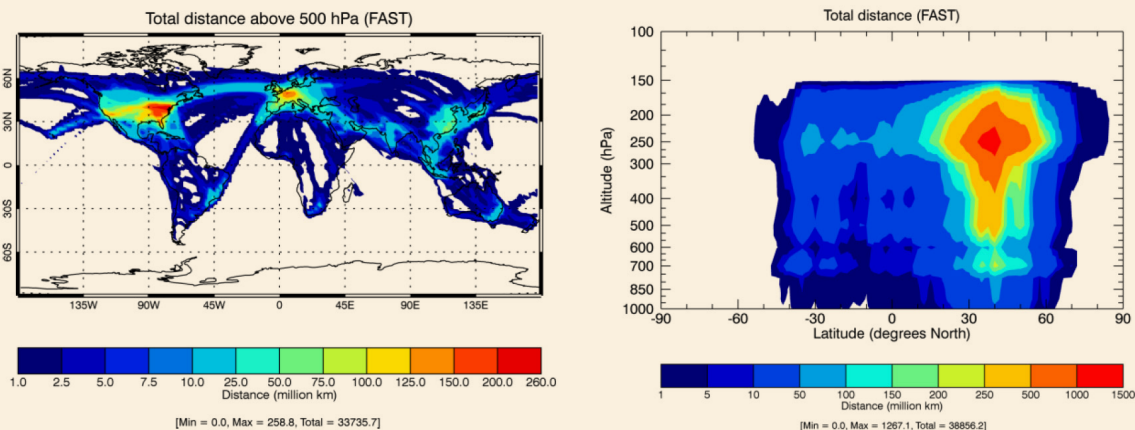


Figure 3. Total distance travelled in the regions where contrails may form (left panel) and distance travelled profile (right panel) for 2006 from the EU FP7 project REACT4C.

EU FP7 PROJECT TEAM_PLAY

TEAM_Play (Tool Suite for Environmental and Economic Aviation Modelling for Policy Analysis) is the EU FP7 Project with the objective of setting up a working tool suite that could be used for policy assessment and strengthening the European modelling capability, and hence ensuring a sustainable growth for the air transport industry when it comes to environmental, social and economic issues. In this project, FAST was used to generate the global aircraft emissions for the year 2006, 2026 and 2050. These global results were used in two experiments by two simple climate models; the first is a pulse emission experiment with the pulse being the 2026 and 2050 CO₂ emissions; and the second a transient experiment where the aircraft and background emissions were assumed to evolve over time. A sample fuel trend from 1940 to 2050 for aviation emissions is illustrated in Figure 4 (left panel) and the resulting CO₂ and non-CO₂ radiative forcing estimates from the simple climate model, LinClim, is depicted in Figure 4 (right panel).

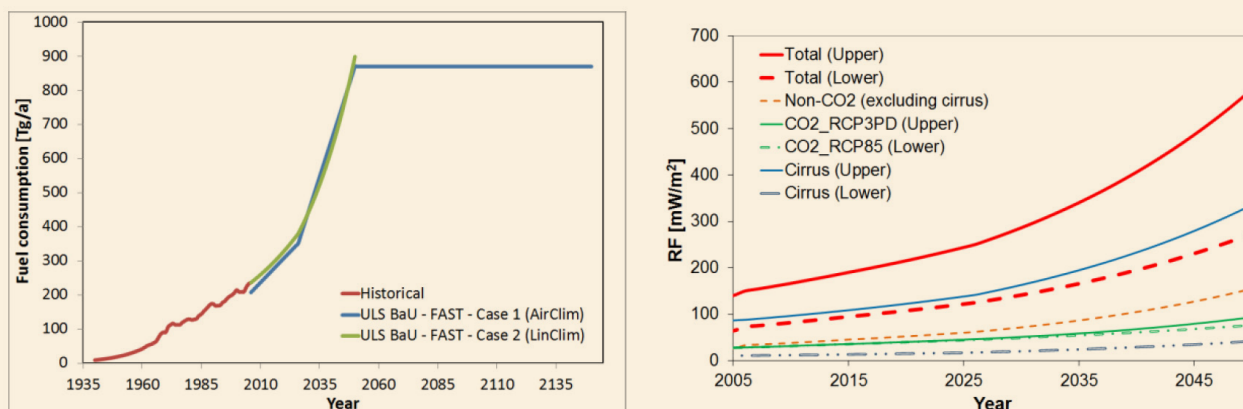


Figure 4. Total annual fuel consumption [Tg/a] from 1940–2005 (Lee et al., 2009) and 2006–2150 for FAST (left panel) and selected RF results from LinClim simulations with FAST input (right panel) from the EU FP7 project TEAM_Play.

SUMMARY

Case studies presented in this paper show the capability of FAST as a modular software that has the capability and robustness to produce output for different applications. It has been validated and verified by the international aviation community and provided diversity to aircraft emissions modelling. It has been used to support studies into the quantification and mitigation of aviation impacts on climate change, taking into account technological and operational options and policy instruments.

ACKNOWLEDGEMENTS

The FAST model development and maintenance is supported by the UK Department for Transport. The case studies presented were funded by: QUANTIFY (EU FP6 Contract No: 003893), REACT4C (EU FP7 ACP8-GA-2009-233772) and (EU FP7 FP7-(AAT)-2010-RTD-1, Project No: 266465).

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AN INTEGRATED MODELLING APPROACH FOR CLIMATE IMPACT ASSESSMENTS IN THE FUTURE AIR TRANSPORTATION SYSTEM – FINDINGS FROM THE WECARE PROJECT

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Abstract. In order to assess the climate impact of technological and operational measures which are introduced to the future air transportation system, the future evolution of the air transportation system must be modelled and analyzed. Within the DLR-project WeCare a modular assessment framework is implemented, which accompanies a 4-layer philosophy for a generic build-up of the passenger air traffic system of the future (Part 1). The four layers consist of the origin-destination passenger demand network, the passenger routes network, the aircraft movements network, and the trajectories network. Due to the global network layer modelling architecture on city pair level, information like how many passengers will travel between certain city-pairs, the (future) routes chosen by the passengers as well as how many aircraft and which size of aircraft will be operated on each route can be provided. Finally, information about the amount, locus and time of emissions can be computed and transferred to climate models for calculating the climate impact. In WeCare, also mitigation strategies by optimizing trajectories are designed and evaluated (Part 2). Mitigation potentials of these less climate-harming trajectories need to be applied on Air Transportation System (ATS) quantity structures and timing to assess cumulative climate impact savable over time.

Keywords: air transportation system, climate impact assessment, evaluation of climate mitigation strategies, scenarios, forecasting, emission inventories

PART 1: SCENARIOS, THE GENERIC BUILD-UP OF THE FUTURE ATS & CLIMATE IMPACT ASSESSMENT

Since the climate impact of aviation highly depends on the amount, species, altitude and latitude of emissions (Koch, 2011) (IPCC, 2013), pure passenger aircraft fleet models with no geo-spatial dimension are not sufficient to assess the global climate impact of aviation. Instead, the spatial distribution of flights is relevant to assess the climate impact of the ATS and the evaluation of potential mitigation strategies and revolutionary new concepts (technological and operational).

A basic research goal of DLR Air Transportation Systems is to explore future evolutions of the global civil ATS. Understanding and modelling the ATS in a comprehensive way is a prerequisite of developing "decision scenarios" (Wack, 1985). To estimate the future realized air passenger demand (APD) on city pair level, not only the assumptions on external socio-economic conditions (e.g. gross domestic product (GDP), population, GDP per capita, ...) are relevant. Likewise, the *internal* scenario concerning the ATS, e.g. how the ATS is changing over time with the introduction of new technologies or new operational concepts has a non-neglectable feedback on realized demand. Realized demand is for example a function of airfares which in turn are depended on cost structures. Cost structures might be changed with the introduction of new technologies and operational measures and thus will have an impact on realized demand.

The ATS is abstracted in four main layers to enable a simulation of alterations in any layer. Network-stakeholder-interactions differ layer by layer. Quantitative decision scenarios may be developed by manipulating systematically and pointedly specific scenario factors and parameters within the model environment according to a well-designed scenario narrative. (Schwartz, 2012) A major focus needs to be the fusion of global ATS network forecasting on city pair level, a fleet renewal model and the discipline of aircraft design to enhance the overall quantitative scenario capability on ATS level. (Ghosh et al., 2015b)

THE 4-LAYER PHILOSOPHY AND THE WECARE PROJECT

The DLR-project WeCare made a big progress towards developing and implementing the idea of modelling the future ATS on a network basis. The WeCare project is about assessing climate mitigating effects of operational and technological changes which are also investigated in the context of the future ATS on a global scale with a time horizon until 2050. Therefore, at first, a generic model forecasting future air traffic on network and fleet basis is required. This is implemented in the model chain called AIRCAST (air travel forecast) based on the 4-layer philosophy (Figure 1).

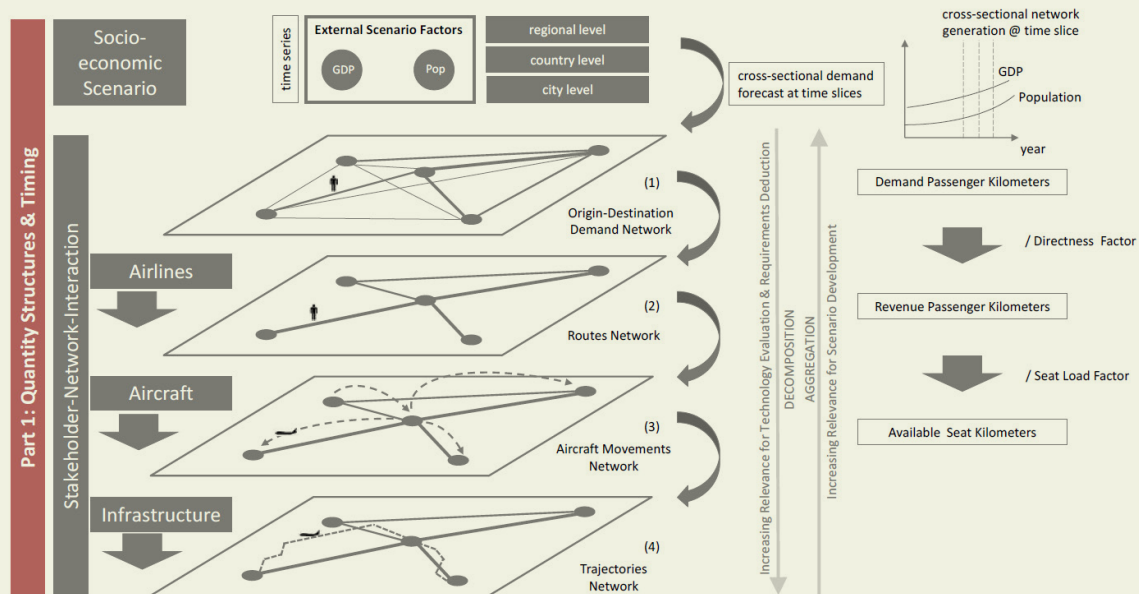


Figure 1. Generic build-up of the future ATS in 4 layers (Ghosh et al. 2015a)

AIRCAST focuses on the structural evolution of global air passenger and aircraft networks abstracted in four main layers. The four layers (see Figure 1) consist of (1) the origin-destination passenger demand network, (2) the passenger routes network, (3) the aircraft movements (ACM) network, and (4) the trajectories network. Each lower layer is derived from the above layer. AIRCAST is used for climate impact assessment and strategy development within the WeCare project. Next, we describe the single layers and the initial starting point of socio-economic scenarios.

EXOGENOUS SOCIO-ECONOMIC SCENARIOS

AIRCAST initializes ATS-networks directly from exogenous socio-economic scenarios. It is designed and planned to use the forecast published by Jorgen Randers "2052" (Randers, 2012) and the five scenarios of the International Futures Global Modeling System (IFs) (Hughes et al., 2006) likewise. In WeCare, the complete run of the modules and experimentation was based on the Randers scenario as a use case. For the time being, it is an alternative aviation scenario which considers worldwide saturation effects of economic growth.

DEMAND NETWORK

Global demand networks are calculated in a two-step approach: (1) topology forecast and (2) forecast of the number of passengers on an edge of the graph. (Terekhov et al., 2015a) (Terekhov et al., 2015b) Elasticities of GDP and airfare on realized air passenger demand are globally analyzed using *Sabre Airport Data Intelligence* (ADI) and *World Bank* data. These are important links between changes of economic wealth (via GDP) and changes through energy cost development and environmental policy measures (via cost and airfare) to demand prediction.

Routes Network

The passenger routes for each demand connection defined in the previous layer are modelled in four steps (Ghosh et al., 2015b):

- Defining plausible passenger routes considering the main transit hubs worldwide and maximum detour factors
- Calculating route probabilities from historical data based on segment probabilities to account for new demand connections
- Allocating the predicted amount of passengers on a demand connection to passenger routes according to the computed probabilities
- Aggregating passengers on the same segment worldwide to get a segment passenger network

The routes network consists of two sublayers: (1) the passenger route network and (2) the passenger segment network. A passenger route from true origin to true destination from a passenger perspective consists of a sequence of flight segments via transfer airports.

AIRCRAFT MOVEMENTS NETWORK

The deduction of aircraft movements is based on the passenger segment network from the previous layer. The frequency-capacity-model FoAM (Forecast of Aircraft Movements) (Kölker et al., 2014) is used to compute aircraft movements on each flight segment worldwide distinguished by seat categories. In a subsequent step, this output is linked to fleet renewal modelling to incorporate the scenario capability of introducing new aircraft concepts into the world fleet. This way, we account for the inertia of the system and transition in technology when creating scenarios as ATS-network evolutions. The aircraft movements network consists of two sublayers: (1) the aircraft movements network by seat categories and (2) the aircraft movements network by aircraft type and aircraft generation.

EMISSION INVENTORIES & TRAJECTORIES NETWORK

The final step in the chain constitutes a simulation of trajectories based on the aircraft movements obtained from the Aircraft Movements Network layer using the Global Air Traffic Emissions Distribution Laboratory (GRIDLAB) developed by DLR. (Linke, 2016) Each mission defined by departure and arrival cities, aircraft type and load factor is simulated under typical operational conditions or by applying new operational strategies, resulting in a network of flight trajectories. For this purpose, DLR's Trajectory Calculation Module (TCM) (Lühns et al., 2014) and Trajectory Optimization Module (TOM) (Lühns et al., 2016) apply simplified equations of motion known as the Total Energy Model in combination with the Base of Aircraft Data (BADA) version 4.1 aircraft performance models by EUROCONTROL (Mouillet, 2013). Based on the aircraft's engine state (e.g. thrust, fuel flow) the engine emission distribution of NO_x, CO and HC species along the trajectory is determined applying the Boeing Fuel Flow Method 2. (DuBois et al., 2006) The amount of CO₂ and H₂O is calculated assuming a linear relationship to the fuel burn. The emission distributions of all flights are mapped into a geographical grid resulting in 3D inventories. These are the essential input for the climate impact assessment tool AirClim (Dahlmann et al., 2016), which determines concentration changes of different radiative forcing agents (CO₂, H₂O, O₃) as well as aviation-induced cloudiness. Based on that, various climate metrics for the given emission scenario can be calculated. This is essential to assess the introduction of new aircraft concepts and operational measures and to simulate the climate impact of a heterogeneous fleet and its evolution over time.

The Trajectories Network can also be used as a basis for models which need that information of energy consumption and flight time on a city pair network level discriminated by aircraft type (specific and generic ones) and aircraft generation (N, N+1, N+2, ...) for future time slices, i.e. future scenarios of ATS network evolutions (see Figure 2).

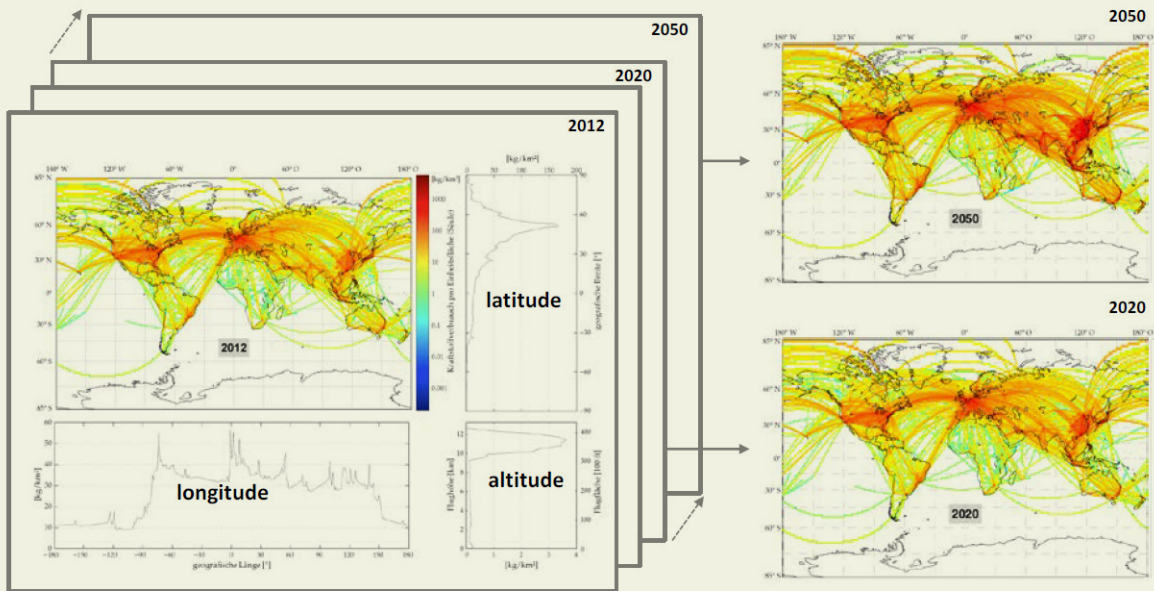


Figure 2. Final result for climate impact assessment as a global scenario capability: spatial distributions of fuel burn and respective 3D emission inventories for future time steps until 2050 according to global developments of the ATS (passenger flows and aircraft movements)

PART 2: FROM POTENTIALS TO SCENARIOS

In other work packages of WeCare various mitigation strategies by optimizing trajectories tactically or strategically have been designed and/or evaluated, e.g. the mitigation potentials of climate-optimized trajectories (Lührs et al., 2016) (see Figure 3) and climate-restricted airspaces (Niklaß et al., 2016).

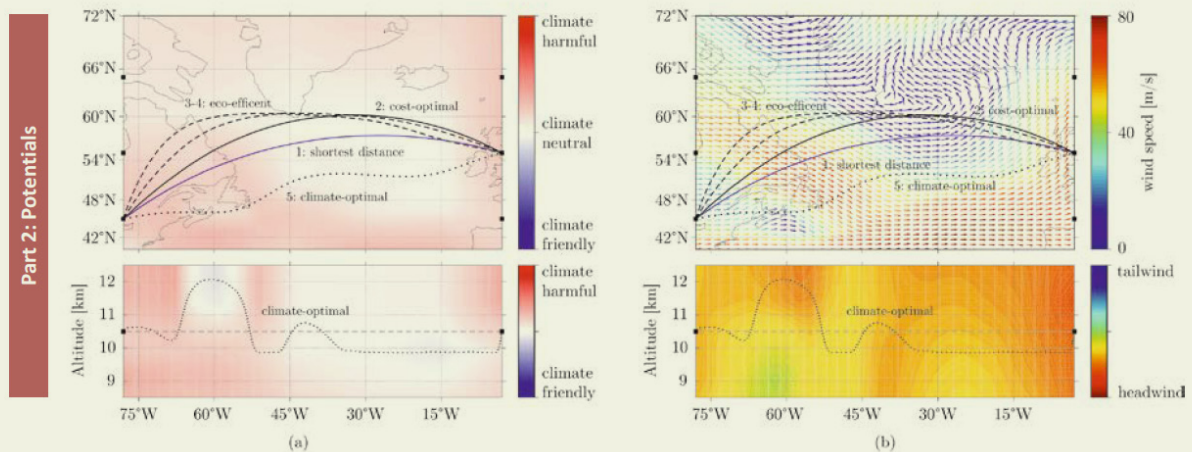


Figure 3. Trajectory optimization: comparison of shortest distance (1), cost-optimal (2), eco-efficient (3-4) and climate-optimal trajectories (5) plotted in (a) total climate change functions and (b) respective wind speeds and directions (Lührs et al., 2016)

Identified potentials of technological and operational mitigation strategies need therefore in a next step to be incorporated into larger scope systems analyses. This can be done with a system like the AIRCAST environment. AIRCAST provides absolute amounts of aircraft movements over time on which a mitigation potential of a specific concept or a set of concepts may be applied with certain times of introduction in the future. Only that way, the *cumulative* climate impact saved compared to a business-as-usual scenario may be quantified and put into perspective to global climate goals.

CONCLUSION

The starting points of modelling the future air transportation system in AIRCAST are exogenous socio-economic scenarios. From those, we develop scenarios of network evolutions. In a first iteration all networks (4 layers) in predefined time steps (in WeCare every five years) until the time horizon are forecasted without applying any future alteration to the system. After that, a scenario of the introduction of new aircraft programs over all seat categories and the introduction of operational measures that should be evaluated needs to be defined until 2050 with all relevant assumptions concerning alterations of cost of operation and quality of travel (Kölker et al., 2015). Especially modelling the feedback of such changes from the supply side of the ATS on the forecast of realized demand and the iterative calculation of all networks is expected to give valuable quantitative insights in the connection between intentional alterations, e.g. to achieve climate targets, and unintended feedbacks of those decisions on the evolution of networks. Modelling future global network evolutions is a means to quantify future shifts in portions of deployed seat categories, shifts of distances flown by seat categories and the geographical shift of aircraft movements induced through heterogeneous air traffic growth by world regions. The scientific value added originates from the consistent modelling of future global ATS networks on city pair level throughout all layers – being global and local at the same time.

Design of mitigation strategies and analyses of their mitigation potentials (Part 2, Figure 3) need to be coupled with modelling of quantity structures and timing of ATS dimensions (Part 1, Figure 1) in order to estimate the absolute cumulative climate impact savable over time.

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POSTER PRESENTATIONS

NO STEP

PP01: COST-EFFECTIVE AND SUSTAINABLE DECARBONIZATION OF AVIATION FUELS

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Abstract. Jet biofuels are becoming a prominent source of aviation energy, especially since their production process ensures sustainability and economic growth. An alternative approach for enabling an extended increase of biomass utilization for the production of greener aviation fuels is co-hydroprocessing of bio-based feedstocks with fossil counter parts as well as hydroprocessing upgrading of intermediates. This approach allows utilization of existing refinery technology and equipment, rendering it a more economically attractive solution. The co-processing of waste cooking oil (WCO) with petroleum feedstock was thoroughly investigated for hybrid jet fuel production, while the stabilization of wood derived bio-oil in two-stage hydrotreatment was also evaluated for drop in jet biofuel production. The results have shown that co-processing of petroleum fraction with biobased feedstocks is a well promising technology for transportation as well as aviation sector, while, the stabilization of wood derived bio-oil via hydrotreatment leads to the production of very light hydrocarbons in the jet and diesel range that can be used as drop in jet biofuels.

Keywords: hydrotreatment, waste cooking oil, pyrolysis oil, jet fuels, hybrid fuels

INTRODUCTION

Aviation currently accounts for ~10% of global transport energy consumption, with a forecast increase in revenue-tonne-kilometres of ~5.1% per year to 2030 and rise by 225% of the Green House Gas (GHG) emissions. For this reason, the aviation industry is putting a lot of effort towards GHG emissions reduction, which can be partially achieved by improving fleet rollover, aircraft infrastructure, as well as engine performance. Nevertheless, the use of renewable aviation fuels is expected to activate the largest reduction of CO₂ emissions, which could reach up to 1.4 billion tons per year by 2050.

The lower fuel quality of conventional biofuels (ex. FAME, bioethanol) and high investment and production costs associated with advanced biofuels (ex. HEFA, BtL), as well as the dependence of drop-in production technologies on energy crops, limit the sustainable growth of these markets. On that basis, co-processing of 2G and 3G bio-based feedstocks (ex. waste lipids, fats, microalgal oils) and intermediates (ex. pyrolysis bio-oils, hydrothermal liquefaction oils, FT-waxes) with fossil-based fractions for the production of partially decarbonized fuels render a promising alternative technology.

The hydroprocessing group of the Centre for Research & Technology Hellas (CERTH) at the Chemical Process and Energy Resources Institute (CPERI) is dynamically involved in co-hydroprocessing liquid biomass and bio-based intermediates with petroleum fractions for the production of partially decarbonized fuels (Bezergianni et al. 2011, Bezergianni et al. 2014a). Technical and environmental assessment confirms the superiority of integrating biomass in refineries vs. stand-alone technologies producing drop in biofuels that are blended with fossil fuels at 10-50% with their fossil counterpart.

The benefits of co-processing include low investment and production costs as existing conversion capacity in underlying refinery units is employed, as well as product quality stabilization which is ensured from the optimal petroleum conversion pathways and final blending systems. Furthermore, the co-processing pathway enables the controlled decarbonization of transportation fuels and gradual crude-oil consumption mitigation, promoting a sustainable and future for aviation and all other transportation fuels.

The aim of this study is firstly to examine co-processing of WCO with petroleum feedstock for hybrid jet fuel production and secondly the stabilization of wood derived pyrolysis oil for drop in jet biofuel production. The experiments took place in the CPERI/CERTH. A hydrotreating continuous flow pilot plant with capacity 60ml/hr was utilised for the experiments, more details about the pilot plant could be found in an author's previous work (Bezergianni et al. 2014a).

RESULTS

Hydrotreating of petroleum fractions with lipids feedstocks offers a unique opportunity to produce a sustainable hybrid diesel fuel completely compatible with existing fuel infrastructure and engine technology. Co-processing of petroleum fractions (i.e. gas-oil) with WCO (from restaurants and households) was examined for hybrid jet fuel production. A commercial NiMo/ γ Al₂ catalyst was utilised according to the results of an author's previous work (Bezergianni et al. 2014b). The results were evaluated in terms of distillation curve, product yields as well as conversion rate. Five blends of gas oil with WCO were investigated (95/5, 90/10, 85/15, 80/20 and 70/30 Gas Oil/WCO). The resulting product known as hybrid fuel has a density ranges from 0.78 to 0.85 g/ml, significantly high cetane number (50–101) and also high net heating value (43.3–47 MJ/kg) (Bezergianni S and Dimitriadis A. 2013). The cold flow properties are also quite diverse based on the catalyst and operating parameters employed, for example pour point is between -20 and 26°C, while the cloud point ranges between -23 and 20°C (Simacek P, Kubicka D 2010). Furthermore, the hybrid fuels are also low sulphur (3–13 ppmwt) and aromatics free (0.1–1.2%wt) fuels, thus they can be considered "clean fuels".

Figure 1 presents the distillation curve A) as well as the jet fuel yields and conversion B) of the products from co-processing of variable blends of petroleum fractions with lipid-containing feedstocks (gas-oil/WCO). The jet fuel yield was estimated as the vol% of the total liquid product that has a boiling range between 193°C and 277°C (see Figure 1). The results have shown that 6 to 9% of liquid product is in the range of jet fuel while the conversion varies from 6 to 7%. The other product is heavier hydrocarbons in the range of diesel. It is obvious that co-processing of petroleum feedstock with biomass based feedstock can render a small percent of jet fuel hydrocarbons which can be further increased by optimising the operating parameters of the hydrotreating process (reaction temperature, reaction pressure, LHSV and H₂/Oil).

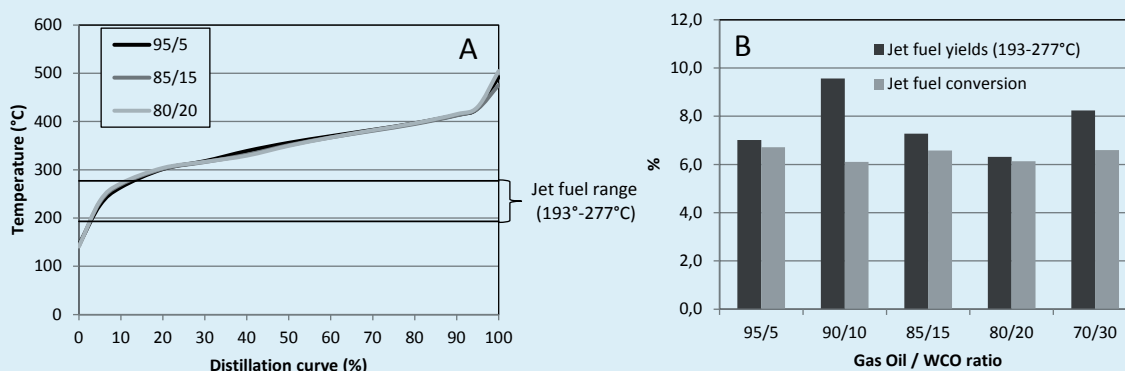


Figure 1. Distillation curve A) and Jet fuel yields and conversion yields B) from co-processing of Gas oil / WCO blends (95/5, 85/15 and 80/20).

Furthermore, the stabilization of wood derived pyrolysis oil was also examined for jet drop in biofuel production in terms of jet fuel yields, conversion and distillation. In general, pyrolysis is a simple way to produce oil from biomass by thermal decomposition at moderate temperatures, ambient pressure and very short reaction time. This process can convert solid biomass and wastes such as wood to higher added-value liquid products (pyrolysis oil). The advantage of this process is that it can be used to the whole biomass without any pretreatment (Bridgwater A. V. 2004). However, pyrolysis oil has disadvantages as an aviation fuel. Pyrolysis oil is a dark brown, free-flowing liquid with about 20-30% water, high acidity and low oxidation stability (Torri et al. 2010). For the above reasons, pyrolysis oil needs further upgrade. Wood-derived pyrolysis oil can be stabilized and converted to a conventional hydrocarbon fuel by converting oxygenates.

Pyrolysis oil of the current study was produced via catalytic pyrolysis of lignocellulosic biomass (wood from tree beech), which was characterized by 21wt% oxygen content, high density (1.051kg/lit) and high acidity. A dual stage hydrotreatment was examined with a commercial NiMo/ γ Al₂ catalyst, incorporating a mild hydrotreatment stage that is aimed in stabilization and pre-conditioning, followed by a more severe hydrotreatment stage allowing further upgrading and production of fuel-like products. A single stage hydrotreatment of biomass (wood) pyrolysis oil renders a heavy (density:1.056 kg/lit), high sulfur (657 wppm), high O₂ (18 wt%), tar-like product with a boiling point range from 100°-670°C, as a result an additional 2nd stage HDT is required. The product from 2nd stage is characterized by lighter hydrocarbons with density 0.8471 kg/

lit, 1% O₂ content, in the range of 78°-580°C boiling point and calorific value 44.7 Mj/kg. Figure 2 presents the distillation curve A) and the product yields B) of the two stage hydrotreatment. The results have shown that after a first stage mild hydrotreating of pyrolysis oil, almost 30% of the products is in the range of jet fuel, while 27% is lighter hydrocarbons and 43% is heavier hydrocarbons in the range of diesel. However, after a second more severe hydrotreatment stage, lighter products could be achieved, the results of two stage hydrotreatment have shown that almost 47% of the liquid products is in the range of lighter hydrocarbons (<193°C boiling point), 24% is in the range of jet fuel (193°-277°C) while almost 30% is in the range of diesel fuel (>277°C). It is clear that high added-value liquid fuels can be produced via hydrotreatment stabilization of wood derived pyrolysis oil.

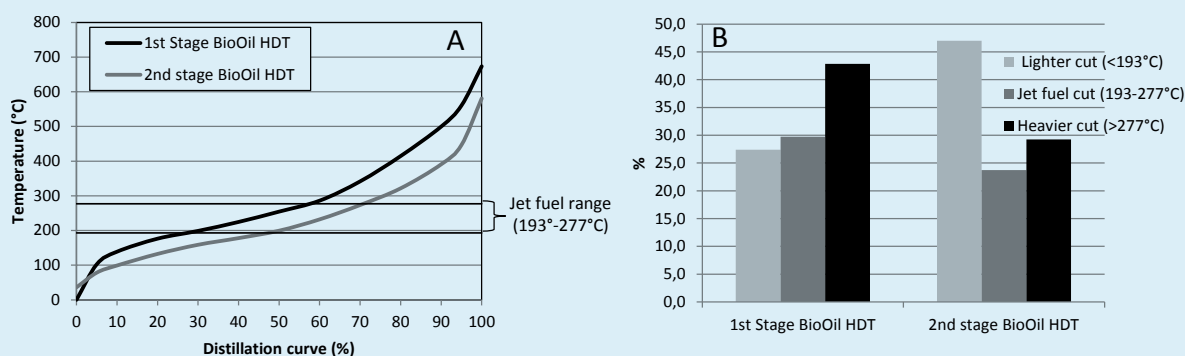


Figure 2. Distillation curve A) and product yields B) from 1st and 2nd stage bio oil hydrotreated

CONCLUSIONS

WCO is considered as an alternative feedstock blend for catalytic hydroprocessing of gas oil. Catalytic hydroprocessing of gas oil/WCO mixtures was evaluated as an alternative approach for integrating residual biomass in the aviation sector by utilising the existing infrastructure of a refinery. The effect of increasing WCO content in the hydroprocessing feed was assessed in terms of jet fuel yields and conversion. The results have shown that the addition of WCO (5% to 30%) in HAGO not only does not affect negative the quality of the final product but rather improves some of its properties without lowering the yield (Bezergianni et al 2014b). Co-processing 5–30% WCO with Gas Oil would render up to 10% jet biofuels.

Moreover, a dual stage hydrotreating upgrade of wood derived pyrolysis oil was also examined in order to produce high quality jet biofuels. Pyrolysis oil in general is not appropriate for aviation sector without upgrading. However a dual stage hydrotreatment technology proved to be very advantageous. The results have shown that a first mild hydrotreating upgrade renders better quality products with lighter hydrocarbons and low oxygen and water content. After a first stage hydrotreating of pyrolysis oils up to 30% of the products are in the range of jet fuel hydrocarbons, while after a second stage hydrotreatment, the final products are even lighter with zero oxygen and water content and high calorific value.

As aviation currently accounts for ~10% of global transport energy consumption, a 10% to 30% jet fuel yields of the described technologies is very promising. It is obvious that, co-processing of lipid feedstock with petroleum fractions as well as hydroprocessing upgrading of pyrolysis oil render a promising alternative technology for aviation sector.

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PP02: EXPERIMENTAL AND COMPUTATIONAL STUDY OF RECIPROCAL INTERACTIONS OF O-NITRILE ELASTOMER AND ALTERNATIVE AVIATION FUEL CHEMICAL CONSTITUENTS

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Abstract. Currently, several processes are being explored for production of the Synthetic Paraffinic Kerosene (SPK) allowing the production of aviation fuel from feedstocks other than crude oil as well as the sand and oil shale. These processes produce a fuel of mainly of normal and iso Paraffins and do not have the spread of hydrocarbons seen in conventional aviation fuel. Despite a number of advantages, one of the most serious concerns of alternative aviation fuels has come from their low aromatic content. This is due to the fact that the ageing seals in the aircraft would face leakage if the concentration of aromatics is too low.

Reciprocal interactions of O-Nitrile elastomer and major hydrocarbon block constituents of alternative aviation fuel were studied experimentally and computationally. For the experimental part, dynamic tests were carried out using a stress relaxation rig under isothermal conditions as well as temperature cycling. In order to try and understand the phenomena better, "Density Functional Theory (DFT)" was used to investigate the molecular interactions of seal constituents and a number of chemical substances representing various classes of major constituents of blend of conventional and alternative aviation fuel including normal, iso, cyclic paraffins together with aromatics.

PP03: HEAT RELEASE MARKERS FOR THE COMBUSTION OF ALTERNATIVE AVIATION FUELS IN GAS TURBINES

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Abstract. The aviation sector has been looking into alternative fuels in order to cope with the growing air transport demand and to moderate environmental concerns. Significant research is conducted on the characterization of various synthetic fuels. These fuels are complex mixtures of components of different chemical classes and the understanding of their combustion characteristics requires the implementation of chemical kinetic based methodologies to delineate any synergistic effects. Heat release rate is an important fundamental flame property that largely characterizes the overall combustion process. Heat release distribution in practical combustors, such as gas turbines, is crucial, not only for the identification of energy intensive flame regions, but also for the understanding and prediction of thermo-acoustic instabilities. There is considerable interest in formulating practical correlations for quantifying heat release rate in flames via appropriate chemical markers, mainly due to difficulties in obtaining a direct estimation of the former. Earlier studies performed in methane/air flames, have identified correlations between suitable kinetic information and heat release rate. However, such correlations are inadequate for unsaturated fuels under rich conditions and for oxygenated fuels under most conditions. The objective of the present work is to investigate the validity and applicability of correlations developed for methane to the combustion of other generic classes of hydrocarbons including alternative and oxygenated fuels and to underline a methodological approach for the development of more general correlations. Proposed correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner-stabilized premixed flames using validated detailed kinetic mechanisms.

Keywords: Chemical kinetic markers; Heat-release rate; Laminar premixed flames; Phenomenological correlation; Practical combustors

INTRODUCTION

Heat release rate is a highly important fundamental flame property that largely characterizes the energetic outcome of the overall combustion process. Heat release distribution in practical combustors is crucial, not only for the identification of energy intensive flame regions, but also for the understanding and prediction of thermo-acoustic instabilities, pulsed combustion and combustion noise (e.g. Hardalupas et al., 2010). Direct measurement of temporally and spatially resolved heat release rate (HRR) in combustion devices is currently timely, costly and impractical. A way to overcome this problem is to formulate versatile correlations between HRR and appropriate chemical markers that can be experimentally determined with acceptable accuracy. Several such correlations have been proposed in the literature and they invariably correlate suitable detailed kinetic information (e.g. species mole fraction and/or elementary reaction rates) to the HRR in fundamental flame environments. Currently, the most reliable approach for HRR quantification involves reaction-rate imaging combining simultaneous CH₂O and OH LIF measurements. The approach has been shown to yield excellent correlations mainly in laminar and turbulent premixed methane flames but its validity for other fuels is currently unclear and has been recently questioned on the basis of experimental and numerical investigations (e.g. Kathrotia et al., 2012).

Alternative aviation fuels are composed of different hydrocarbons, the amount and type of which can differ considerably. Arguably, the composition of the fuel will affect its suitability and performance. Currently, synthetic fuels can be obtained from fossil (coal, gas) and renewable sources (waste, biomass) by many pathways including, among others, gasification applying the Fischer–Tropsch (FT) process, liquefaction, pyrolysis, hydrogenolysis and esterification, etc. Fuel composition consists of a large variety of different species belonging mainly to four chemical families: (i) long-chained unbranched alkanes (n-alkanes), (ii)

long-chained, branched alkanes (iso-alkanes) (iii) cyclo-alkanes (naphthenes) and (iv) aromatics (Braun-Unkhoff et al., 2016).

The present work summarizes and extends previous work by the authors (Gazi et al., 2013) and aims to discuss the applicability of the therein proposed methodology to novel aviation fuels. The objective of the present work is to investigate the validity and applicability of correlations developed for methane to the combustion of other generic classes of hydrocarbons including alternative and oxygenated fuels and to underline a methodological approach for the development of more general correlations. Correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner-stabilized laminar premixed flames utilizing a comprehensive detailed chemical kinetic mechanism.

DEVELOPMENT OF A FLAME DATABASE AND NUMERICAL METHODOLOGY

Although real working conditions of practical combustion devices are characterized by complex flow and chemistry interactions, the validity of any correlation between HRR and appropriate chemical marker needs to be established in a well-controlled environment. A simple but yet realistic fundamental configuration suitable for the application of detailed chemistry is the laminar premixed flame. In the present work flames of different fuel classes, as well as fuel mixtures, have been considered in order to take into account the effect of isomeric structure and the interaction between single, double and triple bonds on HRR patterns. Computations have been performed with CHEMKIN (Reaction Design, 2006).

Table 1 Database of laminar premixed flames considered in the present work (please refer to Gazi et al. 2013 for complete information about flame properties)

#	Reactants (%)	#	Reactants (%)		
A	Methane	1.00	K	Acetylene	2.00
B	Methane (80%) Benzene (20%)	1.00	L	Ethylene	1.90
C	Methane (83%) Allene (17%)	1.25	M	Ethylene	2.00
D	Methane (83%) Propyne (17%)	1.25	R	Benzene	0.70
E	Methanol	0.89	S	Benzene	1.00
F	Ethanol	1.00	T	Benzene	1.78
G	Ethanol	1.00	U	Benzene	1.80
H	Ethanol	1.96	V	Benzene	2.00
I	Ethanol	2.57	W	Benzene	2.00
J	Acetylene	2.40	X	Acetylene (80%) Benzene (20%)	2.00

METHANE FLAMES

The first part of the paper provides evidence on the validity of literature correlations for laminar premixed methane flames. Figure 1a presents computed correlations between the overall heat release rate and the product of formaldehyde and hydroxyl radical concentrations in Flame A, while Fig. 1b shows the corresponding correlation for the net rate of the CH_3+O reaction. It is clear that the latter correlation is superior. Interestingly enough correlations involving the CH_2O and OH species appear to perform slightly better in the doped methane Flames B-D. However, it can generally be argued that both literature-proposed correlations are more than acceptable.

METHANOL AND ETHANOL FLAMES

The next step in the investigation relates to methanol and ethanol flames. The choice of methanol has been based on a number of reasons; it is the simplest alcohol, it has a very similar structure to methane and is adequately experimentally characterized. Furthermore, is considered as an alternative fuel by itself. It should be expected that the HRR correlations shown to be valid for methane flames, would also

be adequate for methanol flames. However, this is not the case as demonstrated in Fig. 3a. Moving further to a higher alcohol, we observe that no such simple correlations can be found for ethanol flames particularly under fuel rich conditions (Fig. 3b).

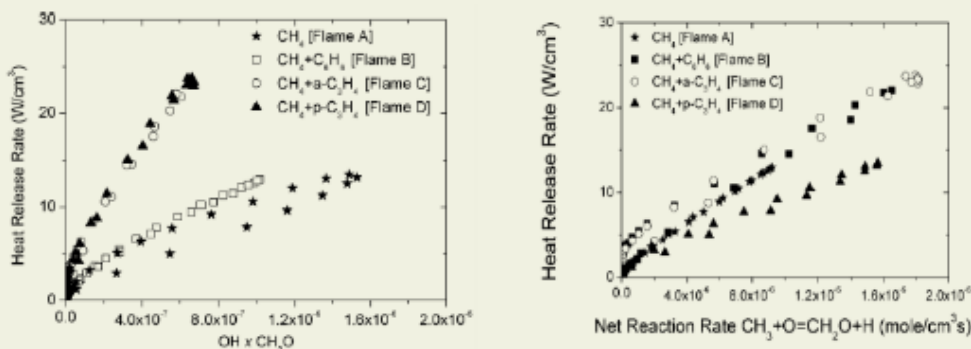


Figure 1. Correlation between HRR and (a) the product of CH_2O and OH mole fractions and the net rate of the CH_3+O reaction in flames A–D

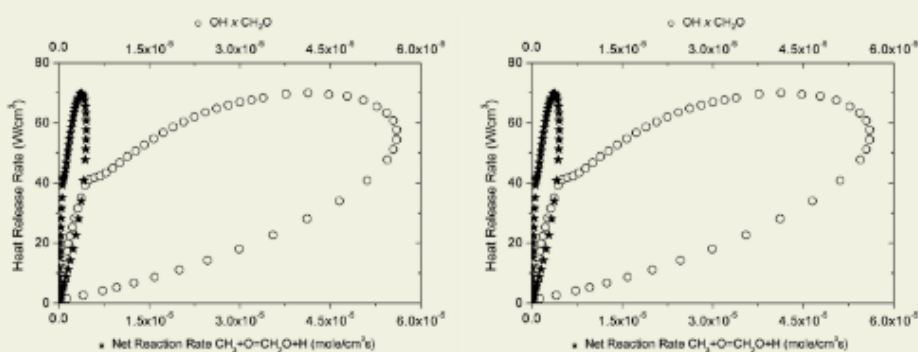


Figure 3. Correlation between HRR and (a) (i) the product of CH_2O and OH mole fractions and (ii) the net rate of the CH_3+O reaction, flame E (b) the product of CH_2O and OH mole fractions, flames G–I.

HIGHER HYDROCARBONS

Acetylene is a major intermediate in hydrocarbon flames and its chemistry is crucial for both heat release and molecular growth paths. Initial fuel consumption paths involve mainly O and OH addition reactions. The former lead to HCCO and triplet methylene radical while the later predominately lead to ketene, which subsequently is also consumed to the ketyl radical. This analysis outlines the crucial role of the ketyl radical in acetylene chemistry. Thus, $[\text{HCCO}][\text{O}_2]$ is an excellent HRR marker, while the formaldehyde conjecture is not. Whether such arguments collectively characterize C_2 fuels has been also investigated. In the case of ethylene the formaldehyde correlation cannot be totally disregarded, although is not the most appropriate. On the contrary, the $[\text{HCCO}][\text{O}_2]$ results in a very good probe, see Fig. 4b. Since the aromatic context in a jet fuel varies, lean to near-sooting benzene flames have been studied herein. The correlation between HRR and the product of CH_2O and OH concentrations is satisfactory, Fig. 5a. The major carbon flow in benzene flames involves initial fuel destruction to the phenyl radical, molecular oxygen attack on the latter, leading to phenoxy radical, followed by expulsion of a CO molecule and formation of cyclopentadienyl radical. Ring opening occurs through cyclopentadiene decomposition to the allyl radical and acetylene. Acetylene is then predominantly consumed to the ketyl radical, even under fuel-lean environments. Thus, the ketyl radical correlation is expected to work not only under rich conditions but also in leaner mixtures, as shown in Fig. 5b.

CONCLUSIONS

The current paper provides an appraisal of appropriate chemical markers for heat release rate correlations. Proposed correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner stabilized laminar premixed flames computed utilizing a comprehensive detailed kinetic

mechanism. It is shown that correlations involving the methyl radical→formaldehyde→formyl radical pathway are adequate for methane flames and only for some lean-to-stoichiometric hydrocarbon flames. This is definitely not the case for oxygenated fuels and particularly under rich conditions. Correlations based on major carbon flow paths seem to work for relatively simple fuels. Generic correlations for rich combustion involving markers related to acetylene breakdown chemistry e.g. the HCCO+O₂ correlation have also been preliminary assessed.

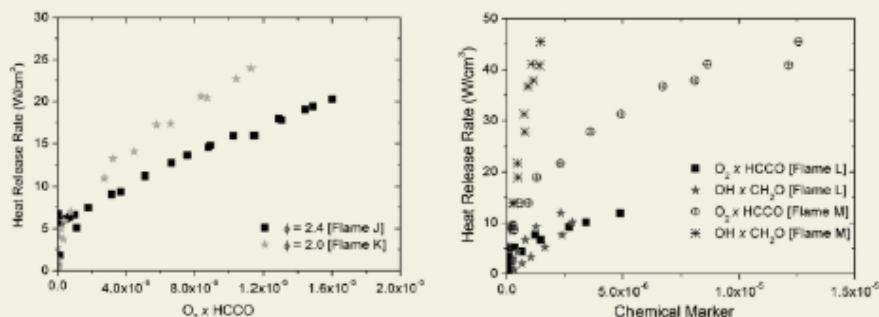
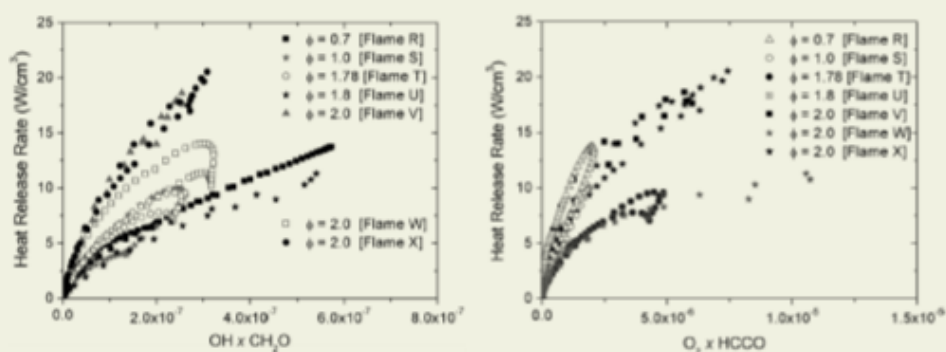


Figure 4. Correlation between HRR and (a) the product of HCCO and O₂ mole fractions for flames J and K (b) the products of HCCOxO₂ and CH₂OxOH mole fractions for flame L and flame M.



Correlation between HRR and (a) the product of CH₂O and OH mole fractions and (b) the product of O₂ and HCCO mole fractions for flames R–X.

ACKNOWLEDGEMENTS

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PP04: METHODOLOGIES FOR AUTOMATIC HYDROCARBON AUTOXIDATION MECHANISM GENERATION

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Abstract. Aviation fuel undergoes oxidation of the hydrocarbon components due to thermal stress, this degrades the fuels properties and causes deposits in the fuel and engine systems. Our research uses computational modeling techniques to understand how the chemical composition of a fuel effects its thermal stability. Computational chemistry techniques are used to calculate the thermodynamic and kinetic data for the oxidation reactions in the fuel.

Keywords: Fuel Oxidation, Modeling

INTRODUCTION

Aviation fuel has the dual purpose in modern aircraft of acting as the energy source and as a heat exchanger to remove excess heat from the engine systems. The increase in fuel temperature causes the aviation fuel to undergo oxidation and form insoluble deposits which can block the fuel systems (Kuprowicz et al 2007). The chemical composition of a fuel has been shown experimentally to effect its thermal stability, with the presence of polar species and high aromatic content increasing the oxidation rate (DeWitt et al 2014). This work attempts to better understand the mechanisms which govern the oxidation of the fuel and the role that changing chemical composition has on the global kinetics of these processes.

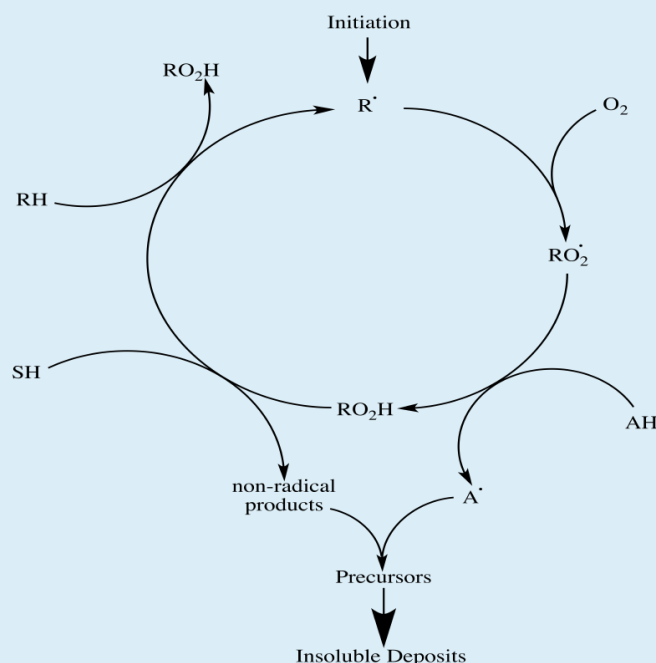


Figure 1. Simple reaction cycle for the formation of oxidation products

Aviation fuels properties are altered by changing the composition, with addition of aromatics increasing the energy density of the fuel, and the range of the aircraft. Increasing the aromatic content has also been linked to increasing the smoke and particulates produced from combustion. For this

reason it would be useful to increase the energy density of a fuel without increasing aromatic content. One solution would be to include higher amounts of cyclic hydrocarbons, as they should burn in the similar ways to normal paraffins (Amara et al 2016). The investigation into the effect that hydrocarbons composition has on the oxidation mechanisms was carried out using quantum chemistry models (Zabarnick et al 2006). The knowledge gained from these calculations builds on the role that each component has on the thermal stability problem. The work presented shows how cyclic hydrocarbons effect the oxidation rate, with the quantum mechanically calculated kinetics and thermodynamics compared to those of aromatic, and straight chain alkanes.

RESULTS AND DISCUSSION

The Calculations were carried out using the Gaussian 09 software, using Density Functional Theory. The calculations were carried out at the B3LYP/6-311G (d,p) level of theory, with electronic structure calculations of peroxides being carried out using CASSCF and CASPT2 theories. The results are compared to experiment and literature.

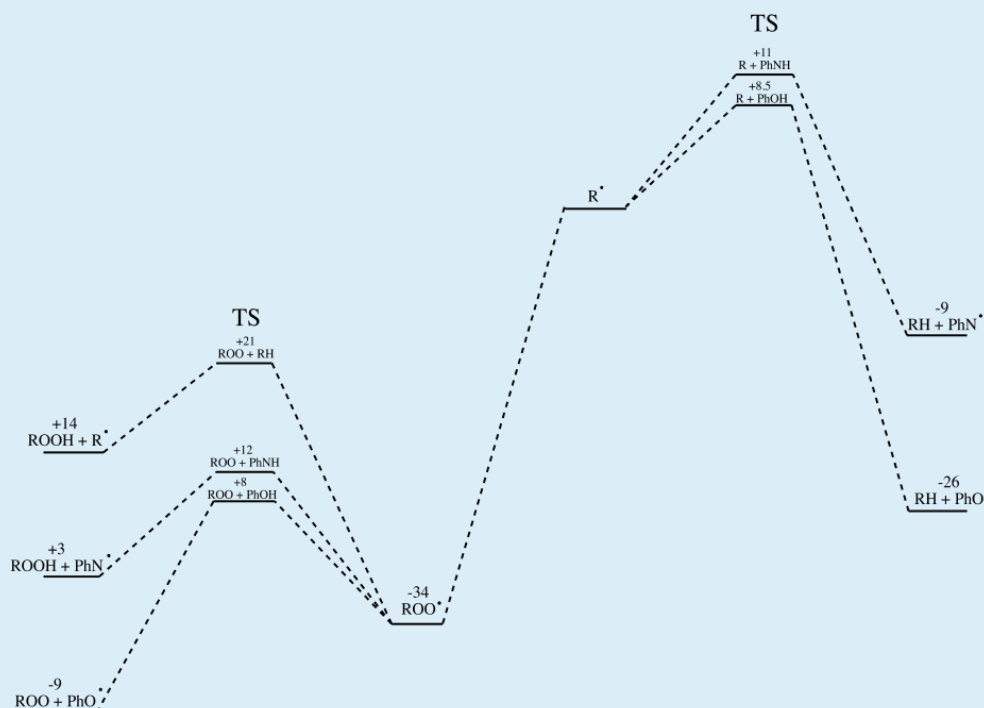


Figure 2. Potential energy surface of the oxidation reactions for dodecane

It was found that cyclic hydrocarbons were more stable to oxidation than aromatic hydrocarbons, with this being linked to aromatic hydrocarbon stabilising the radical species produced during the oxidation process through conjugation. Cyclic hydrocarbons were however more reactive than straight chain alkanes, due to the greater proportion of radical stabilising secondary and tertiary carbons. This supports what is seen in the experiments, with the rate of oxidation increasing as the percentage of cyclic hydrocarbons increase in the test sample. The aromatic and cyclic radicals were more stable and less reactive to further reactions due to the stabilising effects of the hydrocarbon structure. However more investigations are needed to identify the role that structure plays on oxidation rates and deposit formation.

Limitations of the calculations were found when the electron spin states of the species changed during a reaction. This is a particular problem for reaction such as the homolytic fission of peroxides, where it could lead to errors of up 7 Kcal mol⁻¹. This was solved by moving to a theoretical technique that better describes these systems, at greater computational expense.

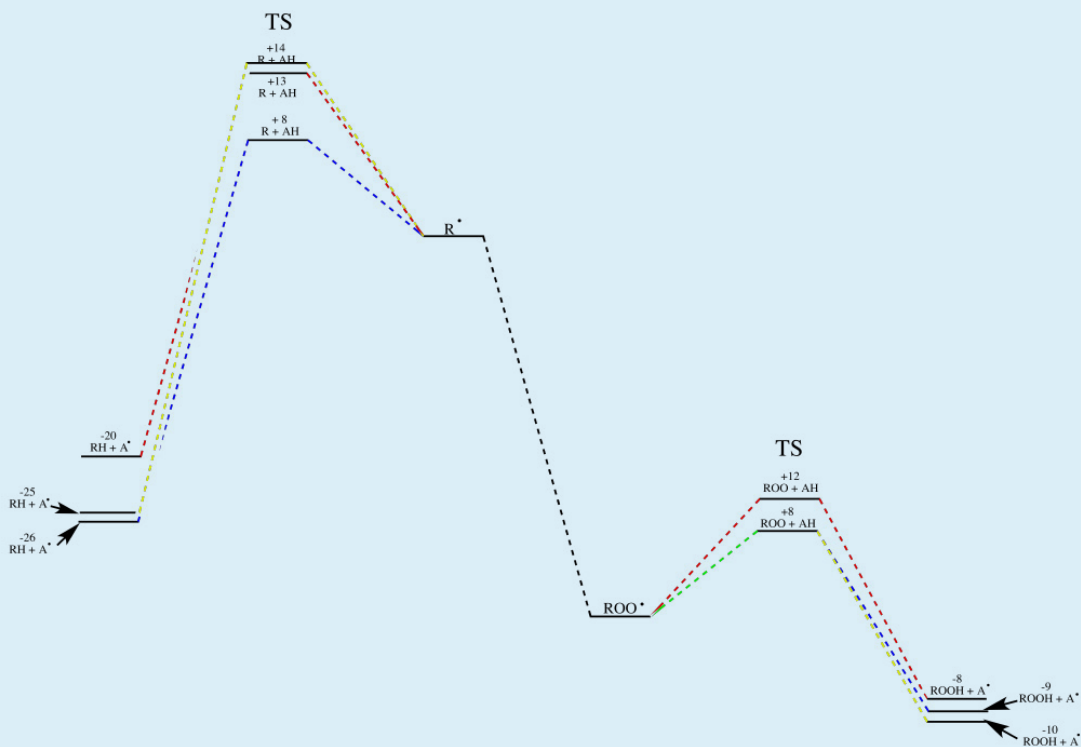


Figure 3. Potential energy surface of the oxidation reactions for dodecane – Blue, Toluene – Yellow and Decalin – Red

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PP06: INTERCOOLED RECUPERATED AERO ENGINE: EARLY DEVELOPMENT STAGES AND OPTIMIZATION OF RECUPERATION BASED ON CONVENTIONAL HEAT EXCHANGERS

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Abstract. In the last two decades, the European Union, in collaboration with main European aero engine manufacturers, Universities and Institutes funded a number of research efforts aiming at the design of innovative aero engines operating on advanced thermodynamic cycles presenting reduced fuel consumption and pollutant emissions, promoting the fulfillment of year 2020 ACARE targets. A part of these activities was focused on an innovative advanced aero engine concept, the Intercooled Recuperated Aero engine (IRA-engine), developed by MTU Aero Engines AG, using an alternative thermodynamic cycle combining both intercooling and recuperation. Under this concept recuperation is achieved by the integration of a heat recuperation system based on heat exchangers mounted inside the hot-gas exhaust nozzle. The recuperation system exploits the exhaust hot-gas energy to preheat the compressor discharge air before the latter enters the combustion chamber, resulting in reduced fuel consumption and pollutants emission. The present paper focuses on the early optimization stages of the IRA-engine recuperation system based on the MTU developed state-of-the-art U-type tubular heat exchanger, performed in AEROHEX and NEWAC projects, aiming mainly at the minimization of heat exchangers pressure losses. The optimization was performed with CFD computations in which the heat exchangers were modelled as porosity models of predefined heat transfer and pressure loss macroscopic behaviour, validated through experimental measurements. For the optimization various customized 3-D models of the recuperation system were developed and investigated which led to considerable pressure loss reduction with positive effects on fuel consumption and pollutants emissions reduction.

Keywords: recuperative aero engines, heat exchangers, porosity models, fuel consumption reduction, pollutant emissions reduction

INTRODUCTION

Commercial aviation presents a history of successful technological advancements affecting the lives of millions of people globally. As air traffic grows at an annual rate of about 5%, the need to increase aero engines efficiency and reduce NO_x, CO₂ and other gaseous emissions becomes more urgent to mitigate their negative environmental footprint, e.g. on global warming. In the last two decades, the European Union, in collaboration with main European aero engine manufacturers, Universities and Institutes funded a number of research efforts aiming at the design of innovative aero engines operating on advanced thermodynamic cycles presenting reduced fuel consumption and pollutant emissions, promoting the fulfillment of year 2020 ACARE targets. A part of these activities was focused on an innovative advanced aero engine concept, the Intercooled Recuperated Aero engine (IRA-engine). This concept which is developed by MTU Aero Engines AG and is presented in Figure 1a is using an alternative thermodynamic cycle combining both intercooling and recuperation. In the IRA-engine cycle, recuperation is achieved by the integration of a heat recuperation system based on heat exchangers mounted inside the hot-gas exhaust nozzle. The recuperation system exploits the exhaust hot-gas energy to preheat the compressor discharge air before the latter enters the combustion chamber, resulting in reduced fuel consumption and pollutants emission.

The present paper focuses on the early optimization stages of the IRA-engine recuperation system, performed in AEROHEX and NEWAC projects, aiming mainly at the minimization of heat exchangers pressure losses since their effect on the overall aero engine cycle was identified as significant. The IRA-engine recuperation system is based on use of various heat exchangers placed in a specific arrangement inside the hot-gas exhaust nozzle and is based on the MTU developed state-of-the-art U-type tubular heat exchanger (HEX)

which is presented in Figure 1b. As it can be seen, the MTU-developed heat exchanger consists of elliptic tubes placed in a 4/3/4 staggered arrangement in order to provide increased heat exchange surface area and thus, increased heat exchanger effectiveness coupled with reduced outer flow pressure losses. The heat exchangers of the IRA-engine are operating as heat recuperators focusing on the exploitation of the waste heat energy of the low pressure turbine exhaust gas so as to preheat the high pressure compressor discharge air right before combustion and decrease the fuel consumption and gas pollutants emissions. Detailed information about this technology is presented in the works of Wilfert and Masse (2001), Wilfert et al. (2007), Schonenborn et al. (2004) and Albanakis et al. (2009).

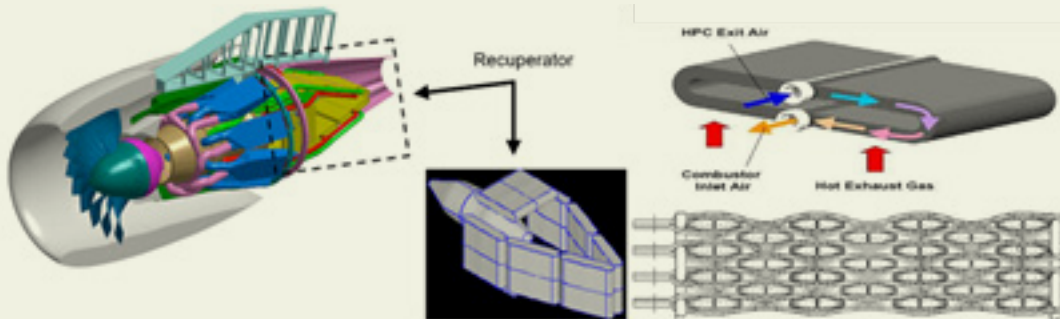


Figure 1a. The IRA - Intercooled Recuperative Aero-engine. 1b. The MTU-heat exchanger.

OPTIMIZATION OF RECUPERATION BASED ON CONVENTIONAL HEAT EXCHANGERS

Due to its direct positioning inside the exhaust nozzle, right after the low pressure turbine, the heat exchangers can impose significant pressure losses which can strongly affect the aero engine performance and the achieved produced work resulting in the degradation of recuperation technology benefits. As it is profound, due to cost and conditions limitations, the conducting of an optimization campaign for the heat exchangers installation inside the exhaust nozzle is of particular importance. For this reasons, the optimization was performed mainly with 3D CFD computations in which the heat exchangers were modelled as porosity models of predefined heat transfer and pressure loss macroscopic behaviour, validated through experimental measurements. Details about the porosity model approach can be found in Missirlis et al. (2009, 2010) and Yakinthos et al. (2006, 2007). The optimization efforts started from the reference (AEROHEX) nozzle configuration, shown in Figure 2.

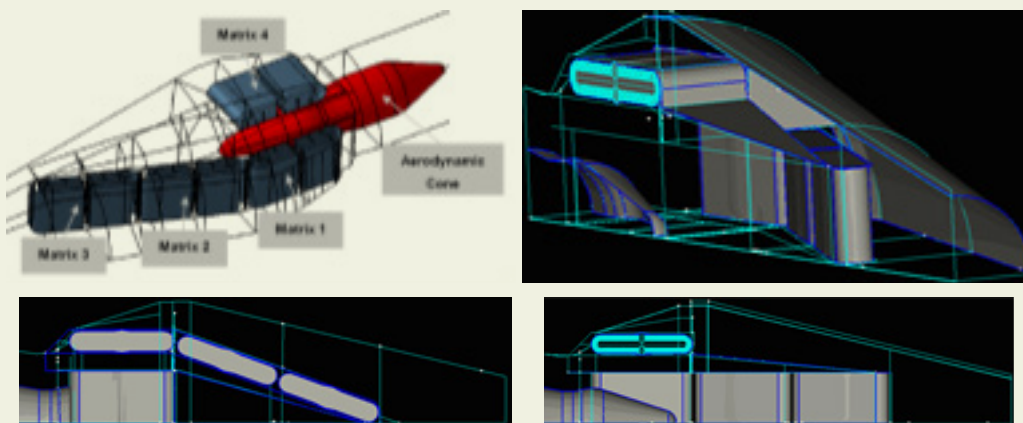


Figure 2. Reference nozzle configuration (AEROHEX) setup– 1/4 nozzle representation

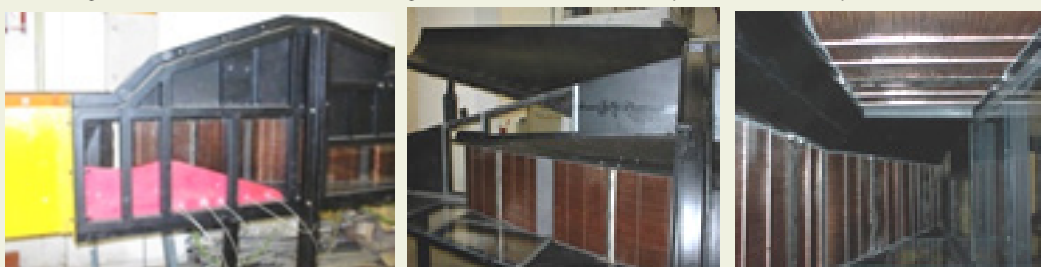


Figure 3. Reference nozzle configuration (AEROHEX) test-rig – 1/4 nozzle representation

In this configuration the heat exchangers were placed in a 0/20/20/0 orientation. For this arrangement experimental measurements on a specially constructed test-rig, presented in Figure 3, were carried-out and CFD computations, mainly with the Shear stress Transport (SST) turbulence model of Menter (1994), following the porosity model approach were performed, Figure 4 shows the CFD grid, and a detailed inside look at the flow was derived, revealing major flow separation regions and secondary flow 3D (swirl) effects resulting in increased pressure losses as presented in Figure 5.



Figure 4. Reference nozzle configuration (AEROHEX) CFD grid – 1/4 nozzle representation

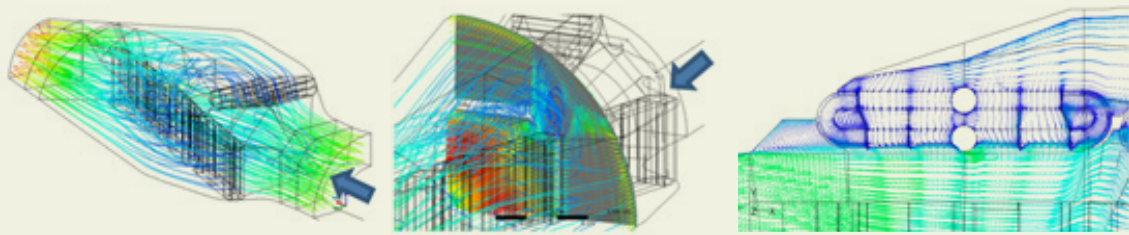


Figure 5. Reference nozzle configuration (AEROHEX) CFD results – 1/4 nozzle representation

Targeting the further optimization of the recuperator various customized 3-D models of the recuperation system were developed, being always based on the MTU-developed tubular heat exchanger, and investigated numerically through additional similar CFD computations. These attempts, performed in the NEWAC project, led to various optimization modifications, presented in Figure 6, which were incorporated in a dedicated test-rig, presented in Figure 7, in which experimental measurements were carried-out for validation purposes.

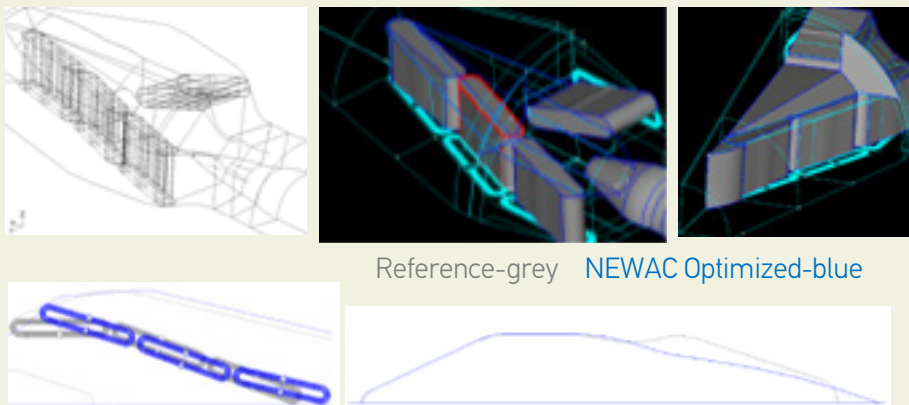


Figure 6. NEWAC optimized case. Modifications in relation to the reference case



Figure 7. NEWAC optimized case test-rig– 1/4 nozzle representation

The following modifications were mainly focused on changes on the orientation of HEX matrices 1/2/3/4 is now at 17/20/13/17 degrees, redesign of the aerodynamic cone in order to minimize the recirculation region downstream the cone, additional changes in the nozzle guiding walls, the addition of an aerodynamic ramp after HEX matrix 3 and adaptation of the HEX bow region covers. These modifications resulted in the significant decrease of the secondary flow losses, due to swirl effects and recirculation regions, and to the achievement of a much more homogeneous flow field distribution (especially through the HEXs of the installation which are placed upstream and encounter significant flow recirculation) which led to the decrease of the flow velocity maxima and to reduced pressure losses. As a result, the NEWAC optimized case provided more than 15% reduced pressure losses in relation to the Reference case, while achieving the same HEXs effectiveness value.

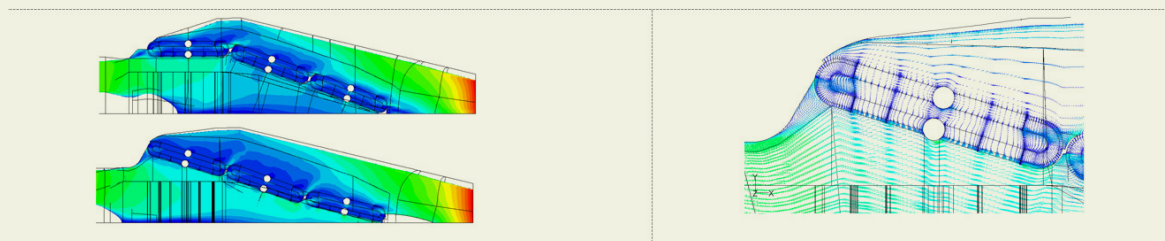


Figure 8. NEWAC optimized case CFD results – 1/4 nozzle representation
(Left: velocity magnitude qualitative comparison in relation to Reference case, Right: velocity flow at the inlet HEXs)

At the final step of the analysis, the major characteristics of the recuperator installation of both concepts were incorporated in GasTurb 11, (Kurzke, 2011) and their effect on the IRA-engine thermodynamic cycle was quantified. The results, showed that the NEWAC optimized nozzle could achieve a specific fuel consumption reduction of ~1.0% with positive effects also on the decrease of pollutants emissions as a result of the considerable pressure loss reduction.

ACKNOWLEDGEMENTS

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PP07: ENVIRONMENTAL IMPACT FUNCTIONS: LINKING ENVIRONMENTAL IMPACT INFORMATION FOR PLANNING ENVIRONMENTALLY-OPTIMAL TRAJECTORIES

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DLR

Abstract. Beyond the desire to minimise fuel use and hence CO₂ emissions, currently the consideration of environmental aspects in en-route flight planning has not been operational practice. The reason for this is a low TRL (technology readiness level) of a flight planning method that considers a multi-dimensional environmental impact assessment and a lack of scientific support to motivate environmental flight planning. The exploratory research project within the SESAR2020 project addresses this gap and has as main objective to explore the feasibility of a concept for environmental assessment of ATM operations working towards environmental optimisation of air traffic operations in the European airspace.

The study will present how a multi-dimensional environmental cost function (ECF) concept is established, which includes air quality impact (for key pollutants) and noise in addition to climate impact. This concept integrates existing methodologies for assessment of the environmental impact of aviation, in order to evaluate the implications of environmentally-optimized flight operations to the European ATM network, considering simultaneously different environmental impacts, comprising climate, air quality and noise impacts. These ECFs are derived from dedicated model output of atmospheric global circulation models, e.g. EMAC, local air quality tools, e.g. Open ALAQS and noise models, e.g. STAPES.

Specifically, a modelling concept for climate-optimisation which has been developed in a feasibility study for the North Atlantic (REACT4C) is expanded to a multi-dimensional environmental impact assessment, covering climate, air quality and noise. Climate cost functions were introduced, to establish a link between climate impact information and flight planning tools, in order to identify climate-optimal aircraft trajectories. This concept is expanded to cover a series of environmental impacts, by providing additional environmental change functions (ECFs) which represent a quantitative measure on impact of emissions and aircraft operations on local air quality and noise. Making available these ECFs in a flight planning tool allows assessing environmental impacts and identifying environmentally-optimal trajectories.

PP08: ECO-EFFICIENT AVIATION: AN OVERVIEW ON FIRST RESULTS FROM THE WECARE PROJECT

Volker Grewe
German Aerospace Center (DLR)

Abstract. Aviation guarantees global mobility. It is also a growing economy and the contribution to climate change by aviation is currently estimated to be roughly 5% of the total anthropogenic warming. A sustainable development is a challenge. The DLR project WeCare contributes to the understanding of mitigation options by taking advantage of spatial variability of non-CO₂ climate effects, i.e. NO_x effects on ozone and methane as well as contrail-cirrus. Various approaches are tested, which range from re-routing of individual aircraft in order to reduce the climate effect with respect to contrail-cirrus and NO_x to new operations, such as intermediate stop operations, and new aircraft concepts. All these concepts have different advantages and disadvantages. They vary in their cost-effectiveness. They also have impacts on travel time, air space controllers work load, etc. These effects are quantified within WeCare and we give here a summary of first results.

PP09: IDENTIFYING CLIMATE OPTIMAL TRAJECTORIES IN UNDER DIFFERENT SYNOPTICAL SITUATIONS

Sigrun Matthes
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Abstract. Mitigation of aviation climate impact is one strategic goal spelled out for a durable development of air traffic. Operational measures to identify climate-optimal aircraft trajectories by air traffic management (ATM) are one option to reduce climate impact. We present results from a comprehensive approach for weather-dependent climate-optimized flight planning applied for a case study the North Atlantic Flight corridor (NAFC) performed within the collaborative project REACT4C (Reducing Emissions from Aviation by Changing Trajectories for the benefit of Climate) funded under the European FP7 programme. Specifically, we present how climate-optimization changes routing preferences depending on the specific synoptical (meteorological) situation. Along with the distinct weather pattern, each day offers a different mitigation potential, expressed as the relation between climate impact mitigation and required investment.

Ultimate goal for climate-optimisation of aircraft trajectories is to identify maximum mitigation gain (in climate impact) for a specific investment, hence minimal marginal mitigation costs. For this purpose consecutively those flights trajectories options are selected which offer the highest mitigation potential taking into account five archetypical weather patterns in NAFC, and traffic samples in eastbound and westbound both direction. Using system approach in optimisation, which consists of identifying amongst all flights those routing options with highest mitigation potential, can result in a cost reduction of 96% of required investment or a mitigation increase by a factor of 5.

The paper presents results from a modelling chain for climate-optimisation in a flight planning tool developed within REACT4C which relies on 4-dimensional climate-cost functions applied to individual weather patterns. Traffic optimization differs between individual weather patterns, hence main characteristics are introduced in brief. Results highlight main characteristics of climate-optimization of flight trajectories, providing an estimate of individual mitigation potentials. Combining these individual optimizations, yield an estimate of the overall global potential mitigation gain of such optimized flight routing measures in terms of climate change.



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