

**18th INTERNATIONAL SYMPOSIUM ON
STABILITY, HANDLING AND USE OF LIQUID FUELS
Louisville, Kentucky USA
September 8 - 12, 2024**

Abstract Summaries

**SESSION 1: FUEL PRODUCTION, OPTIMIZATION AND
CERTIFICATION**

**UTILIZING HYDROISOMERIZATION OF NORMAL PARAFFINS TO IMPROVE
COLD FLOW PROPERTIES AND ENHANCE STORAGE AND TRANSPORT
LOGISTICS**

Victoria Kompanijec, Mahlet Garedew, Chi Chen, Stafford Sheehan, Cheryl Leong
Air Company

Sustainable aviation fuel (SAF) is a revolutionary synthetic alternative to jet fuel, with an aim to significantly reduce the environmental impacts of air travel. Jet fuels need both thermal and storage stability to prevent deposits and degradation over time, ensuring safe and efficient flight operations and improving fuel handling logistics. As such, synthetic fuels should have comparable stability to conventional fuels that are currently approved and in circulation. This can be challenging due to byproducts formed during chemical reactions, so downstream processing of synthetic fuels is often needed. SAF may contain all four of the major hydrocarbon components of jet fuel: isoparaffins, normal paraffins (n-paraffins), cycloparaffins and aromatics. Each of these play an important role in achieving the desired performance and safety of the fuel. Isoparaffins are branched-chain molecules that contribute to improved cold-flow performance: a critical property when operating at high altitudes and for storage at low temperatures. In our CO₂-to-SAF process, we obtain primarily linear n-paraffin chains, so hydroisomerization must be done to form isomers before it can be used for fuel blending. This study investigates the catalytic effect of a precious metal supported on a silica-alumina material in lowering the freezing point of a model fuel, following ASTM methodologies. This study showcases the potential in CO₂-to-paraffin for formulating fuel for use and storage at lower temperatures, given the efficiency and simplicity of the hydroisomerization process.

IMPROVING THE QUALITY OF ADVANCED RECYCLED OILS

Joseph L Stark, Paul Biggerstaff, Randy Garver
Innospec Fuels Specialties

The demand for plastics has steadily increased since production began in the early 1950s due its durable yet light weight properties and flexibility to be used in a variety of forms to improve our daily lives. Plastics are utilized in nearly all aspects of our daily lives in, from healthcare, food packaging, clothing, and building materials just to name a few. Over 400 million tons of plastic are produced globally per year, and this volume is expected to triple by 2050. The majority of plastic ends up in landfills as waste. Currently only around 9% of plastic is recycled through traditional mechanical methods and those plastics suitable for mechanical recycling can only go

through the process once or twice before the plastic degrades beyond additional use. Recent innovations in advanced recycling, such as pyrolyzation, allows for plastic waste to be broken down into its original building blocks. The oil generated through pyrolysis can be recycled infinitely in petrochemical facilities to remake plastic in a circular process. Pyrolysis oil can also be sent to refineries as a feedstock to process units or fractionated directly into fuels. Waste plastic pyrolysis oil (WPPO) generated from advanced recycling tends to be highly olefinic, contain a high concentration of long chain carbon waxes and may be corrosive due to high levels of acidic compounds. In this paper, the cold flow properties, and thermal and oxidative stability properties, of WPPO will be reviewed. Potential solutions for mitigating instability, reducing the potential for fouling issues during process, storage, and transport, and improving the flow properties of these oils will be discussed.

UNIQUE ORGANIC CARBONATE BASED SOLVENTS DERIVED FROM CO₂ FOR SULFUR REMOVAL TECHNOLOGY

Sankaran Murugesan, Onome Ugono, Sai Pinappu

Baker Hughes

The presence of unreactive organic sulfur species in hydrocarbon stream cause both operational and environmental problems. As such regulatory bodies set limits to the allowable amounts of these contaminants present in finished fuels. These serve as the required specifications for those finished fuel streams. In order to meet these specifications several approaches are used to remove the sulfur compounds. Harsh chemicals like caustic are widely employed to remove these sulfur bearing impurities. However, in many circumstances, caustics and other chemicals are unable to effectively reduce the amount of these organosulfur impurities to the required levels. This paper presents the development of an environmentally responsible solvent medium to remove sulfur compounds. This class of solvents (organic carbonates) is derived from CO₂. The efficiency of the extraction of the sulfur compounds was studied for different hydrocarbon stream and also across the two process phases i.e., gas-liquid and liquid-liquid. The sulfur species carrying capacity and number of cycles required for efficient extraction were also analyzed. Furthermore, the regeneration and reuse of this solvent system was also explored. The observations from this study offered an improved process for organosulfur removal comparing to commercially available alternatives.

STORAGE, HANDLING AND COMBUSTION OF A NOVEL HEATING FUEL: EL

Ryan Kerr, Thomas Butcher, Neehad Islam

NORA

The liquid heating market is currently moving towards using more renewable fuels. While biodiesel and hydrogenated vegetable oil, derived from seed oil, and waste materials has had the most impact to date, the industry is looking toward other, cellulosic fuels for the future. One of the fuels that has generated interest is ethyl levulinate (EL). EL is a second-generation biofuel, derived from the mild acid hydrolysis of wood waste and other materials. NORA has developed a process for the evaluation of this fuel through storage, handling, and combustion which can lead to optimization of the role that such a fuel can play in the market. Fuel factors such as conditions under which it is miscible with current fuels, low temperature performance, storage stability, elastomer compatibility, corrosion potential, and combustion performance have been included. The project team is currently working toward the development of a draft specification standard for commercially produced EL. The current areas of focus on EL are the long-term storage changes

of the fuel and the effects it could have on the steel tanks commonly found in the heating oil industry. While this work has been focused specifically on EL the qualification process can be applied to other candidate biofuels for use in this market sector.

SESSION 2: ANALYTICAL TECHNIQUE DEVELOPMENT

USING GC×GC-TOFMS AND COMPARATIVE DATA ANALYSIS SOFTWARE TO GAIN A DEEPER UNDERSTANDING OF CHEMICAL COMPOSITION CHANGES IN FUEL STUDIES

Robert E. Synovec¹, Grant S. Ochoa¹, Timothy J. Trinklein¹, Caitlin N. Cain¹, Austin D. Dobrecevic¹, Matthew C. Billingsley²

¹*Department of Chemistry, University of Washington;* ²*Air Force Research Laboratory/RQRC*

Kerosene-based jet and rocket fuels such as Jet A, JP-8, RP-1, and RP-2 are ubiquitous to aerospace propulsion. There is an ongoing need to more fully assess fuel composition to improve quantitative connections between fuel composition, properties, and system performance. To this end, we apply comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry (GC×GC-TOFMS) and multivariate “chemometric” data analysis to understand how fuel performance depends upon chemical composition, which varies due to production changes and operational handling and use scenarios. Two fuel studies will be presented. First, selective analysis of olefins using bromination chemistry was applied to gasoline, followed by GC×GC-TOFMS analysis of the original and brominated gasoline samples. The data was analyzed to pinpoint chromatographic regions distinguishing the original and brominated samples, with all of the olefins readily discovered. This study has broad implications using selective reaction chemistry to facilitate supervised discovery by targeting compound classes of interest. In the second study, solid phase extraction (SPE) is employed to target polar compounds in fuel. Treating fuel samples with SPE facilitates removal/analysis of specific compound classes, such as oxygenates, allowing for the creation of an altered “pass” sample, identical to the original “neat” sample except for the extracted polar compounds. These neat versus pass samples are analyzed to provide a global discovery of compounds affected by the SPE procedure. This second study has significant ramifications for providing an accurate assessment of the deleterious compounds in fuels, which is essential to confidently relate fuel composition to thermal stability and performance.

CHALLENGES AND INSIGHTS IN APPLYING AVIATION FUEL ADVANCED COMPOSITIONAL METHODS TO DIESEL FUELS

N. Scott Bergey¹, Lena E. Flynn¹, Terrence W. Dickerson¹, Richard A. Kamin¹, Corrianna R. Boucher², Eric M. Johnson²;

¹*U.S. Navy;* ²*Peraton*

The industry focus on understanding aviation fuel thermal stability issues has led to the development of powerful analytical techniques to characterize aviation fuel composition. Some of these methods are readily applicable to diesel fuels and require little or no additional optimization to produce similar quality results, while others require significant additional refinement to be applicable across fuel classes. This work highlights recent developments by the US Navy to expand upon and optimize the joint Air Force/Navy SPE-GC×GC-FID extractable polars methodology to be applied to diesel fuels. This expansion includes the development of a method which

characterizes the LIA content in marine fuels, an analyte class that is uniquely prevalent in diesel fuels and create analytical challenges for GCxGC inlets and column chemistries.

EVALUATING DIESEL BLENDSTOCKS AND COPROCESSED PRODUCTS VIA SPE-GCXGC-QTOF

Richard J. Bell¹, N. Scott Bergey², Grace E. Greene³, Lena E. Flynn², Terrence W. Dickerson², Richard A. Kamin²

¹Peraton; ²U.S. Navy; ³Purdue University

The United States Department of Defense (DoD) uses multiple fuel types for tactical vehicle, ship, and aircraft propulsion. Recent emphasis on trace heteroatomic composition and advanced algorithmic modelling has led to the US Navy developing several analytical tools for trace-level characterization of Navy tactical fuels. Extractable polar nitrogen- and oxygen-containing species have typically been measured using GCxGC analyses using FID and/or single quadrupole MS detectors, but these detectors rely on relative elution times and low-confidence mass spectral assignments to speciate analytes. The United States Navy has recently acquired a state-of-the-art GCxGC-QToF system which significantly improves the 2D resolution as well as mass accuracy of previous instrumentation, allowing for greater molecular specificity. This work highlights recent developments using the GCxGC-QToF system by comparing molecular assignments between petroleum-based diesel fuels and their sustainable production pathway analogs to identify whether analytes eluting in similar regions are truly identical for petroleum versus sustainable diesel fuels or if sustainable production pathways are introducing new trace-level oxygenated moieties.

WATER AND COMPOSITIONAL ANALYSIS IN LIQUID PETROLEUM GASES (LPGS) WITH THE NEW VUV LUMA GC DETECTOR

Dan Wispinski¹, Chris Goss²

¹VUV Analytics; ²InnoTech Alberta

Improved test methods to measure water in LPG have long been an industry need. Propane dryness is monitored with a “functional” valve freeze test. The venting of LPG inherent to the D2713 Valve Freeze method is a safety hazard. The valve freeze test cannot be adapted to on-line analysis or process control. Methanol in the range of 50 to a maximum of 200ppmv is used to mitigate wet LPG problems that occur at sub-saturation levels. This presentation describes a new test method using gas chromatography (GC) separations and the deconvolution (spectral) power of the VUV LUMA for water and methanol (antifreeze agent) in propane. The analysis of ethyl mercaptan (odorant) and hydrocarbon composition of propane (ASTM D2163) is also demonstrated. This single GC run on the VUV LUMA can also detect oxygen, carbon dioxide and hydrogen sulfide.

PREDICTING NON-CO2 ENVIRONMENTAL IMPACTS OF SUSTAINABLE AVIATION FUELS THROUGH PRESCREENING STAGE

Mohammad Reza Ghaani

School of Engineering, Trinity College Dublin, Ireland

As the aviation industry moves towards Sustainable Aviation Fuels (SAF) to reduce its environmental impact, understanding all emissions, not just CO₂, becomes crucial. This study focuses on predicting non-CO₂ emissions, specifically Particulate Matter (PM) and Black Carbon (BC), from SAF using a novel approach. We use 1H-13C Nuclear Magnetic Resonance (NMR)

spectroscopy to analyze the aromatic content of SAF, since aromatics are known to influence PM and BC emissions during fuel combustion. By correlating the aromatic structures identified by NMR with existing emissions data, we develop a machine learning model that predicts the potential for PM and BC emissions in new SAF formulations. This method allows for early-stage assessment of SAF's environmental impact, guiding the development of cleaner fuels. Our initial results highlight the effectiveness of combining NMR analysis with machine learning for environmental impact prediction, offering a pathway towards more sustainable aviation fuel development.

SESSION 3: FUEL SUPPLY CHAIN, STORAGE, HANDLING AND LOGISTICS

TECHNOLOGY DEVELOPMENT OF MOTOR GASOLINE STORAGE IN SALT CAVERNS WITH ASPECTS OF QUALITY PREDICTION, STORAGE AND END-USE.

Arkadiusz Majoch, Jacek Tomaszewski, Łukasz Plis, Zuzanna Rataj
ORLEN S.A. (POLAND)

The growing demand for fuels obtained from crude oil is directly related to the need to increase their stocks. This translates into investments in the expansion of logistics infrastructure, including alternative storage techniques. In Poland, due to favorable geological conditions (availability of salt geological structures), salt caverns are used for long-term storage of hydrocarbons, where crude oil, natural gas and diesel fuel reserves have been successfully stored for years. There are also attempts to apply this technique to the storage of motor gasoline, especially in the face of relatively little practical experience in storage of motor gasoline in salt caverns. In 2016, ORLEN S.A. (refining and pet-chem company) launched the project "Methodology for forecasting and monitoring the quality of gasoline directed for long-term storage in salt caverns, abbreviated as "GASSTO", co-financed by the European Regional Development Fund. The aim of the Project was to develop in laboratory conditions, using the knowledge of ORLEN S.A. employees and external experts, base gasoline blends, the suitability of which for long-term storage in caverns was verified. This was done through an appropriately selected and program of research and testing. Laboratory studies and tests mimicking the conditions of real storage were the basis for developing a method for monitoring gasoline quality during storage in the cavern, as well as technology for producing final gasoline from base gasoline after the storage period. The culmination of the project was the industrial-scale production (40,000 m³) of a gasoline blend selected on the basis of the research and pumped into an real salt cavern. The presentation will cover the results of the project, including an abbreviated review of global and Polish experience in testing the feasibility of storing gasoline in salt caverns and a presentation of the method developed for predicting the properties, production technology and quality monitoring system of gasoline for long-term storage in salt caverns.

NAVIGATING FUEL INTEGRITY CHALLENGES IN BULK STORAGE FACILITIES

Dr. David Evans¹, Nathan Matheson¹, Dr Ulas Yildirim²

¹Defence Science and Technology Group; ²Royal Australian Air Force

Contamination incidents within bulk storage facilities pose substantial operational hurdles for companies and organisations. This paper offers an in-depth analysis of multiple contamination

events within a 5 million litre diesel storage tank. It explores the ongoing struggle between procurement specifications, degradation thresholds, and the essential fit-for-purpose properties when managing in-service issues. Specifically, it investigates a case involving a 5 million litre diesel storage tank utilised as an intermediate quarantine facility, where off-specification fuel was inadvertently introduced into the system. Through this case study, the paper highlights the complexities of maintaining fuel integrity in storage facilities and offers insights into effective mitigation strategies and preventive measures.

RE-EVALUATION OF ASTM D5304: DETAILED COMPARISON OF STORAGE STABILITY METHODS THROUGH THE ANALYSIS OF LIQUID-PHASE CHEMISTRY

Thomas Loegel, Mark Romanczyk, Kristina M. Myers², Robert E. Morris², Jacob Guthrie²
¹Naval Research Laboratory; ²Nova Research, Inc

Evidence suggests that ASTM D5304 may not provide accurate assessments of storage stability for hydrorefined fuels, such as ultralow sulfur diesel (ULSD) or other hydrotreated diesel fuels. ASTM D5304 was developed with legacy high sulfur F-76 fuels, but hydrorefined or alternative fuels that do not contain natural oxidation inhibitors can react non-linearly under the accelerated conditions in ASTM D5304 with respect to ambient storage. Previous attempts to accomplish this critical work was hampered by the lack of sensitivity to track the chemical changes occurring in fuels. High-resolution mass spectrometry (HRMS) demonstrated to be more sensitive than previous GC-MS techniques and able to monitor changes in heteroatomic species within fuel. This study is intended to develop baseline information that can facilitate the development of an improved storage stability test method appropriate for diesel fuels currently being produced focusing on ASTM D5304, ASTM D2274, ASTM D4625, and ASTM D7545. Three aspects of this issue focus on (1) liquid phase chemistry of stressed fuels using HRMS to determine the conditions under which an accelerated test crosses the regime from probable storage related chemistry to forced high temperature reactions (2) linking chemistry to stability performance, and (3) determine potential detection methods and changes that will allow for accelerated storage testing under conditions that more closely approximate ambient fuel storage.

SESSION 4: FUEL QUALITY CONTROL

DEMONSTRABLE QA STANDARDS IN THE SPECIFICATION, PROCUREMENT, DELIVERY AND STORAGE OF LIQUID FUELS FOR USE IN EMERGENCY GENERATORS AND OTHER PLANT

Carl Atkinson
EDF Energy

As end users of liquid fuels, a number of industries and other applications require the systems fuelled to be permanently available. These include essential emergency power supplies for data centres, communications, hospitals, and, together with various essential back-up plant systems, on power stations. In order to ensure that such systems perform as expected on demand the fuel quality must meet strict control standards from initial specification through to its ultimate consumption. In the case of nuclear power stations, particularly, the quality assured process must also be demonstrable. This presentation describes the control standards and quality assured measures in

place and how these standards are maintained and demonstrated from the point of procurement of liquid fuels through to their ultimate consumption. Additionally, the process includes a continual review of external factors that could positively or negatively affect the measures currently in place internal to the organisation (e.g. changes to international or British standards, information gathering via international conferences such as IASH). The presentation also details the corrective action process that is invoked when anomalies or shortfalls are identified, corrective actions monitored through to their close-out on completion, and, the process of effectiveness reviews (or equivalent) to evaluate the success (or otherwise) of measures implemented.

PARTIAL SURVEY OF AVIATION TURBINE FUEL IMPURITIES: CONTROLS AND EFFECTS

Randall C. Boehm¹, Joshua S. Heyne²

¹*Washington State University*; ²*Washington State University and Pacific Northwest National Laboratory*

The standard practice for evaluation of new aviation turbine fuels and fuel additive (ASTM D4054) lists 53 materials (classes-of or specific elements or molecules) whose concentration in fuel should be less than 1%_m. Additionally, 18 properties that could be impacted significantly by trace levels of certain materials in fuel are cited in that method, each with some controlling guidance. In this work we a connection between these fuel requirements and the potential issues they are intended to prevent. Potential issues include excessive deposition of solid or gelatinous material anywhere within the aircraft/engine fuel system or even systems upstream of the aircraft, material compatibility throughout the fuel system and extending into the hot section of the engine and including compatibility with additives, wear considerations, and fuel toxicity or other safety considerations. They may also include factors such as confounding influence on deposit forensics which could make it even harder to diagnose the source of contamination that may lead to an unscheduled engine removal (or worse). Our intention here is to highlight published works that address some of these issues and to document where gaps exist in the archival literature.

MEASUREMENT OF JET FUEL INTERFACIAL TENSION AND ITS RELATION TO MICRO-SEPAROMETER DATA

Shane Kosir¹, Susan Mueller², Zachary West², Paul Wrzesinski³

¹*University of Dayton Research Institute*; ²*University of Dayton Research Institute*; ³*Air Force Research Laboratory*

Surfactants are undesirable compounds in jet fuel since they can compromise fuel filter/separator systems, which could allow dirt and water to pass through and damage engine components. While ASTM standard methods (i.e., D3948 and D7224) are known to respond to some surfactants, there is a lack of knowledge linking these standards to fundamental fuel properties, i.e., fuel-water interfacial tension (IFT) and fuel-air surface tension (ST). The primary focus of this effort was to develop correlations between IFT, ST, and micro-separometer (MSEP) data for various surfactants. IFT, ST, and MSEP were measured for a series of F-24 and Jet A fuels to explore the relationship between the various test methods. It was found that IFT correlated moderately with MSEP for the fuels tested (R² of 0.42) while ST did not correlate with MSEP (R² of 0.02). Two-dimensional gas chromatography (GCxGC) hydrocarbon-type and polars data were collected and analyzed for the fuels. The GCxGC data indicated that IFT was correlated to the total polars concentration, while MSEP was more sensitive to the bulk fuel composition. The effects of corrosion inhibitor/lubricity improver (CI/LI) and firefighting foam (FFF) over a range of

concentrations were studied by doping fuels with known concentrations of each additive and measuring IFT, ST, and MSEP. IFT was found to follow an exponential decay function with additive concentration, while ST was less responsive.

INSIGHT INTO SAMPLING PROCESSES OF AVIATION FUEL²

Moshe Rabaev¹, Liel Mazar¹, Yalfal Siyum¹, Haim Judah¹, Dr. Fred Passman²

¹*Israeli Air Force*; ²*Biodeterioration Control Associates Inc.*

For aviation to be safe and successful, it is essential to have a constant supply of high-quality fuel, which is ensured by using appropriate sampling for testing. This chapter begins with a discussion of official standards as well as other literature related to fuel sampling in different storage locations, during transport, and from aircraft fuel tanks. A description of sampling points from tanks and fuel lines, sampling tools, and containers for samples is provided for specific types of storage vessels. In some cases, problems may occur due to local defects, such as poorly positioned sampling valves, or sloping sections of piping or vessel floors. Methods for ensuring that representative or diagnostic samples are obtained from fuel lines or tanks are discussed. In the context of aircraft fuel tanks, sampling is a particular challenge due to safety concerns and spatial constraints. Aside from routine sampling procedures, accidents, and other flight incidents often necessitate sample collection for forensic purposes. Such cases may require sampling filters installed on fuel lines, dismantling various types of filters, and recovering filter residues. Lastly, a detailed discussion is provided on the important topic of sampling for microbiological tests.

MODIFIED CERAMIC MEMBRANES FOR CARBON CIRCULARITY: FROM LUBE OIL PURIFICATION TO CHEMICAL RECYCLING OF PLASTICS

Pieter Vandezande

Flemish Institute for Technological Research (VITO), Materials and Chemistry Department (MATCH)

For decades, mankind has been living in a ‘make, take, dispose’ economic model. Plastics, with their unrivalled properties and low cost, are an exponent of this way of living. While plastics production reached 391 million tons in 2021, it is estimated that today nearly 50% of the plastic waste in the EU is landfilled, roughly 25% incinerated and only 25% recycled. Another example are used lubricating oils (ULO), equally derived from fossil feedstocks and essential in a wide range of industrial applications, but today recycled only to a limited extent and not in the most energy-efficient way. To mitigate greenhouse gas emissions, recent EU legislation calls for far higher recovery and recycling rates of these materials at the end of their service lifetime. Thanks to their inherently energy-efficient, mild and clean character, as well as flexibility and scalability, membrane processes are fully aligned with current industry drivers towards electrification, carbon circularity and zero/minimal liquid discharge. Therefore, membranes are considered a powerful tool, even key enabling technology, for tackling tomorrow’s separation challenges in chemical related industries. Recovery of base lubricating oils from solvent-free ULOs and of virgin polymers from solvent-based plastics mixtures, targeting removal of critical impurities such as lube oil and plastics additives, calls for robust membranes that can cope with high viscosities and work at elevated temperatures. To address these challenges, tubular ceramic membranes with tailored surface chemistry are being studied on various real life ULO and waste plastics cases. This research fits in the ongoing EU project CUMERI and Flemish project RENOVATE, where VITO is collaborating with several other research institutes and companies on membrane technology development for ULO purification and dissolution-based plastics recycling, respectively. By

facilitating recycling and reuse, both projects aim at tackling the global challenge of climate neutrality while contributing to enhanced circularity and resilience in these industries.

SESSION 5. FUEL CHEMISTRY, RESEARCH AND DEVELOPMENT

IMPACT OF SBCS ON THE BEHAVIOUR OF POLYMER MATERIALS AND EFFECT OF FUEL CYCLING

Mickaël Sicard, Bruno Raepsaet, Duc Minh Le, Yanis Melliti, Frédéric Ser

ONERA

As it travels through the fuel system, kerosene comes into contact with a wide range of materials. To avoid any leaks or malfunctions, it is essential to ensure fuel/material compatibility. A large number of tests are carried out as part of the ASTM D4054 certification process for alternative fuels (SBC). As a result, SBCs can be used safely in blends of up to 50 % in fossil fuels. The next step is to study their behavior in a pure state. The compatibility of three SBCs and three types of O-ring was assessed using the ASTM D4054 procedure. The three SBCs tested were HEFA, ATJ and an alkane/cycloalkane mixture. One of the interests of this study was also to observe the behavior of cycloalkanes, which had not yet been characterized. The results show that these molecules behave more like alkanes. The other objective was to assess the impact of fuel cycling on materials. It is clear that on a daily basis the chemical composition of kerosene varies, especially if SBCs are used. So we also need to assess the behavior of materials subjected to successive fuels. As a first step, simple Jet/SBC or SBC/Jet cycling was evaluated. Cycling had no significant effect on the mechanical properties of the nitrile and fluorosilicone O-rings. Cycling did, however, degrade the properties of fluorocarbon seals. Mass variation was also affected. The last fuel used for cycling had a very marked impact on the variation in mass, which returned to values close to those of the pure fuel.

DIGITAL TRANSFORMATION OF FUEL PROPERTY AND COMPOSITION DATA FOR THE RAPID ASSESSMENT OF CONVENTIONAL AND SYNTHETIC FUELS

Terrence W. Dickerson, Fernando Morales, Fausto Reyher, Richard A. Kamin

Naval Air Systems Command

By leveraging the Department of Defense's vast logistics system and the DOD-developed standardized method for characterization of hydrocarbon composition, the U.S. Navy has accumulated specification property and hydrocarbon composition data for over 1,800 aviation turbine and marine diesel fuels from around the world. The U.S. Navy has designed and implemented a custom, web-based data analysis system to clean, consolidate, display, and analyze this information. This paper presents the Navy's research and development in data analytics to accelerate the rapid assessment of conventional and synthetic fuels based on fuel properties (specification and fit-for-purpose), hydrocarbon composition and their effect on the performance of critical hardware. This paper will summarize the available property, composition, and hardware datasets, analytic tools, and machine learning techniques utilized to assess fuels. Example case studies will be presented to demonstrate the system's use of conventional data techniques and machine learning to provide a comprehensive assessment of a fuel's fit-for-use. The paper concludes with a review of how data analytic tools could be used to enhance evaluations of new

fuels and notable challenges associated with developing those tools and acquiring the requisite datasets.

SESSION 6. FUEL PROPERTIES AND EFFECTS

CHARACTERIZATION OF COMPOSITIONAL EFFECTS ON THE DIELECTRIC CONSTANT FOR BLENDS OF AVIATION FUEL SYNTHETIC BLEND COMPONENTS AND PETROLEUM-BASED AVIATION FUELS

Shane Kosir, April Landsaw, Zachary West, Steven Zabarnick
University of Dayton Research Institute

The dielectric constant is used in aviation for fuel gauging, namely for the determination of fuel volume and density. Synthetic blend components (SBCs) have compositions that may be different from petroleum-based fuels, which can potentially affect the dielectric constant, its relationship with fuel density, and thus the ability to accurately gauge fuel quantity. This work explored the effect of SBC blends with each other and with a petroleum-based Jet A fuel. The dielectric constant was found to be positively correlated with density, with cycloparaffinic kerosene (CPK) blends deviating from the other SBCs. Partial least squares regression using hydrocarbon-type composition features indicates that the dielectric constant is positively correlated with aromatics (i.e., mono and cycloaromatics) and negatively correlated with aliphatics (i.e., iso- and n-alkanes). Clausius-Mossotti (CM) plots were generated using data from 0-40°C to explore the effect of fuel composition on density gauging. The CM slope was found to deviate from Jet A for the SBC/Jet A blends. Specifically, the CM slope decreased for low-aromatic SBCs such as alcohol-to-jet (ATJ) and CPK and increased for high-aromatic SBCs, namely synthetic aromatic kerosene (SAK). R² values were high for the CM plots except for CPK, possibly due to its divergent correlation with density. Despite the variation of the CM slope with fuel composition, the average density error was only 0.15% for all the blends and temperatures tested.

LOW TEMPERATURE BEHAVIOR OF RENEWABLE DIESEL AND BLENDS WITH PETROLEUM DIESEL

Suzanne Golisz, Jessica Grabowski
Innospec Fuel Specialties

Use of renewable diesel (a.k.a. hydrogenated vegetable oil, HVO) is growing worldwide. While it's tempting to think of renewable diesel as a drop-in replacement for petroleum diesel, we have determined that extra consideration is required for the use of renewable diesel in cold climates. This paper is an extension of our previous paper looking at blends of up to 20 volume % renewable diesel in petroleum diesel. We have now widened the range of blending and included blends of renewable diesel in petroleum kerosene. Our primary modes of investigation have been to measure the cloud point, cold filter plugging point (CFPP), and pour point of these blends. Further, we have investigated the role of cold flow improvers and pour point depressants in lowering the CFPP and pour point. We found that additives continue to provide benefits. Lastly, we have evaluated renewable diesel and blends of renewable diesel using a cold stage microscope. These experiments clearly show a difference in the wax crystallization behavior in renewable diesel versus petroleum diesel.

LOW TEMPERATURE DIELECTRIC CONSTANT MEASUREMENT OF JET FUEL CONSTITUENTS TO ENABLE 100% SAF

Harrison Yang, David Bell, Conor Faulhaber, Randall Boehm, Joshua Heyne
Washington State University

Modern aircraft often employ capacitance-based gauging systems that rely on the dielectric constant of the fuel onboard to determine fuel quantity. Aircraft manufacturers have expressed concern over inaccuracies in fuel gauging attributed to variances in the dielectric constant between conventional jet fuels and 100% paraffinic sustainable aviation fuel. Our previous study showed that different hydrocarbon group types exert varying effects on the Clausius-Mossotti relationship. To align with the established experience range for both the dielectric constant and the Clausius-Mossotti relationship, it appears that 100% drop-in SAF will need to incorporate some aromatic compounds. The standard procedure for assessing the dielectric constant (outlined in IP 638) is limited to a temperature range of 10 to 30°C. However, this range does not account for the broader spectrum of temperatures encountered by aircraft fuel, which can range from -40 to 50°C. Currently, there is a notable gap in the literature regarding the measurement of SAF's dielectric constant at lower temperatures. This study aims to bridge this gap by investigating the dielectric constant of SAF and various jet fuel components at lower temperatures, extending the measurement range beyond the current standard.

ENGINE PERFORMANCE AND EMISSIONS: A MODEL-BASED ASSESSMENT OF ADDED VALUES OF SUSTAINABLE AVIATION FUELS (SAF)

Stephan Ruoff, Georg Eckel, Uwe Bauder, Patrick Le Clercq, Manfred Aigner
German Aerospace Center (DLR)

The approval and production of Sustainable Aviation Fuels (SAF) has gained significant momentum in recent years. With the aviation industry's commitment to reducing its environmental and climate impact, SAF offers a promising solution for mitigating CO₂ emissions. Moreover, besides the reduction in greenhouse gas emissions, SAF offers additional benefits, such as reducing non-CO₂ effects or increasing the fuel's energy content. However, besides the constraints imposed by the ASTM specifications, there is also a tradeoff between certain performance and emission metrics. Therefore, a comprehensive tool which can help gaining an overview about different metrics and identifying limiting factors, is developed. In this study, various blend ratios of representative Jet-fuels and Synthetic Blend Components (SBCs) (including ATJ, FT-SPK, and HEFA) are investigated on the added values and current constraints enforced by the ASTM limits. Machine Learning are utilized to predict fuel properties from a given GCxGC composition. Empirical correlations are then employed to predict metrics for performance and emissions, including soot formation and Lean Blow Off (LBO) behavior as well as combustion related subprocesses like atomization and evaporation. The findings indicate that even a low percentage of SBC has a substantial impact on improving jet fuel performance. However, the potential added values depend on the jet-fuel used for blending. Moreover, the addition of SBC significantly reduces the aromatics content in jet fuels, so that the current limits for aromatics are undercut.

FROM MARGINAL FUEL TO 100% FT-SPK: THE IMPACT OF HYDROTREATING ON FUEL SYSTEM PERFORMANCE – THERMAL STABILITY AND LUBRICITY BEHAVIOUR AND IMPLICATIONS FOR FUEL SYSTEM DESIGN

Simon Blakey¹, Ehsan Alborzi², Spiros Siorus²
¹*University of Birmingham*; ²*The University of Sheffield*

The performance of 4 fuels are assessed using the AFTSTU rig, from marginal fuel with a JFTOT breakpoint of 260°C, through to 100%FT-SPK with a breakpoint >340°C. The performance of the fuels are assessed in terms of their interaction with the simulated fuel system in the AFTSTU rig in terms of thermal stability and lubricity performance during an accelerated test procedure intended to simulate 10,000 hours of in-service operation. JFTOT breakpoint and HiReTS tests were also conducted with the fuels. Throughout the testing, improved thermal stability performance was observed as the breakpoint of the fuel increased. The performance of the fuels in the AFTSTU rig give an indication of the anticipated performance on engine over extended periods of operation and show the significant improvement in performance of the 100% FT-SPK compared to conventional fuels. The testing observed undesirable effects as well as improvements, specifically around the lubricity of the 100% FT-SPK which required additive packages to be dosed into the fuel to allow testing in the rig at this extreme of fuel composition. The impacts of this change for fuel system design are discussed and the potential opportunities offered by 100% FT-SPK are quantified in terms of service life and potential for sfc reduction. This study combines work funded from the JETSCREEN, ALFABIRD and QSTP programmes along with industrial funding for the marginal fuel case.

MINIMIZING AROMATICS CONTENT IN 100% 'DROP-IN' SUSTAINABLE AVIATION FUEL

Conor Faulhaber, Randall Boehm, David Bell, Zhibin Yang, Joshua Heyne
Washington State University Tri-Cities

Decarbonizing commercial aviation within the timeframe of current industry goals requires significant upticks in the production and usage of sustainable aviation fuel (SAF). ‘Drop-in’ SAFs produced from renewable energy crop or waste feedstocks can expedite the removal of fossil carbon from aviation fuel by meeting the safety, operability, and performance needs of existing aircraft and engine designs. Current paraffinic SAF pathways often struggle to demonstrate some of these conventional fuel properties, namely dielectric constant and elastomer seal swell, as a result of low aromatic content. To regulate this, SAF blends with conventional fuels are required to contain $\geq 8\%$ aromatics content per ASTM specifications. However, aromatic species in jet fuel are associated with increased sooting and contrail formation, making low aromatic, ‘drop-in’ SAF blends of high interest to the industry. In comparison, cycloalkanes show potential at increased concentrations to induce adequate seal swell but are less likely to meet dielectric constant requirements. Here, an extensive property database of both jet-range hydrocarbons and real SAF products is used to minimize threshold sooting index (TSI) for potential fuel compositions while remaining within the specification or experience range for conventional fossil jet fuel properties, including predicted dielectric constant and seal swell values. These results are used to inform laboratory-producible fuel blends, allowing for experimental evaluation of the bulk property predictions. In addition to improving understanding of aromatics and cycloalkanes in aviation turbine fuel, this work advises fuel producers, regulatory bodies, and engine/airframe manufacturers on compositional pathways towards 100% ‘drop-in’ SAF.

ASSESSMENT OF THE IMPACT OF ALTERNATIVE FUELS ON THE CETANE VALUES AND PROPOSED MODELS FOR CALCULATING IT

Nathalie Brassart¹, Yanis Melliti², Mickaël Sicard², Amandine Herbaut³, Mickaël Matrat¹
¹IFPEN; ²ONERA; ³CETSEO

NATO's Single Battlefield Fuel Policy recommends the use of JP-8 kerosene as a fuel for DIESEL ground vehicles. A minimum cetane number (CN) of 40 is required to assess jet fuel suitability for ground applications. The large chemical composition variability of sustainable aviation fuels (SBC) leads to lower or high CN compared to fossil jet fuel. Therefore, their incorporation into fossil kerosene might be a source of ignition anomalies (low CN), especially when cold or engine efficiency degradation (high CN). Three conventional jet fuels representative of worldwide variability and four SBCs were used to establish a matrix of 36 blends. The aim was to evaluate the cetane number as a function of SBC incorporation rate and composition. A compositional characterization and determination of the main physico-chemical properties of jet fuels, SBCs and their blends were carried out. Moreover, the CN and derived cetane number (DCN) were measured for all fossil fuels with different SBCs concentrations. The results show a linear dependence of the blend CN evolution with the rate of incorporation of the two initial constituents. Furthermore, the CI, CN and DCN values for fossil kerosenes and most SBCs are very close (≈ 2). ATJ, on the other hand, stands out, with a difference of 40. Finally, two models based on different levels of chemical composition of the blend fuel were developed. An original database is thus provided here. It highlights potential limitations for different SBCs while exploring incorporation rates above the current ASTM limit of 50%.

SESSION 8. THERMAL STABILITY

OXIDATION MECHANISM OF SULFUR-CONTAINING COMPOUNDS AND ANTIOXIDANT DEPLETION DYNAMICS: INSIGHTS INTO INTERACTIONS

Jinxia Fu, Scott Turn

University of Hawaii at Manoa

Sulfur-containing compounds (SCCs) are the most abundant heteroatom compounds in petroleum fuel. This study investigates the thermal stability of SCCs in an air atmosphere and their influence on the depletion of commercial antioxidants (AOs). A total of 11 SCCs, encompassing both reactive (thiols, sulfides, and disulfides) and nonreactive (thiophenes and benzothiazole) species, were subjected to analysis. The reaction and degradation processes of SCCs were tracked by monitoring changes in their concentrations over an extended period, while the resulting products after thermal treatment were analyzed to elucidate oxidation and degradation mechanisms. Additionally, the study scrutinized the depletion kinetics of commercial fuel AOs and quantitatively evaluated the impact of SCCs on AO depletion, uncovering antagonistic interactions. Furthermore, the reactions and interactions among the 11 selected SCCs were investigated to explore potential synergetic or antagonistic effects during the thermal treatment. These findings offer comprehensive insights into the behavior of SCCs and AOs under oxidative conditions, providing valuable guidance for the development of more effective AO formulations and sulfur mitigation strategies for the fuel industry.

AN INNOVATIVE MICROFLUIDIC REACTOR FOR TESTING THE OXIDATION STABILITY OF FUELS: APPLICATION TO A SAF SURROGATE AND COMPARISON WITH THE PETROOXY TEST

Ryma Benrabah, Emilien Girot, Jean-Marc Commenge, René Fournet, Philippe Arnoux, Pierre-Alexandre Glaude, Baptiste Sirjean

Université de Lorraine

One potential solution to diminish the aviation carbon footprint is to blend Sustainable Aviation Fuel (SAF) into jet fuels. However, the thermal stability and oxidation stability of standard jet-fuels may be affected by the addition of SAF [1]. In this work, we developed a Si-glass microfluidic reactor with fluid supply made of inert polyether ether ketone (PEEK). The experimental rig PEEK-ACHU (Autoxidation μ Chip Heated Unit) was used to investigate the oxidation stability of a SAF surrogate in and the results were compared to Induction Period (IP) measures obtained in a standard PetroOxy device. A mixture of n-decane and iso-octane was used as the surrogate SAF [2]. The thermal oxidation stability of the mixtures was measured in the microreactor, working at conditions up to 453 K and 30 bar, with a gas-liquid segmented flow that allows the liquid oxidation to occur in homogeneous, self-agitated liquid slugs. PEEK-ACHU allows residence times as long as 2 hours to be reached on a 4-inches diameter chip, a visual access to the reactor and a well-defined kinetic study of the liquid fuel autoxidation. The total hydroperoxide concentration was quantified at the exit of the microreactor using a specifically designed HPLC device with a post-column reactor [3]. For comparison, the same analysis was conducted on the SAF oxidized in the PetroOxy apparatus, with the same residence time. The results of this study show that the microfluidic apparatus is able to perform reliable autoxidation measurement and allows a better understanding of the kinetics. The self-agitation allows a homogenous phase, and the visual access of the reactor is relevant for other applications, such as spectroscopic monitoring of deposit formation.

UNRAVELLING SUSTAINABLE AVIATION FUEL INTERACTIONS: A STABILITY PERSPECTIVE

Dr. David Evans, Rachele Hewitt, Nathan Matheson
Defence Science and Technology Group

The burgeoning demand for Sustainable Aviation Fuels (SAF) has prompted exploration into various production pathways, yielding eight distinct synthetic blending components (SBCs) vital to SAF supply. While prior demonstrations primarily involved single SBC utilization, our research, presented at the 2022 IASH conference, delves into the production of a neat SAF comprising SBCs from multiple pathways. Leveraging fuel derived through catalytic hydrothermal conversion as the base, chosen for its favourable aromatic levels, we crafted blends incorporating FT-SPK, HEFA-SPK, SIP-SPK, and ATJ-SPK at maximum blend ratios. Thorough testing against D7566 requirements for finished fuel, alongside evaluations of thermal conductivity, enhanced thermal stability, and chemical and physical ignition delay properties, revealed an unforeseen interaction in one blend adversely affecting thermal stability, undetectable in isolated SBC testing. Building upon these initial insights, this paper focuses on isolating polar components to elucidate their impact on fuel stability, offering crucial insights for the sustainable aviation industry.

STUDY OF MOLECULAR INTERACTIONS IN THE LATER STAGE OF JET FUEL SURFACE DEPOSITION: COMBINING AB-INITIO DENSITY FUNCTIONAL THEORY WITH EXPERIMENTAL ANALYSIS

Rahimakhanim Babayeva, Ehsan Alborzi, Kevin J. Hughes, Anthony J. H. M. Meijer, M. Pourkashanian
The University of Sheffield

The rapid expansion of the aviation industry requires improvements in operational efficiency and environmental sustainability. For example, modern aircraft engines employ a higher pressure ratio

to enhance efficiency, leading to an elevated thermal load on the engine lubrication system. This, in turn, increases heat sink requirements. Recognising that aviation fuel serves a secondary role as a heat sink prior to combustion, subjected to thermal stress, undergoes thermal degradation. This situation results in the generation of various soluble chemical species and insoluble macromolecules, contributing collectively to the formation of carbon deposits on surfaces in contact with aviation. The formation of surface deposits is linked to the presence of heteroatomic species such as nitrogen, sulphur, and oxygen-containing species, as well as dissolved metals. This research focuses on the combining quantum chemistry simulations using the Vienna Ab Initio Simulation Package (VASP) and small-scale testing, namely PetroOxy/RapidOxy to study the molecular interactions between some of the heteroatomic species and surface in the course of deposition. We utilised PetroOxy and RapidOxy devices to examine the deposition propensity of specific compounds and surrogate fuels, with a particular emphasis on the later stages of deposition when the C-C interactions become more noticeable. This approach allows for a thorough exploration of the stability and reactivity of adsorbates on various metal surfaces, providing insights into the complex physico-chemical interactions that govern deposit formation.

THERMAL AUTOXIDATION OF CYCLOPARAFFINS: THE NECESSITY FOR A FUEL-SPECIFIC CHEMICAL KINETIC MECHANISM FOR SYNTHETIC FUEL

Ehsan Alborzi¹, Yousef Sadat¹, Matthew Dwyer¹, Xue Yong², Simon Blakey³, Anthony Meijer¹, Mohamed Pourkashanian¹

¹University of Sheffield; ²University of Liverpool; ³University of Birmingham

The composition and proportions of hydrocarbon classes in synthetic aviation fuels diverge from those found in conventional aviation fuels. This highlights the need for more fuel-specific chemical kinetic mechanisms to model the autoxidation behavior of various hydrocarbon classes, for example cycloparaffins. A series of small-scale autoxidation tests were conducted to investigate the autoxidation kinetics of decalin and various decalin-solvent blends composed of five normal paraffins. These experiments utilised PetrOxy and a near-isothermal tubular reactor operating at different temperatures. Inline measurements of oxygen consumption in both test setups revealed distinct autoxidation tendencies for decalin and normal paraffins. Density functional theory was employed to compute the activation energies associated with the autoxidative reactions of decalin and its blends.

COMPARATIVE STUDY OF SURFACE DEPOSITION PROPENSITY ON TWO TYPES OF METAL SURFACES (STAINLESS STEEL AND NICKEL ALLOY) UNDER AERO-ENGINE REPRESENTATIVE CONDITIONS

Xue Yong¹, Ehsan Alborzi², Hassan Ghadbeigi², Morteza Roostaienia³, Simon Blakey⁴, Mohamed Pourkashanian²

¹University of Liverpool; ²University of Sheffield; ³Virginia Polytechnic Institute and State University; ⁴University of Birmingham

It is known that, during thermal oxidative stability, the first stage of fuel deposition processes involves the adsorption of fuel species onto the walls. Stainless steel is often utilised as a substrate for deposition due to its prevalence in inner surfaces along fuel lines in a jet fuel system. In addition to stainless steel, Ni alloys are also employed in the fuel injection system within modern jet engine architecture. However, the molecular interactions between aviation fuel constituents and these surfaces are poorly understood and were investigated in more detail here. Two types of burner feed arms were utilised in the Aviation Fuel Thermal Stability Test Unit (AFTSTU) to replicate

conditions representative of an aero-engine. The deposited tubes were characterised using Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray (EDX) analysis. The chemical composition of aviation fuels (both major constituents and heteroatomic species) were quantified, using comprehensive two-dimensional gas chromatography with thermal modulation. We employed the plane-wave Density Functional Theory (DFT) Vienna Ab-Initio Simulation Package (VASP) to model the fundamental interactions between adsorbates and different wall models.

FURTHER STUDIES OF JET FUEL OXIDATIVE DEPOSIT FORMATION IN QUARTZ CRYSTAL MICROBALANCE EXPERIMENTS

Krege M Christison, Gregory B Boursalian

Chevron

When analyzed by Quartz Crystal Microbalance (QCM) under oxidative conditions there is no deposit formation in hydrocracked jet fuel components due to the severe hydrotreating used in their production, which generally eliminates reactive, polar, and heteroatom-containing molecules. Previous research has shown that the addition of quinolines, aliphatic amines, and cyclohexylpyridines to a hydrocracked jet fuel component leads to increased deposit formation during QCM analysis. Furthermore, the addition of reactive sulfur compounds, specifically mercaptans and sulfides, along with the nitrogen compounds, increases the deposit formation observed. It was also observed that the delayed oxidation from the addition of alkyl phenols led to lower overall deposit formation when combined with reactive sulfur and nitrogen compounds. These previous studies have inspired additional avenues of investigation. A larger quantity of the previously identified cyclohexylpyridine compound has been synthesized for further experimentation. The addition of reactive sulfur compounds on their own are of interest, especially since they are prevalent in unhydrotreated jet fuel components. Certain refinery processes lead to oxidation of mercaptan molecules, forming disulfides, and possibly other sulfur oxides. Therefore, these compounds have been explored, both on their own and in the presence of nitrogen compounds that are known to form deposits. Nitrogen oxides have not been explored previously but could be present due to oxidative processes in refineries and are therefore added to this test matrix.

SESSION 9. MICROBIOLOGICAL CONTAMINATION / MONITORING

GENOMICS AND TRANSCRIPTOMICS ANALYSIS UNVEIL CONSERVED FUNGAL ADAPTIVE MECHANISMS ESSENTIAL FOR THRIVING AND PROLIFERATING IN TOXIC HYDROCARBON ENVIRONMENTS

Osman Radwan¹; Oscar N. Ruiz²

¹University of Dayton Research Institute; ²Biomaterials Branch, Materials and Manufacturing Directorate, Air Force Research Laboratory

Fungal contamination in fuel has substantial effects on production, transport, and storage. This project aimed to comprehend fungal adaptation to toxic fuel environments through advanced genomics, transcriptomics, and bioinformatics tools. Genomes of filamentous fungi and yeast species, including *Byssoschlamys* sp., *Lecanicillium* sp., *Fusarium fujikuroi*, *Aspergillus versicolor*, *Graphium* sp., *Yarrowia lipolytica* ATCC20496, and *Meyerozyma guilliermondii*, were sequenced using next-generation sequencing, followed by bioinformatic analysis for genome

assembly and annotation. Comparative genomics and local BlastP searches against databases such as Pfam, COG, and KOG revealed that fungal genomes harbor gene functional categories linked to energy production, carbohydrate, amino acid, and lipid transport, and metabolism. Additionally, RNA-Seq technology was employed to profile gene expression in fungal species growing in either Sodium Acetate or Jet A fuel. The study included three fungal species: *Hormoconis resiniae* ATCC22711, *Byssoschlamyss* sp., and *Y. lipolytica* ATCC20496. RNA-Seq data unveiled differentially expressed genes and pathways crucial for microbial adaptation to hydrocarbon fuels, demonstrating similar regulatory patterns across diverse fungal species. These genes involved in the uptake and extrusion of hydrocarbon via membrane protein channels and efflux pumps, iron acquisition, hydrocarbon degradation using monooxygenases and hydroxylases, and biofilm formation. Results suggest that fuel fungal adaptation take place via conserved global mechanisms that provide the capacity to the fungal cell for survival and proliferation to the toxic environments. The global mechanisms identified through this study may become important targets for potential applications in developing biomanufacturing and fungal detection-mitigation technologies for fuel system biodeterioration prevention.

GRAPHENE OXIDE-BASED BIOFILTRATION: UNVEILING ITS POTENTIAL IN ESTABLISHING MICROBIAL FUEL FILTER

Moshan S. Kahandawala¹, Osman Radwan¹, Forood Karimzadeh¹, Amanda L. Barry-Schroeder¹, KA Shiral Fernando¹, Oscar N. Ruiz²

¹*University of Dayton Research Institute*; ²*Materials and Manufacturing Directorate, Air Force Research Laboratory*

Microbial contamination in fuel poses challenges in military and civilian applications, leading to reduced fuel quality, stability issues, tank biocorrosion, filter plugging, and coating degradation. Graphene Oxide (GO) is a promising nanomaterial for various biomanufacturing and biotechnological applications. In this study, we investigated the potential of developing a GO-based microbial fuel filter capable of efficiently removing bacteria with a diameter as low as 0.5 μm without causing a significant increase in pressure. The development progressed from a laboratory prototype to a field-ready filter for practical applications. The developed filters were designed with the goal of achieving a pressure loss below 7 PSI and a removal efficiency surpassing 90% for contaminated fuel (>4000 CFU/L), as determined by initial field assessments. Samples collected at intervals, where 100,000 gallons of fuel passed through a 10 GPM filter consisting of four 2.5 GPM filter modules, demonstrated no impact on fuel quality. Endurance testing using a 2.5 GPM filter module revealed a removal efficiency exceeding 99% after passing 25,000 gallons of fuel, removing over 10 billion cells. Similarly, endurance testing with the 0.3 LPM filter indicated a removal efficiency of over 99% after passing 700 gallons of fuel, eliminating more than 100 million cells. Both filters demonstrated the ability to remove over 99% of microbial cells from contaminated fuel, at low concentrations of approximately $2.45\text{E}+03$ CFU/L. This highlights their crucial role in effectively eliminating biocontamination in its early stages. In summary, the GO-based biofilter proves to be a practical and effective solution for removing microbes from contaminated fuel in real-world field applications.

CORRELATION BETWEEN MICROBIAL BIOMASS IN AIRCRAFT FUEL TANKS AND AVIATION FUEL SAMPLES WITH CFU COUNTS OBTAINED BY CULTURE METHODS

Lucy Owen, Gareth Williams, Graham Hill

ECHA Microbiology Ltd.

IATA recommend microbiological testing of drain samples from aircraft fuel tanks to detect microbial growth. IATA guidance classes microbial contamination results from culture-based (colony forming units; CFU) tests as Negligible, Moderate or Heavy. Moderate and Heavy results instigate preventative and/or remedial action. Other types of tests should show broad agreement with contamination categories defined for CFU tests. However, the relationship between CFU results and the amount and type of microbial biomass/biofilm in fuel tanks is not fully understood. This study aimed to investigate the correlation between quantity and type of microbial biomass in aircraft tanks and aviation fuel samples with CFU results. The findings of visual inspections of aircraft fuel tanks (n=11) were compared to IP 613 CFU results for drain tank samples taken over several occasions. A correlation between CFU count and tank inspection observations was found; Heavy results were obtained by IP 613 for 3 of 4 fuel tanks with visible microbial contamination. Moreover, 346 aviation fuel samples were assessed by CFU tests (IP 385 and IP 613) and results compared with a graded severity of biomass contamination determined by phase contrast microscopy. Correlations between CFU counts/IATA contamination level and biomass contamination grade were confirmed. Fuel samples with Moderate and Heavy contamination are likely to contain significant microbial biomass, and, in the case of Heavy contamination, clumps of fungal hyphae and/or microbial extracellular polymeric substances. Overall, the results of this study support the justification for remedial actions triggered by Moderate and Heavy CFU test results (IATA limits).

SESSION 10: GROUND FUELS - GASOLINE, DIESEL AND BIODIESEL

FORMULA 1 RACING FUEL EVOLUTION INFERRED FROM REGULATION CHANGES

David Abdallah¹, James Turner², Vincent Pereme²

¹*EMTEC*; ²*Federation Internationale de l'Automobile*

Although it has been said many times that they are similar, F1 fuels have always differed from commercial pump fuels, but the actual details are kept under tight wraps by the fuel suppliers who have put a lot of effort into their development. Understanding these fuels and their differences has been a challenge. However, some details can be gleaned from evolving fuel regulations over the years that seek to limit the use of certain components and rein in compositional departures from commercial fuels. The paper reviews the history of F1 fuel specifications and highlights changes to fuel compositions and properties over time. It also discusses the rationale behind those changes, shedding light on the Formula 1 race fuels used throughout the history of the sport.

DEMONSTRATING IMPROVED COMBUSTION AND ENVIRONMENTAL IMPACTS FROM THE USE OF DIESEL DETERGENT ADDITIVES

Mary Dery, Gavin Medine, Eric Payne

Innospec Fuel Specialties

In 2022, the EPA adopted the Clean Trucks Plan which mandated the reduction of emissions and harmful air pollutants from heavy duty (HD) trucks. Reduced emissions that form smog and soot will apply to HD engines and vehicles beginning in model year 2027. The transportation industry is making changes to comply with these new regulations. Diesel technology has evolved to reduce

the impact of petroleum-based combustion on the environment. This includes the incorporation of aftertreatment systems to trap or reduce particulate and gaseous emissions like NO_x, CO and hydrocarbons. Burning fuel mixtures that include renewable and biodiesel further reduce a fleet's carbon footprint. Diesel performance additives are known to clean up deposits in a diesel engine that prevent optimal combustion of the fuel. Diesel performance additives also help to reduce emissions and enable the use of more biodiesel and renewable fuels. This presentation will review some of the recent findings and positive impacts of diesel detergents in field trials from around the globe.

GASOLINE CHEMISTRIES AND EFFECTS ON PROPERTIES

Zainab Saihati

Saudi Aramco

The world's increasing demand for liquid fuels has highlighted the need for a deeper understanding of fuels fundamental chemistries to optimize properties and aid us for the transition to liquid low carbon fuels. This abstract discusses the importance of understanding the various types of gasoline chemistries to aid in properties prediction and their effects in order to enhance fuel quality and performance. Delving into the chemical composition trends of gasoline fuels and their properties will enable us to build the understanding of such complex chemistries and potentially find innovative ways to synthesize low carbon fuels to reduce environmental impacts. The following paper will be looking at the relationship between the different components and chemical groups using Gas Chromatography techniques to identify correlations with key properties such as RON, density, RVP, and distillation. The correlations can be a potential predictive tool for gasoline properties and further the understanding of properties and how they could be enhanced by the use blend components selection.

SESSION 11: FUEL TESTING AND TEST METHODS

COMPARISON OF DERIVED AND INDICATED CETANE NUMBER FOR AVIATION TURBINE FUELS AND CORRELATION WITH LEAN BLOW OUT

Jon Luecke, Robert McCormick

National Renewable Energy Laboratory (NREL)

The introduction of sustainable aviation fuel (SAF) into aviation turbine fuels requires approval as described in ASTM D4054 to ensure compatibility with preexisting aviation hardware. Derived cetane number (DCN), measured using an Ignition Quality Tester (IQT) as described in ASTM D6890, is currently required to be in the range of 35–60 to meet the D4054 fit-for-purpose requirements due to previously developed correlation of DCN with measured phi for lean blow out. Additional ASTM methods for determining cetane number (CN) exist, the latest being ASTM D8183, which uses a device called the Advanced Fuel Ignition Delay Analyzer (AFIDA) to measure indicated cetane number (ICN). This method requires 40mL of fuel versus 100mL for DCN, a significant advantage for early stage SAF fuel development. Here we present DCN and ICN results for set of fuels that includes NJFCP A-1, A-2, A-3, C-1, C-2, C-3, C-4; additional commercial jet fuels and blends with SAF, and several pure compounds, with ICN ranging from 28–65. ICN values were measured to be 2 units on average higher than DCN values for CN>40, whereas ICN measurements for CN<35 were determined to be 2 units on average lower than DCN.

A crossover equivalence in the region of cetane numbers from 36-38 is indicated. This dataset provides guidance for inclusion of D8183 ICN data into the D4054 specification as an alternative, lower volume method for measuring CN. Additionally, an approach that reduces the fuel requirement of D8183 from 40mL to 25mL is described.

GENERATION OF NOVEL DATASET FOR DENSITY, DIELECTRIC CORRELATION, AND CHEMICAL COMPOSITION OF INDIVIDUAL AND MIXTURES OF HYDROCARBON CONSTITUENTS IN AVIATION FUEL

Syarir Akram Bin Jamaluddin¹, Dr Xue Yong², Dr Ehsan Alborzi¹, Professor Mohamed Pourkashanian¹

¹*The University of Sheffield;* ²*University of Liverpool;*

Sustainable aviation fuel (SAF) and jet fuels both consist of a mixture of different types and ratios of hydrocarbons, which have a broad range of properties. This results in grand challenges and high costs for the fuel producers and jet engine manufacturers in ensuring the technical suitability and safety considerations. To address these challenges, a dataset of properties for individual, and mixtures of hydrocarbon fuel constituents is highly desired. One example of these properties is the density and dielectric constant properties which are key factors for aircraft capacitance gauging systems providing real-time fuel information to pilots. Therefore, this study utilized a combination of molecular dynamics (MD) simulations and experimental measurements to construct a comprehensive dataset for density and dielectric properties of individual, binary, ternary, and quaternary mixtures of hydrocarbon constituents of drop-in fuels across different ranges of temperatures. The results of this study demonstrate strong agreement with experimental data, offering valuable insights for early-stage fuel screening and production optimization. This work will establish a basis for further exploration into complex multicomponent SAF blends and advancements in developing more precise and efficient aviation fuel surrogate mixtures.

INCREASING THE LEVEL OF DETAIL OF COMPOSITIONAL ANALYSES WITH GCxGC-FID/ QMS FOR PRESCREENING OF SUSTAINABLE AVIATION FUELS

Hannes Lüdtkke, Florian Pütz, Uwe Bauder, Markus Köhler, Andreas Huber, Patrick Oßwald
Institute of Combustion Technology, German Aerospace Centre

To evaluate sustainable aviation fuels (SAF) and other complex samples, non-targeted comprehensive analysis is required. The commonly selected method for this purpose is the two-dimensional gas chromatography (GCxGC) as it provides high peak capacities and generates detailed compositional information through multiple separation mechanisms. The obtained results are the basis for probabilistic property models that are able to estimate a number of key properties without the need for additional experimental measurements. Applications for this Prescreening methodology is preliminary feedback prior to approval processes and the possibility for support during the optimization and design of novel SAFs production routs. However, the quality of predictions is dependent on the degree of detail provided by the compositional data. GCxGC results are usually categorized for carbon number and group type. Since the different isomers are not accounted for, but can differ significantly in their properties, uncertainties arise when predicting the properties of a fuel. The DLR GCxGC system is equipped with a dual detector setup comprising of a quadrupole mass spectrometer (qMS) and a flame ionization detector (FID). This ensures the capability of simultaneous identification of uncommon fuel compounds while maintaining a sensitive and universal quantification method. Nevertheless, MS proves to be not

always sufficient for complete structural isomeric differentiation. In an attempt to improve the detail of classification through identification of smaller subgroups, an investigation on the correlation of structurally influencing parameters to the separation behavior was carried out. The impact of higher compositional detail on the prediction of different properties is discussed.

SGMM - A NOVEL MODEL UTILIZING COMPOSITIONAL SUBGROUP INFORMATION FOR INCREASING ACCURACY OF FUEL PROPERTY PREDICTION IN PRESCREENING

Florian Pütz, Hannes Lüdtke, Astrid Ramirez, Uwe Bauder, Patrick Le Clercq, Andreas Huber
DLR (German Aerospace Center)

The prescreening process developed by Heyne, Rauch, Le Clercq, and Colket has become an important element in supporting development of new sustainable aviation fuel production pathways and increases the likelihood of successful ASTM approval. Prescreening involves the determination of the fuel composition at a molecular level using two-dimensional gas chromatography (GCxGC). Based on the composition, probabilistic machine learning models can then predict the properties of the fuel. However, a major limitation results from the inability of GCxGC to precisely resolve molecules on the level of structural isomers, which leads to serious disadvantages when predicting fuel properties. This limitation is particularly relevant for properties that differ significantly due to the isomeric structure of the molecules, such as freezing point and viscosity. Since these properties are strongly isomer dependent, the assumption that all known isomers can be present in the fuel has a particularly negative impact on both the inaccuracy and uncertainty of fuel property predictions. To address this challenge, the German Aerospace Center (DLR) is developing a method to identify subgroups within GCxGC bins. Building on this, we introduce the novel SubGroupMeanMatrix (SGMM) model that integrates these subgroups into the property prescreening framework to improve prediction accuracy and reduce the prediction uncertainty. In this study, we explain the methodology behind this new model and evaluate its impact on the accuracy of property prediction for selected representative aviation fuels as well as limitations of the new model.

DEVELOPMENT AND EVALUATION OF RUGGED PORTABLE SENSOR FOR IN-FIELD MEASUREMENT OF CORROSION INHIBITOR/LUBRICITY IMPROVER ADDITIVE

N. Scott Bergey¹, Corrianna R. Boucher²; Eric M. Johnson², Lena E. Flynn¹, John J. Buffin¹, Terrence W. Dickerson¹, Richard A. Kamin¹

¹*U.S. Navy*; ²*Peraton*

The US Navy has developed and tested an in-line field additization cart that injects the three required F-24 additives into unadditized D1655 fuel. Fuel system icing inhibitor and static dissipator additive both have readily field-portable measurement techniques available to validate that the in-line injection correctly blended the additive to its specified concentration as required in AFLP-3747. Since there is currently no portable measurement technique to measure corrosion inhibitor/lubricity improver (CI/LI) additive, the US Navy has spearheaded development of a simple, portable, and inexpensive field kit to reliably quantify CI/LI. This work showcases the final prototype kit and the processes used to optimize and simplify the measurement technology to maintain viability across challenging environmental conditions.

SESSION 12: POSTER SESSION

PERFORMANCE AND STORAGE STABILITY OF RENEWABLE FUELS WITH STATIC DISSIPATIVE ADDITIVE

Asha Patel, Sankaran Murugesan, Don Wolfe

Baker Hughes

Renewable fuels are becoming an increasing part of the fuels offering for domestic and commercial applications, and more recently an emphasis towards production of Sustainable Aviation Fuels (SAF). In the industry, different renewable feed stocks are used to make renewable fuels such as vegetable oils, used cooking oils and various biomasses using different catalytic conversion process to produce renewable fuels. The properties of renewable fuels are related to the feeds and processes used in their manufacture. Generally, in traditional distillate fuels, Static Dissipative Additives (SDA) are used to facilitate the safe dissipation of electrostatic charges through the liquid hydrocarbon, by reducing the accumulation of hazardous surface charges. However, in case of renewable fuels, the investigation of conductivity improver performance has not been explored. This presentation gives a comprehensive study of conductivity performance of SDA in three different renewable fuels in comparison with conventional ULSD. Detailed discussion of the SDA performance with regard to dosage variation, temperature and long-term fuel storage stability is considered.

EFFECT OF CHEMICAL COMPOSITION ON FREEZE POINT OF HYDROCARBON MIXTURES

David C. Bell, Randall Boehm, Zhibin Yang, Joshua Heyne

Washington State University

Accurate property predictions for the freezing point of hydrocarbon fuels is an ongoing challenge in the aviation fuel community. Freezing point has historically been attributed to high concentrations of n-alkane species and high temperatures at the upper distillation curve values (T90 and FBP), but these models are strictly correlative methods based around experience with conventional fuels. For alternative fuels, the applicability of these methods is uncertain. Recent work has suggested that freeze point is determined by the concentration of a limiting species, where the balance has negligible impact. This work tests this hypothesis and improves a method for freeze point predictions for complex fuels. In this work, low concentrations of high freeze point components are added to low freeze point solvents to isolate the impact of several explanations of freeze point behavior. These include the impact of aromatics on solvency, the impact of mixture complexity, and the impact of structural similarity. The results of this study show that mixtures of fuels will result in freeze points lower than any of fuels on their own and demonstrate the basis for a widely applicable prediction method for alternative and conventional aviation fuels.

DEFINING QUALIFICATION REQUIREMENTS FOR RENEWABLE DIESEL FUELS

David Evans, Tori Guarnera, Rachele Hewitt,

Defence Science and Technology Group

The aviation industry maintains stringent guidelines for qualifying synthetic blending components, governed by ASTM D4054. Following approval by the ASTM D02.J subcommittee, the new Synthetic Blending Component (SBC) is integrated into ASTM D7566, a process closely overseen

by Airframe and Engine OEMs, fuel producers, and industry experts. Conversely, the diesel industry lacks a comparable mechanism to assess SBC quality for diesel fuel. Although ASTM D975 permits non-conventional feedstock, it emphasizes the potential need for additional testing. Diesel engine OEMs generally accept SBCs, and sometimes neat synthetic diesel, provided they meet ASTM D975, EN950 or EN15940 performance standards. The US Navy has established a rigorous qualification testing protocol outlined in Navy Standard Work Package 44FL-005, which aligns with ASTM D4054 and is considered the gold standard in technical requirements. With the renewable diesel production market expanding rapidly, there's an imperative to establish minimum testing standards to mitigate risks that is readily accessible by industry. This paper proposes minimum technical requirements based on the ASTM D4054 Fast Track approach to ensure performance and fit for purpose requirements are satisfied and introduces additional specifications for diesel fuel containing synthetic components.

INSIGHTS INTO SCALING UP HEFA-SPK PRODUCTION

Jesse Vilja, Neste, Kati Sandberg, Reetu Sallinen, Oscar Nyman
Core R&D

It is widely recognized that for the aviation industry to reach net-zero emissions by 2050, sustainable aviation fuels (SAF) are relied upon. Consequently, a rapid scale-up of global SAF production is required already during this decade. With the final investment decision made in 2018, Neste's Singapore refinery's expansion utilizing the proprietary NEXBTL™ technology was completed in 2023. Combined with the upcoming modification to Neste's Rotterdam refinery, which will enable SAF production in addition to Renewable Diesel, Neste will reach SAF production capability of 1.5 Mt/a in 2024. In the NEXBTL™ process, various fatty acid and fatty acid ester feedstocks are converted through hydroprocessing, isomerization and fractionation into HEFA-SPK, a synthetic blend component (SBC). Utilizing infrastructure dedicated for SBCs, at Neste Singapore and Rotterdam the tank farm setups include several positively segregated product tanks, and jetties inserting the SBCs into the global supply chain. In compliance with ASTM D7566, the SBC is blended downstream in the global blending terminal network at maximum 50 vol-% with conventional jet fuel, resulting in a drop-in jet fuel. Quality assurance principles set by the industry standards EI/JIG 1530 and EI 1533 are followed throughout the supply chain. The ASTM D7566 certified HEFA-SPK can in neat form and over its lifecycle reduce GHG emissions by up to 80 % compared to conventional jet fuels. Furthermore, when incorporated into jet fuel blends it can reduce aeroengines' particulate emissions, and thus reduce aviation's non-CO₂ emission impact.

UPDATE TO THE DEVELOPMENT OF A SHIPBOARD TEST KIT FOR DISSOLVED COPPER IN A JET FUEL PROTOTYPE FIELD TEST KIT

Kristina Myers¹, Thomas Loegel², Robert Morris¹, Jacob Guthrie¹
¹Nova Research, Inc.; ²Naval Research Laboratory

Recently, the Navy has been investigating functionalized filtration technologies to selectively remove copper from fuel. In order to utilize this system, there is a need to monitor copper content in the filter effluent. We have revisited the bathocuproine (BCP) colorimetric methodology. The chemistry was further refined and some work was performed to extend the method applicability to both jet and diesel fuels. An upgraded and more capable data acquisition and analysis kit was also developed. A range of copper concentrations were obtained by combining a copper-free JP-5 with that same fuel doped with copper from copper metal, as well as a set of copper-bearing fuels from

Navy ships. The analyzer performed adequately at copper concentrations from 400 to 50 µg/kg, which was deemed adequate for the intended purpose of monitoring copper filter breakthrough. However, it was found that fuels from a particular aircraft carrier displayed negative results due to decreased absorbance when BCP was added with respect to the reagent blank. Chemical characterizations of these anomalous JP-5 fuels were conducted in an effort to determine any anomalous species responsible for this behavior. Investigations into alternate reducing agents, protocols, and reagents were also conducted in order to develop a test method to accommodate these outlier fuels.

CETANE IMPROVER EFFECTIVENESS IN SEMI-SYNTHETIC JET FUELS AND RELEVANCE OF CETANE NUMBER IN AERONAUTICAL COMBUSTION

Mikael Orain¹, Mickaël Sicard¹, Amandine Herbaut², Nathalie Brassart³, Mickaël Matrat³
¹ONERA; ²CETSEO; ³IFPEN

Safe operation of diesel engines requires a fuel with a cetane value over 40. However, kerosene may be used in land vehicles as the single fuel on the battlefield. Kerosene cetane value is yet lower than that of diesel. It is then possible to add a cetane improver (CI) to increase this value. Nowadays, the incorporation of alternative fuels (SBC) raises the question of the effectiveness of this additive. Moreover, some SBCs have very low cetane values. In order to study the behavior of two different CI, a fuel matrix, composed of JP-8/ATJ and JP-8/HEFA-ARO blends were additivated at different levels. The derived cetane number (DCN) results show that an increase of SBC content decreases the cetane boost. Comparison of the two CI shows that both have similar responses. Although the cetane number was developed to characterize the behavior of a fuel in a diesel engine, recent studies have shown that it would be possible to use it to characterize a fuel in an aeronautical combustor. To support this hypothesis, droplet sizing and ignition tests were carried out on different SBCs for different temperatures and pressures. The results show that there is no clear influence between drop sizing and the fuel. The ignition tests, performed in a model combustor, exhibit significant variations between the fuels. However, considering only the cetane value does not allow to explain the results. These are highly dependent on fuel temperature, and therefore almost certainly on parameters such as viscosity and surface tension.

HANDLING, MAINTENANCE AND SAFETY USE OF AVIATION FUEL - INFORMATIVE BULLETINS

Maor Saban, Liel Mazar, Yalfal Siyum, Haim Judah, Moshe Rabaev
Israeli Air Force

Optimal care and maintenance of aviation fuels and infrastructure is of crucial importance for ensuring the safety of passengers, personnel and the environment. In order to increase the awareness of fuel technicians, engineers and decision makers about safety issues concerning the maintenance and handling of fuel in the field, we have produced numerous informative bulletins. These are written in simple language without much jargon, making it possible to convey important and essential knowledge in an easy, digestible manner for the layperson. Topics covered in the bulletins include information about "Apple Jelly", microbial contamination, fuel filters, static electricity, aviation fuel additives, laboratory tests, critical fuel properties, fuel contaminations and real fuel-related aircraft safety events - emphasizing how a minor human mistake can have major safety implications. The bulletins have greatly raised the awareness of our organization's personnel in their handling of aviation fuel, and therefore we find it essential to share them with the global community.

EXPERIMENTAL QUANTIFICATION OF THE HYDROPEROXIDE CONTENT IN SURROGATE JET-FUELS ON HPLC DEVICE

Ryma Benrabah, Pierre-Alexandre Glaude, Boris Roux, Philippe Arnoux, René Fournet, Baptiste Sirjean,

Université de Lorraine, CNRS, LRGP

Hydroperoxides are major products of the autoxidation of hydrocarbon fuels and play a central role in oxidation kinetics. The quantification of hydroperoxide is a key factor for the qualification of jet-fuel and is determined through a standardized method. A recent review and comparison of different iodometric methods of quantification determines that an HPLC-P-cR device is highly precise with a high reproductivity. In this work, we optimized an HPLC coupled with an iodometric post-reaction to detect and quantify the hydroperoxide content in liquid fuels. This setup separates the different oxygenated fractions and offers more extended information on the reaction products. Different surrogate jet-fuels were aged in a PetroOxy and then passed in this device to analyze the content. n-Decane and cumene were used as surrogate jet-fuels. The oxidation of n-decane yields decane hydroperoxides and other oxygenated compounds that were observed in the liquid chromatography. The different compounds were separated and the nature of hydroperoxides and their dimers was investigated. The aged cumene is analyzed after the experiment in the HPLC device and the separation showed that only 3 products of oxidation are formed for cumene which allowed a validation of the chemical pathway of liquid phase oxidation of cumene.