ANL-23/13

WORKSHOP ON **SUSTAINABLE AVIATION FUEL END-USE RESEARCH OPPORTUNITIES**

Summary Report from Virtual Workshop
February 15–16, 2022

U.S. DEPARTMENT OF ENERGY

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prepared by

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LIST OF ACRONYMS

AFRL	Air Force Research Laboratory
AI	artificial intelligence
ARL	Army Research Laboratory
ASCENT	Center of Excellence for Alternative Jet Fuels and Environment
ASTM	American Society for Testing and Materials
BETO	Bioenergy Technologies Office
C#	Number of carbon atoms in a hydrocarbon; e.g. C16 – 16 carbon atoms per molecule
CFD	Computational Fluid Dynamics
CO	carbon monoxide
CPU	Central Processing Unit
CRADA	Cooperative Research and Development Agreement
CRATCAF	Combustion Rules and Tools for the Characterization of Alternative Fuel
DCN	derived cetane number
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
EERE	Energy Efficiency and Renewable Energy
EPA	U.S. Environmental Protection Agency
FAA	Federal Aviation Administration
FOM	figure of merit
GHG	Greenhouse gases
HyChem	Hybrid Chemistry
ICAO CAEP	International Civil Aviation Organization Committee on Aviation Environmental Protection
IQT	Ignition Quality Tester
JudO	Jet Fuel Blend Optimizer
LBO	lean blowout
LLNL	Lawrence Livermore National Laboratory
LTO	Landing and take-off
ML	machine learning
MOU	memorandum of understanding

NASA	National Aeronautics and Space Administration
NGO	non-governmental organization
NIST	National Institute of Standards and Technology
NJFCP	National Jet Fuels Combustion Program
NOx	nitrogen oxides (=NO + NO_2)
NRC	National Research Council
NREL	National Renewable Energy Laboratory
nvPM	non-volatile particulate matter
OEM	original equipment manufacturer
ORNL	Oak Ridge National Laboratory
PACE	Partnership to Advance Combustion Engines
PAH	poly-aromatic hydrocarbons
PM	particulate matter
RCM	rapid compression machine
RDD&D	research, development, demonstration, and deployment
RQL	Rich-Quench-Lean
SAF	Sustainable Aviation Fuel
SAFER	Sustainable Aviation Fuel End-Use Research
SATF	Synthetic Aviation Turbine Fuels
SERDP	Strategic Environmental Research and Development Program
SNL	Sandia National Laboratories
UHC	Unburned hydrocarbons
USDA	U.S. Department of Agriculture
VTO	Vehicle Technology Office

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EXECUTIVE SUMMARY

On February 15-16, 2022, the U.S. Department of Energy's (DOE's) Vehicle Technology Office (VTO) within Energy Efficiency and Renewable Energy (EERE) convened a workshop to assess the end-use research opportunities for Sustainable Aviation Fuels (SAF). This report summarizes the proceedings and findings of the workshop, which the U.S. Department of Energy's Argonne National Laboratory hosted as a virtual event. During these two half-days, invited members of national laboratories, industry, government, and academia connected virtually to share perspectives on SAF research needs for improving end-use adoption.

DOE's goal is to produce in the near-term, 3 billion gallons of SAF per year by 2030 as a part of the SAF Grand Challenge announced by the White House involving USDA, DOT, and DOE.[1] This will necessitate unprecedented public-private partnerships and enhanced collaborations between fuel scale-up and end-use researchers. This workshop identified gaps and research opportunities in the space of end-use research. Below is a short summary of key gaps and opportunities identified by the invited speakers for the workshop.

FUEL PROPERTY CHARACTERIZATION: For candidate SAF developed by Bioenergy Technologies Office (BETO) and industry

- Develop blending relationships between multiple SAF
- Develop and publish liquid (density, viscosity, surface tension, vapor pressure, specific heat, heat of vaporization) and vapor (thermal conductivity) property data as a function of temperature and pressure
- Understand effect of fuel structure impact on properties and thereby on gas turbine engine performance

CHEMICAL KINETICS: For selected SAF, develop surrogate fuel

- Develop kinetic mechanism that can predict nitrogen oxides (NOx), carbon monoxide (CO), smoke/particulate matter (PM), auto and forced ignition characteristics across the flight map; develop reduced mechanism
- Rigorously validate kinetic mechanisms with rapid compression machine (RCM) and shock tube data, flame speed characterization, and emission data from flow reactors

FUEL INJECTOR FLOWS AND SPRAYS: Identify one or two common atomizer geometries of relevance

- Perform detailed internal flow experiments and simulations under engine-relevant conditions with Jet A and selected SAF to quantify differences in droplet distribution and mixing fields
- Perform controlled coupling spray measurements (spray and flame wall interaction and pyrolyzing sprays), leveraging lab assets that may not have been formerly leveraged by the aero-propulsion community/industry
- Develop/advance spray models for SAF under engine-relevant conditions and understand operation under transcritical conditions

IGNITION AND COMBUSTION: Identify single-cup configurations that is of interest to industry

- Improve understanding of forced ignition and turbulence/chemistry interaction processes

- Further study influence of fuel properties on lean blowout (LBO), relight, and cold-start, starting with Jet A and subsequently extended to selected SAF; use datasets to improve models
- Enhance combustion models with machine learning (ML)/artificial intelligence (AI) tools for further acceleration of simulations

EMISSION AND CONTRAILS:

- Improve fundamental understanding of non-volatile PM (nvPM) nucleation and morphology for Jet A and selected SAF
- Understand impact of fuel sulfur content on PM and contrails
- Improve existing empirical models for soot and contrail formation

HEAT TRANSFER:

- Develop understanding of liner heat transfer coefficients for SAF
- Perform high-fidelity simulations and complementary experiments to improve liner cooling models
- Improve radiative heat transfer models for Jet A and extend to SAF

DOE national laboratories have significant expertise in addressing multiple research needs as demonstrated by the Co-Optima project, a collaboration between BETO and VTO.[2] Core capabilities and tools developed under Co-Optima can be leveraged in the new collaboration being designed by national laboratories under the supervision of VTO. Our national laboratories have extensive capabilities in performing fundamental and applied research by generating new data and developing computational tools that will help industries work together to optimize future fuels and design the next generation of aircraft engines. We envision that DOE's research program will be complementary to FAA, NASA, and other government agency end-use research programs.

BACKGROUND

Workshop Objectives

The SAF Grand Challenge is the result of the DOE, DOT, and USDA launching a government-wide memorandum of understanding (MOU) to develop a comprehensive strategy that will attempt to reduce the cost, enhance the sustainability, and expand the production and use of SAF on a commercial scale. SAF is a fuel produced from bio- or other sources used to power aircraft that has similar properties to conventional jet fuel but with a smaller carbon footprint. Depending on the feedstock and technologies used to produce it, SAF can reduce life cycle GHG emissions dramatically compared to conventional jet fuel. The SAF Grand Challenge's goal is to achieve a minimum of 50% reduction in life cycle greenhouse gas emissions compared to conventional fuel and to supply sufficient SAF to meet 100% of aviation fuel demand by 2050. This increased SAF production will play a critical role in a broader set of actions by U.S. government and the private sector to reduce the aviation sector's emissions, on a pathway to full decarbonization by 2050. Through this MOU, the DOE, DOT, and USDA intend to accelerate the research, development, demonstration, and deployment needed for an ambitious government-wide commitment to scale up the production of SAF to 35 billion gallons per year by 2050. A near-term goal of 3 billion gallons per year is established as a milestone for 2030.[1]

An interagency team led by the DOE, DOT, and USDA worked with EPA, other government agencies, and stakeholders from national labs, universities, non-governmental organizations (NGOs), and the aviation, agricultural, and energy industries is developing a SAF Grand Challenge roadmap, "Flight Plan for Sustainable Aviation Fuel." The roadmap (Figure 1) outlines a whole-of-government approach with coordinated policies and specific activities that should be undertaken by the federal agencies to support achieving both the 2030 and 2050 goals of the SAF Grand Challenge. This roadmap ensures the alignment of government and industry actions and the coordination of government policies to achieve the goals of the SAF Grand Challenge. This includes coordination in the formation and execution of plans in research, development, demonstration, and deployment (RDD&D) to ensure sharing of approaches, tools, assumptions, and insights across agencies' research centers at the DOE national laboratories, FAA's Center of Excellence for Alternative Jet Fuels and Environment (ASCENT), and other entities.

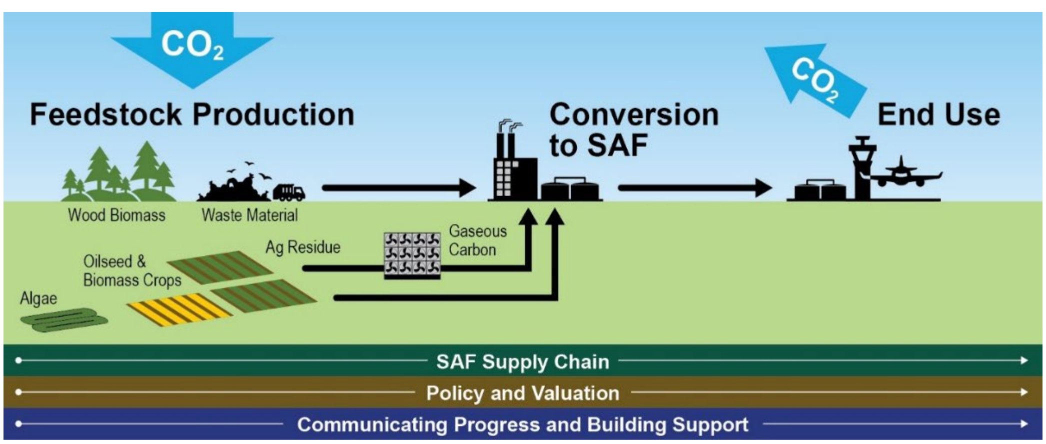

Figure 1. Graphic representation of the SAF Grand Challenge Roadmap*[1]*

Enabling the end-use of SAF is a key focus area for the SAF Grand Challenge roadmap. This includes facilitating the end-use of SAF by civil and military users by addressing critical barriers, including efficient evaluation of fuel, engine and aircraft performance and safety, advancement of certification and qualification processes, expansion of existing blend limits, and integration of SAF into fuel distribution infrastructure. VTO's interest is primarily focused on the end-use aspect and accelerating the adoption of SAF in commercial aircraft engines.

The VTO and Argonne convened this workshop to understand end-use research opportunities with SAF. We brought together experts from relevant aviation fuel end-use backgrounds to determine SAF adoption challenges and identify collaborative opportunities to address them. We encouraged industry, academia, and other government entities to voice ideas, so that we can help VTO shape a program focused towards accelerating the optimization of fuels and ensuring safe and reliable jet engines. To the best of our knowledge, there is no other integrated effort to address challenges highlighted above from an end-use standpoint to complement the SAF Grand Challenge. To ensure that the industry can de-risk SAF incorporation in 2030 and beyond, end-use research must accelerate and be tightly integrated with industry.

This workshop report summarizes the key gaps and opportunities identified during the workshop. Small differences in fuel physical and chemical properties between Jet A and SAF may result in differences in internal flows, atomization, and mixture formation, which may result in different combustion and emission behavior. Workshop presenters identified needs for data generation for all these physical and chemical processes with SAF (Figure 2) and emphasized the need to develop efficient and predictive computational tools.

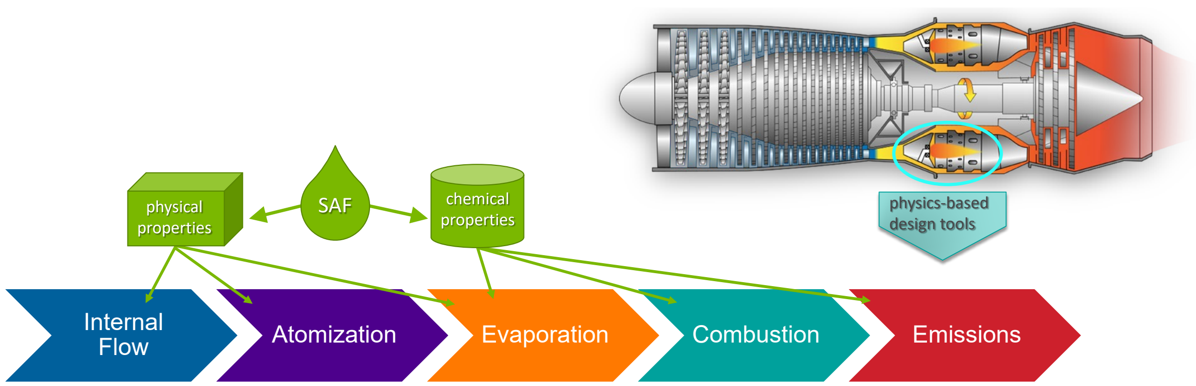

Figure 2. Graphic representation of physio-chemical processes in gas turbine engine

FUELS OF INTEREST AND CHARACTERIZATION NEEDS

Current Status

DROP-IN VS. NON DROP-IN

A drop-in fuel is one that can be substituted for jet fuel, based on meeting all specifications of jet fuel as specified in ASTM D1655.[3] All other fuels, by definition, would be non drop-in, even if most specifications are matched.

The DOE's decarbonization goals within the SAF Grand Challenge necessitate that petroleum-derived jet fuel is replaced in its entirety by SAF by 2050. SAF concentrations in jet fuel blends are currently limited to 50 vol% regardless of the fuel properties, and at least one SAF is limited to 10 vol%. Obtaining approvals for new SAF compositions and processes is time-consuming and costly for all fuels and can be the largest technical barrier to introducing a new fuel. Currently, there are no current "drop-in SAF". There are only approved pathways that can be blended with Jet A/A-1 and then become drop-in (or more precisely, be reidentified as Jet-A/A-1 under ASTM D7566). The amount of time and cost is highly dependent on whether the SAF is qualified to be drop-in or non drop-in. Fuels with significant differences from Jet A/A-1 (and significantly different from currently approved synthetic fuel pathways) are likely to require more time and cost for approval compared to synthetic fuels that are more similar to Jet A/A-1 or to currently approved pathways.

FAA certifications for jet turbine engines, which prioritize aircraft safety, are organized around ASTM standards and the resultant certification is valid only for the fuel specified. For all commercial jet engines, the fuel used for certification is Jet A/A-1, as defined in ASTM D1655. While this standard was originally developed for petroleum-derived fuel, there is an allowance for synthetic fuels (e.g., not petroleum-derived fuels) to be treated as Jet A/A-1, meaning that they are a drop-in fuel. The process for a fuel to be classified as a drop-in consists of two steps:

1. The fuel must be evaluated for compatibility according to ASTM D4054, which consists of a 4-tiered compatibility review, starting with evaluating fuel properties through full-scale engine testing and aircraft flight test. Per ASTM D4054, Tier 1-4 screening requires 10, 80, 10,000, and 225,000 U.S. gallons, respectively.[4]
2. If the fuel is deemed to be a drop-in, a description of that fuel (properties, composition, and production pathway) is added to ASTM D7566 and it can be treated as Jet A/A-1, when blended with Jet A/A-1, up to the specified concentration as long as the required properties of the blend meet specifications.[5]

Currently, ASTM D7566 lists seven approved synthetic fuel pathways blended with Jet A/A-1 that are approved for use as drop-in fuels, and all are primarily hydrocarbons with only trace levels of oxygenates or heteroatoms permitted. These SAF can differ from petroleum-derived Jet A/A-1 in relative content of n-paraffins, iso-paraffins, cyclo-paraffins, and aromatics as well as the individual constituents. The drop-in terminology applies to the blended fuel (SATF blended with Jet A/A-1), as nearly all currently available SAF are non drop-in as neat fuels. An ASTM Task Force was formed in 2021 with an effort to modify ASTM D7566 drop-in standard to allow 100% SAF (which includes permitting blends of multiple SAF). The seven SAF in ASTM D7566 approved for use in blends as drop-ins are shown in Table 1, including the biomass feedstock, processing technology, and maximum allowable blend concentration.

Table 1. Pathways currently listed in ASTM D7566 and approved for use as drop-in blendstocks.

Name	Acronym	Biomass Feedstock	Processing	Composition	Max Concentration in Jet A/A-1 Blend
Fischer-Tropsch (FT) Hydroprocessed Synthesized Paraffinic Kerosene	SPK	Any/not specified	□ FT process using iron or cobalt catalyst to produce paraffins and olefins □ Subsequent processing[a]	□ Paraffins (report mass%) □ Cycloparaffins (< 15 mass%) □ Aromatics (< 0.5 mass%)	50 vol%
Synthesized Paraffinic Kerosene from Hydroprocessed Esters and Fatty Acids	HEFA	□ Mono-, di-, and triglycerides □ Free fatty acids □ Fatty acid esters	□ Hydroprocessing and deoxygenation □ Subsequent processing[a]	□ Primarily paraffins (report mass%) □ Cycloparaffins (< 15 mass%) □ Aromatics (< 0.5 mass%)	50 vol%
Synthesized Iso-Paraffins from Hydroprocessed Fermented Sugars	SIP	Fermentable sugars	□ Fermentation of sugars into farnesene feedstock □ Hydroprocessing to produce iso-paraffins (primarily farnasane) and fractionation	□ Saturated hydrocarbons (> 98 mass%) □ Farnasane (> 97 mass%) □ Hexahydrofarnesol (< 1.5 mass%) □ Aromatics (< 0.5 mass%) □	10 vol%
Synthesized Kerosene with Aromatics Derived by Alkylation of Light Aromatics from Non-Petroleum Sources	SPK/A	Any/not specified	Blend of: □ SPK □ Aromatics derived from non-petroleum sources through alkylation between FT-derived olefins and light aromatics (primarily benzene)	□ Paraffins (report mass%) □ Cycloparaffins (< 15 mass%) □ Aromatics (< 20 mass%)	50 vol%
Alcohol-to-Jet Synthetic Paraffinic Kerosene	ATJ-SPK	□ Ethanol □ Iso-butanol	□ Dehydration □ Oligomerization □ Hydrogenation and fractionation	□ Paraffins (report mass%) □ Cycloparaffins (< 15 mass%) □ Aromatics (< 0.5 mass%)	50 vol%
Synthesized Kerosene from Hydrothermal Conversion of Fatty Acid Esters and Fatty Acids	CHJ	□ Free fatty acids □ Fatty acid esters	□ Catalytic hydrothermolysis □ Subsequent processing[a]	□ Paraffins (report mass%) □ Cycloparaffins (report mass%) □ Aromatics (8.4 – 21.2 mass%)	50 vol%
Synthesized Paraffinic Kerosene from Hydroprocessed Hydrocarbons, Esters, and Fatty Acids	HC-HEFA	□ Algae-derived hydrocarbons, free fatty acids and fatty acid esters[b]	□ Hydrogenation and deoxygenation □ Subsequent processing[a]	□ Paraffins (report mass%) □ Cycloparaffins (< 50 mass%) □ Aromatics (< 0.5 mass%)	10 vol%

[a]Subsequent processing can include hydrotreating, hydrocracking, hydroisomerization, polymerization, isomerization, and fractionation.

[b]Botryococcus braunii species of algae is currently the only recognized bio-source. Additional esters and fatty acids can be approved as source material by the ASTM committee once sufficient data are available.

By contrast, a non drop-in SAF has yet to be approved for use. Such an approval would require an alternative fuel standard to Jet A/A-1 (ASTM D1655). ASTM also has a 100% non drop-in Synthetic Aviation Jet Fuel group to define the specifications of non drop-in fuels for the future. This ASTM Task Force would develop a standard that original equipment manufacturers (OEMs) could use, if desired, to certify their equipment. Time and cost estimates have not been given for developing such a standard because the problem is open-ended with numerous potential pitfalls, such as resistance to microbial contamination, differences in electrical capacitance for accurate fuel level readings, and more. Furthermore, an alternative fuel standard would require all jet engines to be certified twice: first, to use the non drop-in fuel and, second, for Jet A/A-1 or drop-in fuel. Other additional concerns were voiced: implementing infrastructure investments and accompanying processes to segregate a non drop-in from Jet A/A-1 to prevent cross-contamination or misfuelling, both of which could be safety concerns. For these reasons, many industry stakeholders see non drop-in SAF as an intractable problem, even though some airlines express interest.

The use of SAF is growing rapidly; 45 airports are distributing SAF, and offtake agreements exist for over 21 billion liters of SAF. Additionally, numerous flight demonstrations have taken place with 100% SAF, including a commercial flight from United Airlines. A multi-agency collaboration (USDA, DOT, DOE) has initiated the ambitious SAF Grand Challenge, which seeks to scale-up production and deployment of SAF to 3 billion gallons/year by 2030, and to 35 billion gallons/year by 2050. The intent of the MOU between DOE, DOT, and the USDA is to accelerate the R&D required to meet this demand.

NATIONAL JET FUELS COMBUSTION PROGRAM

The National Jet Fuels Combustion Program[6] (NJFCP) began in 2014 and included industry, academia, and government agencies designed to accelerate the adoption of drop-in SAF through four main goals:

1. Reduce the time and cost of ASTM approvals
2. Reduce the quantities of SAF needed for approvals
3. Reduce engine manufacturer risk and uncertainty in the adoption of SAF
4. Improve modeling tools to assess fuel impacts on combustor performance

The technical areas of work in the NJFCP were designed to develop a better understanding between combustor performance, fuel composition, and/or fuel physical and chemical properties. The NJFCP defined primary figures of merit (FOM) that reflected the metrics that OEMs are required to meet as part of any combustor development program or fuel approval effort. The measured values of FOM are dependent on the fuel properties, which are functions of the fuel composition, and is dependent on both the feedstock and the process used to develop those fuels. Ultimately, the feedstock, processing, and composition for each approved SAF is described in ASTM D7566, and many more fuel candidates are currently progressing through the approval process.

Developing a better understanding and predictive capability between fuel composition and engine performance was central to the NJFCP. As is implied by the definitions for the fuel feedstock, processing, and composition for each individual fuel definition in ASTM D7566, SAF is a broadly encompassing term. It can include fuels like farnesane, which are selective to a single molecule, and SAF can also include complex chemical mixtures with hundreds or thousands of individual components. Even with a given chemical classification and carbon number (e.g., C16 iso-paraffin), different isomers can exhibit different properties and performance. This challenges some of the longstanding property correlations that have evolved with petroleum-derived fuels (e.g., the temperature dependence of viscosity can be different for SAF).

The NJFCP sought to develop screening methodologies for new potential fuel candidates that used small fuel quantities. An α screening tier relied on comprehensive two-dimensional gas chromatography (GC x GC) analytical techniques for chemical speciation and distillation predictions used only 1 mL of fuel, and a β screening tier measured a range of physical properties using 10-140 mL of fuel. These fuel requirements contrast drastically from the ten gallons of fuel required for the early stages of the ASTM process. This information was used to predict critical properties and, ultimately, the fuel's usability. This pre-screening information was designed to aid in identifying and eliminating potentially undesirable fuels at an earlier stage, allowing resources to be used more productively. It also served to develop the Jet Fuel Blend Optimizer (JudO), which was useful in predicting the liquid fuel properties with SAF blends.[7, 8] It should be noted, though, that α and β screening tiers are still under development and their applicability and effectiveness for screening SAF candidate fuels is still to be validated.

The NJFCP's technical work was organized around common custom fuels that could be used by all the participants consisting of three petroleum-derived "category A" fuels, all of which met the Jet A/A-1 standard but constituted a best-case, average, and worst-case scenario with regard to viscosity, volatility, and hydrogen content.[9] It also consisted of a series of alternative "category C" fuels (initially five, later expanded to nine). All C fuels consisted of hydrocarbons within the Jet A/A-1 boiling range, but differed in distillation curve, cetane number, viscosity, and hydrocarbon composition.

The NJFCP focused on these technical areas relating to fuel performance and modeling:

- Chemical kinetics combustion experiments
- Chemical kinetics model development and evaluation
- Advanced combustion tests
- Combustion model development and evaluation
- Atomization tests and models
- Referee swirl-stabilized combustion rig evaluation and support

The current status of atomization and combustion modeling (technical areas 4 and 5) are covered in later sections of this workshop report. An overview of the remaining areas (technical areas 1,2,3, and 6) is provided here.

The chemical kinetics combustion experiments and modeling were conducted to reflect a conceptual model of jet fuel combustion where fuel rapidly decomposes, controlled by pyrolytic processes; then, the combustion rate and flame structure are governed by oxidation of the pyrolysis products rather than directly by the parent fuel. The intent was to navigate extensive and complicated uncertainties associated with parent fuel oxidation for typical jet fuel constituents. Shock tube experiments with optical diagnostics and gas sampling were conducted with the different fuels at multiple temperature and pressure conditions to identify the pyrolysis products. For the chemical kinetic mechanism development, a central element of the approach was the implementation of lumped fuel pyrolysis chemistry with detailed kinetics for smaller ($\leq$C7) hydrocarbon intermediate species. Thus, a complex fuel is modeled as a single species with a fixed integer-based elemental composition (e.g., C_mH_n) which decomposes rapidly into combustion intermediates ranging in size from hydrogen to toluene. This Hybrid Chemistry (HyChem) approach[10] is understood to be valid when modeling chemical kinetics at high temperatures (>1000 K) within many engine operating scenarios, where large aviation fuel components rapidly decompose prior to oxidation reactions. Simplifying the fuel-specific chemical kinetics in this way enables the semi-empirical fitting of fuel-specific pyrolysis chemistry measurements from fundamental experiments without detailed knowledge of the complex fuel or a complicated surrogate formulation. Versions of HyChem models were successfully developed for the reference fuels JP-10, A-1, A-2, A-3, C-1, and A-2/C-1 blends. While detailed HyChem models for aviation fuels are typically small (100~200 species), further reductions to as few as 35 species were also demonstrated.

The advanced combustion tests consisted of three parts:

1. Lean blowout (LBO)
2. Ignition for cold start and high altitude
3. Turbulent flame speed measurements

Aircraft encounter LBO when fuel to the engine is reduced significantly, such as during descent for landing; if blowout occurs, the engine loses propulsive power. Prior to the NJFCP, it was believed that LBO could be attributed to physical properties of the fuel (e.g., viscosity, density, and distillation temperature) and impact on the resultant spray. The NJFCP found that LBO correlated more significantly to derived cetane number (DCN), which is primarily a measure of the chemical reactivity of the fuel. It should be noted, though, that if the atomization quality is sufficiently deteriorated by a very low injection pressure, the LBO does correlate to physical properties. By contrast, ignition for cold start and high-altitude relight was found to be primarily dependent on the physical properties, and specifically the viscosity and surface tension of the fuel. The turbulent flame speed measurements supported the conceptual model of jet engine combustion where the fuel was first pyrolyzed in a fuel-rich zone, and then the rate of reaction was governed by the pyrolysis products. Since many of the fuels yielded similar distributions in pyrolysis products, the turbulent flame speed of many of the fuels was similar, with a notable difference being fuel C-1, which consisted of branched paraffins and had a low cetane number, and an unconventional boiling curve.

The referee combustor rig, which employed a single swirl-cup burner, contributed to numerous aspects of the NJFCP, including the advanced combustion tests and providing data for non-reacting flow, spray, and reacting flow model validation. In addition to these, emissions and combustion efficiency data were also collected. Particulate emissions correlated most strongly with the hydrogen-to-carbon ratio of the fuel, with higher hydrogen content producing lower particulate emissions. Combustion efficiency correlated most strongly with the density of the fuel, with higher fuel density producing a lower combustion efficiency, e.g., higher emissions of CO and unburned hydrocarbons.

Gaps and Opportunities

1. SAF Scale-up

It was noted that, to meet the SAF Grand Challenge, a massive scale-up of approximately 1,000 times current-day production is required by 2050. This scale-up is primarily a SAF production challenge, but end-use challenges were also noted. There will be regional and seasonal variability in available biomass feedstocks as well as SAF production process differences between facilities. The magnitude of the performance differences within the approved SAF production routes and property ranges listed by ASTM is currently unclear. Maintaining quality control of the fuel properties is paramount to ensuring safe operations with SAF. Thus, there is a need to better understand what range of fuel property and composition variability is acceptable with SAF.

Further, ample opportunities exist for producing biofuels that do not qualify as drop-in SAF, and potentially do so at significantly lower cost. Currently, however, these fuels cannot be used in aircraft due to onerous approval challenges. Thus, a remaining gap is to better understand whether a non drop-in biofuel could help the SAF scale-up in order to meet the SAF Grand Challenge, either in the form of fuel blends or as intermediate chemicals that can provide feedstock for further conversion to produce drop-in SAF.

2. Small Volume Screening of SAF

Scaling-up SAF production to meet the SAF Grand Challenge will likely require the development and approval of additional SAF formulations. The volume of any single SAF required for ASTM D4054 certification to be qualified as a drop-in biofuel exceeds 235,000 US gallons, and even the small SAF volume of 10 gallons needed for the first tier of the screening process can be a barrier for research teams developing milliliter-quantities of fuel at bench scale. The small-volume screening tiers (α and β) developed during the NJFCP made significant strides, but further development and validation remains. These screening tiers focused largely on physical properties, but additional work is needed to link the fuel screening to engine performance. Ideally, the results of the small-volume screening processes could be extrapolated to predict the results of the tier 4 tests, which currently require 225,000 U.S. gallons.

3. Development of Improved SAF (Jet A +)

All drop-in SAF blends need to meet the requirements of Jet A/A-1 to ensure ASTM qualification and backward compatibility with fuel infrastructure and the existing fleet. However, SAF have the potential to meet and exceed these requirements in certain strategic ways. In particular, a SAF with a higher hydrogen-to-carbon ratio and a higher DCN than the average Jet A could produce lower soot emissions, resulting in fewer contrails (discussed in more detail in the *Emissions and Contrails* section), and be more resistant to LBO. Additional research is needed to understand what a Jet A+ formulation could be and provide feedback to researchers working to develop SAF processes.

4. Transferability of Results to Full-Scale and Next Generation Combustors

Testing done during the NJFCP, including the combustor rig testing, was performed using a single swirl-cup combustor and a reference combustor geometry. Each OEM has its own proprietary combustor design that affects engine operation and LBO performance. The extent to which the impacts of fuel properties, based on the results from the NJFCP, are applicable to each engine design at each OEM is proprietary to the OEMs.

Further, rich-quench-lean combustors are representative of most current commercial combustion systems and are designed to keep local temperatures in the combustor sufficiently low (to minimize NOx production) while retaining combustion stability. However, fuel-lean combustion offers significant reductions in criteria pollutants (soot and NOx in particular). Since the NJFCP focused primarily on RQL combustor configurations, additional work is needed to understand how fuel composition and properties affect combustion in fuel-lean combustion systems.

5. Better understanding of blending multiple non drop-in SAF

As mentioned earlier, most of the drop-in SAF only meet the fuel property requirements of Jet A/A-1 in blended form and do not meet the fuel property specification in neat form. A SAF that does have drop-in fleet-wide compatibility is ideal in many ways but is not necessarily required. This is because a blend of different SAF from different processes may be able to compensate for each other's deficiencies. This categorization is commonly referred to as "red apple, green apple, and banana." A red apple means it is identical to Jet A (drop-in), a green apple has one property outside of the Jet A specification, and a banana has more than one property outside of the specification. A simple example of how blending different components to make a red apple can be demonstrated with aromatics. A hydroprocessed synthesized paraffinic kerosene (SPK) contains an insufficient level of aromatics to meet the drop-in requirements (green apple), whereas another SAF may have an aromatic concentration that is too high to meet the drop-in requirements (green apple). While neither of these individually meets the Jet A/A-1 specifications, it is possible that a blend of SAF could meet the required specifications (to qualify as red apple). The aromatic content is only one example of many composition and property targets that could possibly be achieved by blending multiple different SAF together. Greater understanding of the SAF blending landscape, particularly as it pertains to achieving 100% SAF, is an area that requires significant research.

6. SAF Surrogates

Computational investigations of SAF, and SAF-blended fuel combustion may necessitate the use of surrogates for these fuels. Additionally, the unavailability of the NJFCP fuels may require the development of surrogate fuels. Both physical and chemical behaviors need to be considered. It has already been demonstrated that the physical behaviors of these fuels do not follow similar temperature dependencies and it is unclear if the HyChem approach to modeling the chemical kinetics of all SAF is appropriate. For NJFCP, full engine and auxiliary power unit tests demonstrated consistent figures of merit as the single-cup configuration. For the newer fuels, it would need to be assessed if a simple configuration is sufficiently comprehensive to define targets for model, or surrogate fuel performance.

INTERNAL FLOWS AND SPRAYS

Current Status

Fuel injection and combustible mixture preparation determines the performance and emissions characteristics of modern gas turbine systems[11, 12, 13, 14] found in aircraft. Liquid fuel delivery, atomization, and mixing with flowing air are achieved in the atomizer hardware of the engine combustor, which typically feature complex, and often proprietary, geometries to promote targeted fuel distributions, equivalence ratios, and mixing to influence global performance enhancements. These devices exploit various fluid injection and breakup strategies to achieve desired performance across many FOM. The design process for these devices often relies on empirical and analytical models for simplified canonical multiphase flows, which does not account for many of the interaction and complex geometries of the production hardware. Fundamental insights into fuel-air injection, mixing, and subsequent combustion and emissions will lead to development of a robust and efficient computational workflow. For successful predictive capabilities, the following physics need to be captured, which are influenced by internal nozzle flows and atomization:

1. Droplet sizing, vaporization rates, Fuel-air mixing/uniformity

The injection of fuel and early fluid dynamic phenomena relating to multiphase mixing and atomization are primary processes in the combustor. Fuel physical properties govern the injection, flow rates, breakup of liquid into droplets, distribution, and mixing with the flowing air. Primary atomization, the process where a continuous liquid stream or film disintegrates into discrete ligaments or droplets, remains difficult to simulate or predict accurately for realistic operating conditions and geometries in the atomizer. The complexities of modern atomizer designs may dictate that primary atomization occurs and fuel re-coalesces before undergoing a separate atomization mode (e.g., the hybrid airblast atomizer[15]), further challenging predictive abilities. Capturing the multi-scale and multi-physics associated with this realistic early process is difficult if not impossible for current engineering-level models.

2. Flame location/dynamics, leading to operability (ignition, LBO blowout)

Distribution of the liquid fuel, dependent on fuel properties and inflow conditions, can result in non-uniformities in flame shape and stabilization. This may be due to variable liquid properties dependent on upstream conditions, and may differ between fuels (e.g., at low or high temperatures). The fuel distribution was shown to be a primary influence on ignition viability, particularly at operating conditions where physical properties diverged between test fuels during the NJFCP.[16] Furthermore, LBO is particularly sensitive to flame shape and non-uniformity, which can be derived from fuel physical properties and also an amplification of a geometric non-uniformity of the fuel nozzles and atomizer.

3. Durability (liner heat transfer, combustor dynamics)

Increased OPR for modern engines has pushed the energy density of gas turbine combustors toward material limits for combustor liners.[17] Fuel distribution, flame shape, and combustion stability, influence the heat transfer conditions at the combustor liner, and can lead to durability issues. Spray behavior, dependent on fuel properties, can influence these effects.

4. Emissions

Combustion efficiency and performance is directly linked to the fuel distribution, evaporation, and air-mixing processes. The combustion behavior, therefore, dictates the emissions profiles. Beyond the statistically steady condition, the liquid injection and atomization process produce a distribution of liquid droplets and ligaments, which evaporate and combust. Fuel physical properties, particularly deviations seen at extreme conditions, can contribute to the atomization performance, and therefore, emissions profile.

5. Temperature profile/pattern factor

Linked to flame shape and combustion performance on the full combustor scale, the pattern factor can be the result of cup-to-cup variability in spray behavior, as influenced by fuel properties. For the same reasons as flame location and shape varies, differences between individual fuel injectors can result in non-uniformities in heat release, causing non-ideal thermal gradients.

A spectrum of modeling fidelity is currently used (in conjunction with AI/ML) to serve engine design. This process currently hinges upon experimental testing of representative flows and analogous systems used for modeling. Improvements to spray modeling accuracy will enable fuel effects on combustor performance to be differentiated and to benefit combustor design.

Spray experiments were conducted through NJFCP at LBO and cold ignition conditions.[18] While the largest differences in spray distribution were seen due to changes in operating conditions, spray distribution differences were also observed across the wide ranges of fuel properties, most severely for the low pressure, low fuel flow rates, low temperatures associated with high altitude ignition. Test conditions, injector geometries, and spray diagnostic methods were all limited under the NJFCP. Thus, the full picture of the effect of fuel properties on sprays is incomplete.

Furthermore, weighting of different fuel property parameters “remains elusive”—this weighting changes at different conditions.[19] Additionally, simulations were not able to capture the fuel property effects and there is a need to explore more of the design space, exercising model validation. Fuel properties’ influence on primary FOMs, i.e., LBO, cold start, and high-altitude relight, further showed that small differences in fuel properties such as kinematic viscosity, density, surface tension, distillation curve, CN, and flashpoint resulted in performance differences for the FOMs. The relative importance of these properties across the flight map operating conditions are not well understood. Also, modeling tools are not sufficiently mature or consistent across the industry to capture these complicated fuel-engine interactions.

Gaps and Opportunities

Panelists during the workshop identified several gaps and opportunities:

1. Accurate measurement of boundary conditions and real geometry characterization

High quality data sets, for controlled experiments at realistic operating conditions are of high value for model validation. Critical to the databasing of experimental results, is ensuring complete information about the inflow temperatures, pressures, and velocity profiles. As-built geometry, namely the fuel nozzles and atomizer, is included in this detailed case definition, as variability from design can be influential to the combustor performance.

2. Internal and Near-nozzle flows of Jet A/A-1

Quantitative data are needed of flow inside fuel nozzle and of liquid atomization very near the nozzle exit based on experiments and high-fidelity simulations using Jet A/A-1 and SAF to improve our physical understanding. The physical models, with conventional fuels, are still in need of improvement, prior to introducing effects of fuel physical property variability. The large uncertainties that remain in this regime are due to difficulties in acquiring high-quality experimental validation data.

3. Transcritical/supercritical spray morphology

Diagnostics capable of capturing transcritical/supercritical behavior from experiments using Jet A/A-1 and SAF are needed with corresponding validated simulation tools. High temperature and pressure conditions are not only difficult to achieve, but the high-density flow environment leads to diagnostic challenges, which have limited the availability of high-quality experimental validation data. Diagnostics utilized for similar high temperature and pressure, though static, conditions for diesel combustion are applicable to contribute to this area. Similarly, modeling methods developed for diesel conditions may be validated by this growing database for flowing applications. The effects under these conditions are not well understood for Jet A/A-1 and it is possible that SAF will behave differently, based on their unique physical and chemical properties.

4. Improved accuracy/efficiency from high-fidelity nozzle flow and spray simulations

Not to be understated is the need for trusted flow and spray simulations, validated by high-quality experimental data sets. Furthermore, improvement of the time-to-result for these simulations is paramount, especially to inform the parametric exploration of effects on fuel sprays.

5. Fast transfer to lower-level models

Automated procedures to go from high-fidelity simulations and detailed experimental data sets to “engineering models” for complete combustor simulations is desired. Detailed simulations are not anticipated to be adequately fast enough to practically serve in the design cycle. Therefore, physical accuracy that can be validated in the high-order models needs to be transferred to engineering level models, possibly leveraging data-driven methods.

6. Experiments and models differentiating multi-component liquid preferential vaporization

All fuels are blends of multiple components such as n-alkanes, iso-alkanes, cyclo-alkanes, and aromatics. The fuel composition strongly influences the vaporization behavior of the fuel spray droplets due to the varied volatility of the different sub-components. Capturing this phenomenon is particularly critical, since the subsequent combustion behavior and emissions are influenced by the local fuel-air ratio.

7. Database development

While some of the above data and modeling tools exist for conventional Jet A fuel, these datasets need to be developed in an organized fashion for SAF and blends of interest. Maintaining standardization of conditions, techniques, and data formats will accelerate the adoption of the data for validation.

Many of these gaps can be addressed using tools, models, and methodologies developed under PACE and Co-Optima programs, interpolated to middle-weight jet fuel. These tools need to be further validated with appropriate geometries and operating conditions of interest. Similar to procedures developed under PACE, detailed internal nozzle flow simulations can be coupled with spray simulations to improve the efficacy and predictive capability of the simulations.

High precision nozzle geometry metrology has been demonstrated through these former programs to and the results contribute to more accurate predictions of spray morphology. Both neutron and X-ray computed tomography techniques can contribute to characterizing as-built internal geometries of nozzles, for thick parts (neutron) and those needing high spatial resolution (X-ray).

Regarding an understanding of near nozzle physics, and challenges related to supercritical spray diagnostics, X-ray imaging reveals unique spray evolution for realistic injectors since it is not influenced by beam-steering effects of high-density environment conditions. Capabilities need to be enhanced for high pressure and temperature conditions so that the spray morphology details are obtained at more relevant conditions of interest to industry.

There was also interest in generating data in simplified geometries to rigorously validate models first and then increase the complexity of geometries and operating conditions to ensure that the models remain predictive. The Aero-spray atomizer (funded by NASA) and manufactured by Woodward for X-ray testing at Argonne provides a balance between simplified geometry (modelable) and pertinent atomization physics of interest to industry. Several instances of the generic atomizer can be manufactured, common boundary conditions defined, and complementary experiments can be conducted to build a more complete picture of the spray morphology for model validation.

COMBUSTION AND HEAT TRANSFER

Current Status

Combustion and heat transfer phenomena occur at a broad range of conditions in a gas turbine engine. The inlet conditions for the combustor can vary in pressure from 0.4 atm to 70 atm and in temperature from 200 K to 1000 K. Switching fuels is known to impact several critical factors of the engine operation. These include the combustion behavior, combustor's operability, and durability; coking of the nozzle, swirler, and liner; heat release rates; combustion dynamics (noise and stability limits); efficiency; and emissions. The premise of drop-in fuels is that the fuels closely mimic the performance of the Jet A/A-1 fuels in terms of the above combustor performance characteristics. That is, the effort is focused on producing alternate fuels that behave the same way for a given engine design ("Fuels for Design"). Even with drop-in SAF blends that meet the Jet A/A-1 as defined in ASTM D7566, variations in the SAF composition are known to impact some of the performance parameters, and engine emission performance. However, if this view is expanded to consider non drop-in SAF designed for enhanced operation in other words consider changes to engine design to exploit some of the desirable properties of fuels ("Design for Fuels"). For example, fuels with low or negligible aromatic content would result in significantly reduced particulate matter (soot) and fuel properties like a higher thermal stability boost efficiency by enabling more fuel heating. Other benefits could include increased range and durability.

Several previous collaborative efforts of academia, industry, and government made significant progress in understanding combustion processes for alternate fuels/SAF (funding from NIST, NASA, AFRL and SERDP). The CRATCAF program (begun in 2010) was initially established to understand the impact of alternative fuels on the performance, operability, and durability of gas turbine engines, and to validate a methodology for cost-effective screening procedures for new fuels.[11, 12] The NJFCP evolved from CRATCAF (begun in late 2014) with a greater emphasis on establishing experimental tests for early fuel screening and improving modeling capabilities. The NJFCP facilitated collaborations between university partners, industry, and government agencies and assembled several experimental capabilities including shock tubes, component combustion experiments, single cup combustors, and the referee rig. The combustion experiments focused on LBO and ignition at conditions selected to amplify fuel sensitivities[16, 20]. While these efforts have expanded the understanding of combustion and heat transfer phenomena for SAF, there remains a relatively sparse amount of data at gas turbine engine conditions for model validation due to the testing costs and diagnostic challenges in confined, liquid-fueled experiments.

The NJFCP's CFD team performed benchmark simulations to predict the LBO limit in the referee rig using two fuels. The simulations were performed using nine code and submodel combinations and several of these correctly predicted the trend in the LBO limit between the two fuels.[21] Altitude relight modeling was also performed and while the simulations predicted the ignition probability as a function of equivalence ratio, the error bars were large.[21] The CFD effort behind these benchmarks was substantial and overall showed a good qualitative prediction of LBO and altitude relight. However, the benchmark was not definitive as to the choice of submodels, chemistry kinetics model, and flowfield resolution needed to be quantitatively predictive. The benchmark faced an additional challenge: the uncertainty in the temperature boundary conditions and wall heat transfer model limitations. The NJFCP did not have an opportunity to measure the accuracy of emission predictions from the CFD models. Additionally, as learned through the DOE Co-Optima and PACE programs, current combustion models fall short of predicting the spray-flame structure and soot morphology.

Gaps and Opportunities

Two major low lifecycle carbon fuel programs focused on the impact of fuel properties on combustion system performance, recently ended in the United States: the NJFCP on sustainable aviation fuel for gas turbine engines and the Co-Optima program funded by the DOE to co-optimize fuels and engines for on-road vehicles. This presents an opportunity to now pursue research jointly across the two communities. Such a collaboration would more rapidly build the foundational knowledge, predictive tools, novel diagnostics, and experimental insight and validation to remove barriers for broader and more diverse SAF utilization. Some of the opportunities identified in this session include:

1. Expansion of existing facilities

The existing experimental facilities for the NJFCP and Co-Optima programs can be augmented with new measurement techniques, instrumentation, and sensors to understand the fuel property impacts more accurately on the combustion characteristics, turbulence-chemistry interactions and heat transfer in the combustor. Advances in AI/ML and data science can exploit the higher spatial-temporal resolution of new diagnostics to further improve accuracy and fuse experimental knowledge with predictive simulation. As an example, the NJFCP referee rig would be able to measure more accurately the impact of SAF on critical combustion phenomena (forced ignition, lean blow out, pattern temperature, coking, emissions, and flame dynamics) while producing high-quality validation data for CFD prediction.

An opportunity also arises to expand the existing experimental facilities to fill the scale-gap between canonical combustion experiments (e.g., shock tubes, rapid compression machines, jet-stirred reactors, and diffusion flames) and more complex jet engine combustor representatives (e.g., NJFCP referee rig, multi-cup sector, and full annular set). Experiments at the small scale can study coupled turbulent combustion phenomena with greater resolution, less uncertainty of the boundary condition, and relatively small fuel testing volumes (1 liter or less), compared to the larger, more representative geometries. For example, a constant volume spray chamber can provide highly repeatable delivery of SAF at a large range of conditions (300 – 1800 K and 0.4 to 350 atm) suitable for reproducing the conditions in the central and outer recirculation zones of the combustor. The build-out of experimental facilities at this scale and coupling them with the existing resources from NJFCP and Co-Optima is key to developing predictive CFD. These experiments provide understanding and validation data for individual and reduced subsets of the physical (sub-) models in jet engine combustor simulations (for heat transfer, spray breakup and mixing, turbulence chemistry interactions, emissions formation, and flame extinction/ re-ignition).

2. Development of Chemical Kinetics models for SAF

An expanded joint effort between the former NJFCP and Co-Optima teams would allow for the fuel-flexible HyChem model to be combined with the detailed hydrocarbon and bioderived palettes, mechanism compression, surrogate optimization, and detailed soot models funded by the DOE. This integration of experience would allow for a greater number of SAF chemistries to be created with greater accuracy per species/reaction, and permit the inclusion of key International Civil Aviation Organization (ICAO) emissions (CO, UHC, NOx and nvPM) in the predictive models. Another important point to consider is the accuracy impact of the trade-off between computing cost of the fuel/emissions chemistry resolution and spray breakup/mixing resolution.

3. Ignition behavior

Ignition is a challenging problem encompassing cold-start, high-altitude relight, and autoignition and spans temperature ranges of ~220 – 1300 K. Different SAF can have varied coupling between kernel formation, heating, fuel vaporization and subsequent ignition. An exhaustive understanding of this can be enabled through experiments and simulations for a range of configurations starting from simplified geometries to complex rig tests.

4. Combustion physics at relevant temperatures

Most experiments currently focus on pressure ranges of ~ 0.8-5 atm and Mach number of < 0.2 in combustors. However, an assessment of fuels at realistic conditions requires pressures in the range of 0.5- 40 atm and 0.05-0.4 Mach number to capture the high-speed, high turbulence intensities and compressibility effects. Full-scale engine testing is necessary for the fuels of interest under different flight operating conditions. Facilities at universities and AFRL etc. can be leveraged for this purpose. Availability of such data from industry will also be highly beneficial. A complimentary effort needs to occur for multi-phase reacting flows within the combustors with improved combustion models that can capture turbulence-chemistry interactions and handle large chemical mechanisms efficiently. Additionally, toolboxes for advanced diagnostics can be developed and used in tandem with the CFD model to understand precursors and how they change for different SAF for critical phenomena such as lean blow out, high-altitude relight.

5. Heat transfer

For improved thermal efficiency, reduced fuel consumption and pollutants, gas turbines need to be operated at higher pressures (and hence higher temperatures). This necessitates the improvement in heat transfer techniques for enhanced durability of these systems. Convective heat transfer for wall cooling is a challenge for current engines even with conventional jet fuels and is expected to have similar challenges for SAF. The development of new cooling technologies is possible through experiments of simplified geometries and extending these technologies by development of improved modeling to assess the performance on realistic geometries. Radiative loading can be expected to be different between conventional jet fuel and SAF due to the changes in the C/H ratio of the fuels. Integration of improved radiation models with combustion models can allow for improved temperature prediction within the combustors and allow for more accurate prediction of emissions.

6. Combustion Dynamics

Combustion instability is a complex problem and is determined by a combined impact of the geometry and the flame behavior within the combustor. Around 2020, Phase 1 of the FPCI program focused on fuel properties for combustion instabilities in a simplified rig with pre-vaporized air. However, an understanding of the impact of fuel properties for spray combustion within realistic geometries remains elusive. This is particularly relevant for SAF as a change in the physical and chemical properties can inherently change the flame dynamics leading to alteration in the response of combustion instability. Developing models to predict the onset of instability as a function of liquid properties and key geometric features, using a combination of experiments and simulations, will help assess the effects of SAF on combustion dynamics and ground level noise.

EMISSIONS AND CONTRAILS

Current Status

SAF decarbonization goals do not consider flight cycle pollutants; standards for these aircraft emissions are set instead by environmental regulatory bodies such as the US Environmental Protection Agency.[22] To ensure globally uniform regulatory frameworks, these bodies largely adopt emissions standards produced by the International Civil Aviation Organization Committee on Aviation Environmental Protection (ICAO CAEP).[23] Initial ICAO CAEP emissions standards in 1981 focused on local air quality pollutants such as NOx, nvPM, CO, and UHC produced during ground-level operations and in the LTO portions of the flight cycle. These standards are continuously updated based on independent expert review and assessment of “challenging but achievable” mid-term (10-year) and long-term (20-year) engine technology goals and have been expanded to include emissions at cruise conditions.[24] It is important to note that ICAO CAEP standards are focused on the engine rather than the fuel, and thus are not directly tied to new SAF approval. Nonetheless, ASTM D4054 Tier 3 and 4 SAF screening require a combination of ground-based and flight tests, and fuels that lead to deteriorated emissions performance during testing relative to petroleum derived Jet A/A-1 are unlikely to receive positive recommendations by OEM review boards.

Following are the two dominant combustor architectures of aero-engine gas turbine combustors:

1. **Legacy Rich-Quench-Lean (RQL) combustors** with swirl -stabilized flame and fuel-rich primary zone followed by liner mounted dilution jets used to reduce NOx production, dilute the fuel-rich mixtures and control combustion temperatures. For RQL combustors, most nvPM is formed in the primary zone with rich mixtures (hence high equivalence ratios) due to the mixing of injected fuel, air, and recirculated burned gases and most of it is oxidized in the quench zone resulting from the dilution jets. NOx is produced in the high temperature regions of the combustor. NOx is controlled by quickly quenching and limiting the residence time in high temperature regions. However, quick quenching also prevents the oxidation of fuel and CO and results in higher UHC and CO emissions. Hence several competing factors are at play.
2. **More modern lean burn combustors** where flame stabilization is accomplished using a fuel-rich pilot and fuel staging into the fuel-lean main combustion zone. For lean burn combustors, nvPM emissions are predominantly formed in the pilot but are generally lower, relative to RQL designs, due to the comparatively smaller fuel-rich zone. Lean burn combustors use less or no dilution air, with most air supplied through the dome end. The lean main zone helps reduce NOx, UHC, CO emissions.

Each combustor type features a large burnout zone that enables oxidation of most formed nvPM, UHC, and CO. Both involve trade-offs between NOx, nvPM, UHC, CO, operability (ignition and LBO) and other combustor characteristics.

Pollutant emissions are highly dependent on the fuel (chemistry and physical properties), and mixture preparation within the combustor and oxidation processes within the turbine and nozzle. Prediction, accordingly, depends on a detailed understanding of all these processes and their highly non-linear coupling. It is also important to note that different parts of the flight cycle and ground-level operations necessitate different operational envelopes. For example, at takeoff (where full power is required), higher inlet combustor pressures and temperatures and large fueling rates will accordingly result in a substantial increase in formed nvPM and NOx. Emissions sources at cold start, idle, and taxi as well as from periodic fuel venting must also be considered.

In addition to air quality and environmental impacts, aircraft emissions are thought to contribute significantly to anthropogenic climate change. Contrail cirrus cloud formation is suspected to have greater effective radiative forcing than that of aircraft CO_2 emissions, as cloud trapping of radiation from the earth's surface dominates over cloud shading. Emissions of NOx are known to cause a short-term increase in tropospheric ozone that can result in effective radiative forcing at par with aircraft-emitted CO_2.[25] Hence, emitted aircraft CO_2 is roughly *only a third of the net radiative contribution* to global warming from aircraft.[26] While climate forcing emissions are not yet directly addressed by ICAO CAEP standards, these are under active discussion and there is a reasonable chance that these will be regulated in the future.

Contrails form where there is high water vapor concentration in the exhaust plume and atmosphere. In most cases, soot particles act as the condensation nuclei. Once exhausted, the water quickly freezes, and the ice crystals grow. Secondary condensation and collision add to existing particles. While the nucleation process is connected to the hydrophobic or hygroscopic properties of soot particles, there is limited understanding of how fuels and local combustion conditions affect these emitted particles. For example, if different SAF have different morphology and number density of emitted particles, as high ethanol blends are shown to do for automotive engines, the propensity for contrail formation may increase, even if total mass or number of emitted particles remains constant.

Gaps and Opportunities

The gaps and opportunities include further understanding of the particulate matter formation and the formation of contrails:

1. Particulate Matter Formation

Soot particle formation is driven by the formation and growth of poly-aromatic hydrocarbons (PAH), much of which formed due to pyrolysis reactions (i.e., no oxygen). The four stages of soot formation include soot inception, growth, agglomeration, and soot particles. Measurements are needed for SAF candidate components to determine the minimum PAH size needed to support particle growth as a function of pressure and temperatures. These measurements also provide validation for the fuel and particle formation models built from fundamental reaction kinetics. Sectional methods are typically used to model the soot formation process. Additional research is needed on sectional methods to determine the model structure requirements to accurately capture the inception process. For soot growth and agglomeration understanding the impact on the number of representative particles and their key dimensions (e.g., atom number, C/H ratio, surface area, active sites, methylation, morphology *etc.*) is important. Most of the soot produced in the primary zone is oxidized in the downstream/dilution zone, with the residual amount being the soot emitted. Soot oxidation can occur at rates nearly as fast as inception and growth. As a consequence, the final particulate matter levels are hard to predict as the net production is determined by the difference of two very large numbers. Improvements to accurately capture oxidation via O_2, OH and atomic oxygen, and consideration for other contributing molecules are warranted to accurately predict SAF emissions using the sectional model. Advances in particle formation experiments are also needed to validate the model predictions and oxidation pathways over the range of conditions important for cleaner engine operation. Collaborations can be established with OEMs, NASA, AFRL, etc., to characterize exhaust soot emissions under ground-level testing and use those data to compare to soot generated in bespoke experimental conditions.

2. Contrails

A study by NRC Canada demonstrated that a fuel with 92% paraffinics and 8% aromatics reduced contrails significantly, thus providing evidence that substantial decreases in contrails are possible with changes in fuel composition.[27] However, major gaps remain before an accurate prediction of contrails with different fuel compositions, sulfur content, operating conditions, and atmospheric conditions. Water droplet nucleation processes from emitted soot at flight conditions are not understood, including the effects of soot particle morphology, dependency on size for soot nucleation, influence of exhaust and ambient water concentration on ice crystal formation and growth, and the influence of jet exit mixing processes. Opportunity exists to develop well-controlled atmospheric test facilities and feed in realistic exhaust streams (nvPM, temperature, water content, flows) and study nucleation processes using in situ diagnostics (e.g., lasers, X-rays). In addition, reactor, spray, and combustor soot experiments with fuels with varying sulfur content can be performed. This data can be used for developing microphysics modules, new soot and water nucleation kinetics that can be predict nucleation and ice crystal formation with varying fuel composition. Such modules can be coupled with CFD to characterize the early development of near-field contrails.

3. Atmospheric Chemistry

Whether pollutant emissions are at flight or ground conditions will strongly influence the associated impact on radiative forcing. Most commercial aircraft fly at the upper portion of the troposphere, where emitted NOx can more readily interact and influence ozone layer concentrations in the stratosphere depending on transport conditions. Emitted particulate from inorganic impurities has unknown impact on atmospheric chemistry.

ANTICIPATED NEXT STEPS

VTO is interested in establishing a program that accelerates SAF adoption to decarbonize the aviation sector by leveraging unique capabilities at DOE labs. Such a consortium would deliver fundamental science, computational tools, and new data for industry to design next-generation engines in collaboration with BETO, FAA, NASA, etc. Broadly, the scope for national laboratory research focus will be on:

- Developing data-knowledge-tools to accelerate SAF adoption for aero-propulsion based on workshop inputs provided by industry (GE, Honeywell, Pratt & Whitney, Raytheon, Rolls-Royce, etc.), academia, and other relevant government agencies (AFRL, ARL, FAA, NASA, etc.).
- Conducting research across a broad range of operating conditions (flight map) to understand and predict the effects of fuel physical and chemical properties on combustor dynamics.
- Transferring computational tools, data, fuel property, and kinetic mechanisms to industry (via CRADA, etc.) and enhance their existing workflows. Disseminate key findings via high-impact papers and SAF review meetings.
- Integration with university-based community groups, such as the International Sooting Flame Workshop (ISF), the Turbulent Non-premixed Flame Workshop (TNF), and Chemical Kinetics workshop.

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APPENDIX A: WORKSHOP AGENDA

Tuesday, February 15, 2022

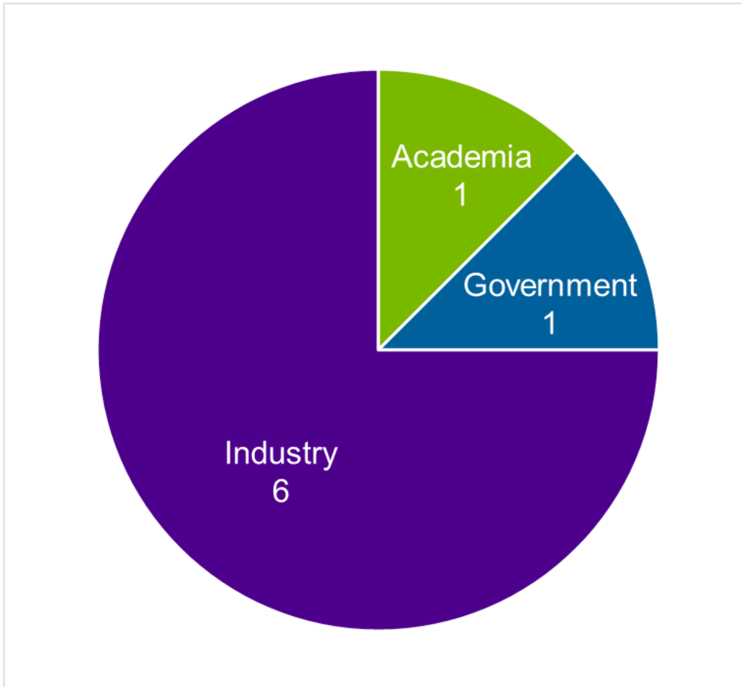
11:00 – 11:05 a.m. (CST)	**Welcome Address**	
		Paul Kearns, Director at Argonne National Laboratory
11:05 – 11:10 a.m.	**SAF Efforts in DOE and Collaboration Opportunities**	
		Michael Berube, Deputy Assistant Secretary for Sustainable Transportation, DOE - EERE
11:10 – 11:15 a.m.	**Workshop Objectives and Mechanics**	
		Brandon Sforzo (Argonne National Laboratory)
11:15 – 11:45 a.m.	**Keynote – National Jet Fuel Combustion Program Summary**	
		Med Colket (Retd. UTRC)
11:45 a.m. – 12:45 p.m.	**Panel Discussion: Next Steps – 100% SAF/Non drop-in SAF Qualification**	
		Moderator – Tim Lieuwen (GT)
		Panelists – Mark Rumizen (FAA)
		Gurhan Andac (GE Aviation)
		Stephen Kramer (Pratt & Whitney)
		Anna Oldani (FAA)
		Anthe George (Sandia National Laboratory)
12:45 – 12:50 p.m.	**Break**	
12:50 – 1:20 p.m.	**Keynote - Fuels and Characterization**	
	Joshua Heyne (University of Dayton)	
1:20 – 2:20 p.m.	**Panel Discussion: Fuel Property Characterization Needs**	
		Moderator – Tonghun Lee (UIUC)
		Panelists – Paul Wrzesinski (AFRL)
		Yuxin Zhang (GE Aviation)
		Mathew McNenly (LLNL)
		Brad Culbertson (Honeywell)
		Corinne Drennan (PNNL)
2:20 – 2:50 p.m.	**Breakout Room Discussions**	
2:50 – 3:00 p.m.	**Report out from Note Taker**	
3:00 p.m.	**Adjourn**	

Wednesday, February 16, 2022

11:00 – 11:05 a.m. (CST)	**Welcome Back** Sibendu Som (Argonne National Laboratory)
11:05 – 11:35 a.m.	**Keynote – Internal nozzle flow and sprays** Brandon Sforzo (Argonne National Laboratory)
11:35 a.m. – 12:35 p.m.	**Panel Discussion: Computational and Experimental needs for Sprays** Moderator – Vince McDonell (UCI) Panelists - Michael Benjamin (GE Aviation) Xiaoyi Li (RTRC) Eric Mayhew (ARL) Jeff Moder (NASA) Gina Magnotti (Argonne National Laboratory)
12:35 – 12:45 p.m.	**Break**
12:45 – 1:15 p.m.	**Keynote – Combustion, Heat Transfer and Emissions** Keith McManus (GE Research)
1:15 – 2:15 p.m.	**Panel Discussion: Computational and Experimental needs for Combustion** Moderator – Jackie O'Connor (PSU) Panelists – MS Anand (Rolls Royce) Andrew Caswell (AFRL) Steve Zeppieri (Pratt & Whitney) Lyle Pickett (Sandia National Laboratory) Debolina Dasgupta (Argonne National Laboratory)
2:15 – 2:45 p.m.	**Breakout Room Discussions**
2:45 – 2:55 p.m.	**Report out from Note Taker**
2:55 – 3:00 p.m.	**Closeout Comments** Sibendu Som (Argonne National Laboratory)
3:00 p.m.	**Adjourn**

APPENDIX B: PARTICIPANT FEEDBACK: SUMMARY OF QUESTIONNAIRE RESPONSES

Questionnaires were sent to 25 affiliate groupings of invitees; eight responses were received.



Below are the questions from the questionnaire with aggregate responses.

1. **What are the perceived risks of Drop-in 100% SAF (e.g., safety, reliability, engine durability, emissions)? Non drop-in?**

Responses indicated an overall concern for both drop-in and non drop-in fuels. The table below summarizes the themes of the responses with the number of occurrences.

durability	4
operability	3
sealing	3
lubricity	2
reliability	2
safety	2
stability	2
autoignition	1
cavitation	1
coking	1
controls	1
emissions	1

endothermic capabilities	1
fuel switching	1
icing	1
temperature stability	1
viscosity	1

2. **What drop-in and non drop-in fuels are of interest for your organization?**

Several responses indicated that all fuels were of interest, especially those qualified for commercial use. Specific answers included:

- JP-10
- RP2
- HEFA/FT blend
- ATJ
- HEFA
- DMCO
- ATJ-SKA
- HEFA-SKA
- CHJ
- SPK+SKA
- CPK-0
- SPK

3. **Relative to your application, what areas do you feel are most in need of better understanding from a computational modeling standpoint, and why?**

The table below summarizes the areas of response with the number of occurrences.

primary and secondary atomization	5
thermal stability	3
vaporization in subsonic/supersonic cross-flow	3
chemical kinetics	2
coking	2
heat transfer	2
ignition	2
PM formation	2
supercritical fuel injection	2
acoustics	1
chemical property correlations (DCN, distillation curve, radical index)	1

4. **What are the most important elements to improve the predictive capabilities of simulations, and why?**

Responses varied, as follows:

- Understand fuel distribution (liquid and vapor).
- Prediction of coking and endothermic behavior.
- Improved chemical kinetics models.
- Understand fuel behavior near and above critical point.
- Combustion dynamics.
- Turbulence-chemistry interaction.
- Ignition predictions.
- Simpler lean blowout methodologies.
- Emissions models.
- Atomization models.
- Advancements in large-scale HPC, or improving simulation cost.
- Increased computational capability and accessibility.
- High-quality near-field spray/vaporization database at relevant conditions.
- Single droplet experimental validation data.
- Full spray experimental validation data.

5. **Currently, what is the accuracy of engineering simulations vs. experimental data?**

Several replies did not respond to this question as it was not applicable to them. Others responded as follows:

- PM and combustion dynamics are not predictively accurate.
- Reliant on experiments for ground truth.
- Time accurate, scale-resolved simulations do not achieve accurate results prior to experimental validation.
- Combustion simulations are between TML [Tool Maturity Level] 1 and 2[a]
- Predictive accuracy is spatially lacking enough precision to eliminate tests.
- Directional accuracy is typically correct.
- Peak temperatures are not accurate nor precise enough to eliminate test.

---

[a] Tool Maturity Level 1: "Analytical process is exploratory in nature. Fidelity of predictions is largely unproven. Provides some physical insight but cannot reduce development testing."

Tool Maturity Level 2: "Proven capability for comparative assessment, ranking or trending. Experimental validation is still necessary. Can drive development or assessment plan and test matrix."

DOI: 10.1186/2193-9772-1-2

6. What code(s) is/are used in your organization for engineering simulations?

Ansys Fluent	5
In-house codes	2
Metacomp CFD++	2
CART3D	1
CONVERGE	1
FUN3D	1
KESTREL	1
Overflow	1

7. What codes(s) is/are used in your organization for high-fidelity scale-resolved simulations?

Ansys Fluent	3
In-house	2
CELESTE	1
CharLES	1
CONVERGE	1
Loci-CHEM	1
PowerFlow	1
REACTMB	1
US3D	1
None	1

8. What physical processes and geometries require additional scale-resolved simulations?

Several replies did not respond to this question as it was not applicable to them. Others responded as follows:

Atomization	3
Ignition	2
Acoustics	1
Cooling	1
Entire combustor/diffuser system	1
Flame Stability	1
Real-gas effects	1
Vaporization	1

9. What is the extent of use of AI/ML techniques towards accelerating simulations, design optimizations, and data synthesis?

Several replies did not respond to this question as it was not applicable to them. Others responded as follows:

Limited or N/A	5
Combustor simulations	1
Design optimization	1
Students are encouraged to pursue usage	1

10. For internal flow experiments, RANK operational regime in greatest need of characterization.

Several respondents could not comment on this ranking. Other responses were as follows:

Acceleration/cruise	3
High altitude relight	3
Climb	1
Cold start	1
Initial pre-ignition conditions	1
Mixed	1
Takeoff	1

11. For external sprays experiments, RANK operational regime in greatest need of characterization.

Several respondents could not comment on this ranking. Other responses were as follows:

High altitude relight	3
Takeoff	2
Cold start	1
Cruise	1
Transient chop	1
Warm start	1

12. Would/how the previous rankings change for simulations?

All respondents indicated that the rankings would not change, with one replying that the experiments and modeling should be coupled

13. What are the typical chemical mechanism sizes used for modeling?

Several organizations could not comment, with several others indicating that they use typical skeletal or reduced mechanism sizes. Three responded that their mechanisms had 10s of species and 100s of reactions.

14. For SAF what additional flame speed, ignition delay, and speciation data is desired?

Flame speed	2
Ignition delay	2
Any standardized data	1
Detailed combustion data	1
High fidelity chemical kinetic models	1
Highlighting of difference between Jet A models and SAF	1
Speciation data	1

15. Please provide information on ignition and turbulent combustion modeling approach(es) used in your organization.

Not all organizations were able to respond to this question.

Laminar chemistry for low-order models	2
Standard Fluent submodels	2
SAGE	1
In-house codes	1

16. Is it expected that contrail formation will be regulated in the future, and if so, how?

Responses were mixed for this question, with some replies as follows:

Unsure	3
Unlikely	2
Probably	1

17. Can additional data (experimental, simulation) and geometries be made available from your organization (under proper contractual agreements) to accelerate national lab research?

Maybe	4
N/A	2
Yes	2

18. What kind of validation/verification would the OEMs like to see before adopting newer models and/or tools in practice?

Several were unable to reply to this question, while others provided the following responses:

Benchmark at condition	3
Validation in generic geometry	2

19. What are workforce development needs for end-use research with SAF?

Several replies were unable to answer this question. Several others are as follows:

N/A	2
Collaborative	2
More familiarity with chemical aspects	1
Transfer of atomization and kinetics domain-knowledge	1

APPENDIX C: ATTENDEE LIST & AFFILIATIONS

ABDA

Glenn Liston

Aerodyne

Richard Miake-Lye

Aerojet Rocketdyne

Scott Claflin

Jeff Stout

Air Force Research Laboratory

Matt Billingsley

Cam Carter

Andrew Caswell

Edwin Corporan

Stephen Hammack

Tim Ombrello

David Peterson

Brent Rankin

Paul Wrzesinski

Alder Fuels

Derek Vardon

Argonne National Laboratory

Muhsin Ameen

Debolina Dasgupta

Sinan Demir

Guadalupe Franchini

Scott Goldsborough

Don Hillebrand

Alan Kastengren

Paul Kearns

Doug Longman

Gina Magnotti

Chi Young Moon

Pinaki Pal

Chris Powell

Riccardo Scarcelli

Brandon Sforzo

Sibendu Som

Suresh Sunderrajan

Meltem Urgun Demirtas

Michael Wang

Chao Xu

Army Research Laboratory

Mike Kweon

Eric Mayhew

Jacob Temme

BETO

Jay Fitzgerald

Boeing

Steven Baughcum

JP Belieres

Joseph Ellsworth

James Kinder

Ilya Kosilkin

Boom

Ben Murphy

Combustion Consulting Services, LLC

Med Colket

Colorado University Boulder

Peter Hamlington

DOE

Michael Berube

Siddiq Khan

Reyhaneh Shenassa

Mark Shmorhun

Ben Simon

Trevor Smith

Jim Spaeth

DOE BETO

Marykate O'Brien

Zia Haq

Mark Shmorhun

DOE-VTO

Dave Howell

Gurpreet Singh

Kevin Stork

Mike Weismiller

DOT

Kristin Lewis

FAA

Nate Brown

Ileri Levent

Anna Oldani

Mark Rumizen

GE Aviation

Gurhan Andac

Michael Benjamin

Kwanwoo Kim

Zhang Yuxin

Joe Zelina

GE Global Research

Paul Glaser

Nick Magina

Keith McManus

Joanne Morello

Umesh Paliath

Krishna Venkatesan

Changjin Yoon

Georgia Institute of Technology

Ben Emerson

Tim Lieuwen

Adam Steinberg

Honeywell

Brad Culbertson

Rudy Dudebout

Jon Fein

Nagaraja Rudrapatna

Liangyu Wang

Fang Xu

Lanzatech

John Holladay

Lawrence Livermore National Laboratory

Goutham Kukkadapu

Matt McNenly

Chiara Saggese

Scott Wagnon

Russell Whitesides

Tanusree Chatterjee

NASA Glenn Research Center

Zhuohui He

Yolanda Hicks

Kathleen Tacina

Jennifer Klettlinger

Kumud Ajmani

Francisco Guzman

Jeff Moder

NASA Langley

Tom Drozda

Rich Moore

National Research Council Canada

Pervez Canteenwalla

Andrew Corber

Nanthan Ramachandran

Navair

Jan Herzog

Richard Kamin

Andrew McDaniel

NREL

Craig Brown

Marcus Day

John Farrell

Gina Fioroni

Robert McCormick

Shashank Yellapantula

NRL

Ryan Johnson

ONR

Steve Martens

Oak Ridge National Laboratory

Haiying Chen

Scott Curran

Dipti Kamath

Michael Kass

Vladislav Lobodin

Josh Pihl

Andrew Sutton

Jim Szybist

Todd Toops

Robert Wagner

Martin Wissink

Pennsylvania State University

Jacqueline O'Connor

PNNL

Corinne Drennan

Pratt & Whitney

Margaret Adamson

Sean Bradshaw

Stephen Kramer

Baris Sen

Purdue University

Bob Lucht

Raytheon

Harry Cordatos

Zissis Dardas

Sean Emerson

Miad Yazdani

Raytheon Technologies Research Center

Peter Cocks

Jeff Cohen

Wookyung Kim

Xiaoyi Li

Lance Smith

Steve Zepperi

Rolls Royce

Papaaye Aye-Addo

Masha Folk

Heeseok Koo

MS Anand

Brad Belcher

Brad Wall

Sandia National Laboratories

Marco Arienti

Damian Carrieri

Isaac Ekoto

Anthe George

Julien Manin

Lyle Pickett

Dario Pintor Lopez

Shell

Griffin Valentich

Stanford University

Ron Hanson

Matthias Ihme

Trinity College Dublin

Stephen Dooley

UCI

Vince McDonnell

UDRI

Scott Stouffer

Steven Zabarnick

University of Illinois at Urbana-Champaign

Tonghun Lee

Alex Solecki

University of Connecticut

Tianfeng Lu

University of Dayton

Randall Boehm

Alex Briones

Matt Dewitt

Tyler Hendershott

Josh Heyne

Jeffrey Monfort

Williams International

Matthew Brouwer

Kyle Chavez

Jamey Condevaux

Woodward

Carthel Baker

Bidhan Dam

Angela Kimber

Ashley Moore

World Energy

Greg Buczynski

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