



Project 024(B) – 2016 Period of Performance

University Participants

Penn State University

- P.I.(s): Randy L. Vander Wal, Professor, Energy and Mineral Engineering, Materials Science and Engineering
- FAA Award Number: Grant 11712482, Amendment No. 13-C-AJFE-PSU-008
- Period of Performance: Aug. 18th, 2014, Sept. 30th, 2016
- Task(s):
 1. Develop Database. Include mass and number nvPM emission data for fuels, engine, measurement method(s) and engine conditions.
 2. a) Compare current ground nvPM predictive methods to measured values from NASA campaigns.
b) Compare current cruise scaling approximation to measured cruise values from NASA's ACCESS.
 3. Correct current engine condition predictive methods using proprietary GE cycle deck data.
 4. Compare current methods using accurate engine condition inputs.
 5. Formulate new predictive relationships for nvPM with engine thrust level.
 6. Evaluate whether a universal relation or separate ones are required for Jet-A and alternative fuels.

Project Funding Level

FAA funding: \$149,975

GE Aviation is the Industrial Partner supplying matching funds, level \$150,000, with \$1,724,895 available to the FAA COE AJFE ASCENT program, administered through Washington State University.

Investigation Team

Professor Randy L. Vander Wal, Penn State EME Dept., with responsibilities for project management, reports, interfacing with FAA program manager, and mentoring the graduate student supported on this project.

Mr. Joseph P. Abrahamson, Graduate student. Responsibilities include data assembly, analysis and predictive relation assessment, as integral towards completion of a Ph.D. program.

Project Overview

Relationships between fuel components, engine operating conditions and emissions are necessary to understanding their formation and achieving mitigation. Present synthetic paraffinic kerosene (SPK) aviation fuels differ from petroleum derived aviation kerosene by their high paraffin (~ 53% n-paraffin, 47% iso-paraffin, FT Shell), naphthene content (~ 87% cycloparaffin, 12% iso-paraffin, FT Sasol), but most notably absence of aromatics (< 0.5%) and negligible organo-sulfur compounds. Future alternative may have substantially higher cycloparaffin content while hydrotreated depolymerized cellulosic (HDCJ) fuel may even (re)-introduce aromatics, adding to composition variability and need for understanding emissions from varied components and their mixtures.

With the emerging use of alternative fuels and varied compositions markedly change non-volatile PM (nvPM) emissions. Number density and mass changes are found, and hence emission index (EI). These measures in particular are relevant to potential regulations. These quantities can vary with engine power, and are strongly dependent upon fuel components, namely paraffin, naphthene and aromatic content. The value of these studies is that assembling data across platforms, fuels and measurement methods will build a comprehensive picture of PM emissions dependence upon components, engine type, power level and minor fuel species such as sulfur.

Objective(s)

Nonvolatile PM emissions from aircraft engines are primarily comprised of soot particles formed in the engine combustor. The amount of soot formed within a specific combustor design can change by more than an order of magnitude as engine thrust increases from idle to takeoff, due to increasing combustor pressure, temperature, and fuel-air ratio. In order to understand the influence of fuel properties on nvPM emissions from a specific engine, it is important to separate fuel effects from changes in emissions due to differences in combustor operating conditions, which are affected by engine thrust level, ambient conditions, altitude, flight Mach number, and engine deterioration.



Research Approach

Emerging use of alternative fuels markedly change non-volatile PM (nvPM) emissions. Number density and mass changes are found, with emission index (EI) being the most uncertain given its derivation by smoke number. These measures in particular are relevant to future regulations. These quantities can vary with engine power, and are strongly dependent upon fuel components, namely paraffin, naphthene and aromatic content.

In light of this situation emissions data from the FAA CLEEN program, NASA-led ACCESS campaigns, and related NASA Aviation Particle Emission Experiment (APEX) I, and Alternative Aviation Fuel(s) Experiment (AAFEX) I & II campaigns has been collected. These campaigns and tests investigated alternative fuels, varied fuel components and assessed the role of and aromatics. To-date there is no comparison(s) between these studies or compilation of results into a unified database. The value of these studies is that assembling data across a range of studies, conducted using one engine class, representative of rich-dome style combustors, platforms, fuels and measurement methods will build a comprehensive picture of PM emissions dependence upon fuel composition and engine thrust at ground and cruise.

Previous studies have used simplified relationships to estimate emissions as a function of engine operating conditions. A more detailed two-step process is planned to correct for these effects in this proposed study. GE Aviation has detailed proprietary analytical models for each GE and CFMI engine type to predict pressures and temperatures throughout the engine as a function of thrust and inlet conditions. The first step in the proposed study is to use this type of model to calculate combustor inlet pressure, temperature, and fuel-air ratio at operating points where nvPM emissions have been measured, and re-evaluate current predictive methods using correct engine operating conditions. By comparison to ground and cruise nvPM emission data, deficiencies in current formulations can be identified and new predictive relations can be developed. With relations benchmarked against measurements, and confidence in engine operating conditions, measured nvPM from alternative fuels may be used to guide parameter formulation in these new predictive relations so as to expand their applicability to alternative fuels. Thereafter these relations will be assessed by comparison to nvPM test data from other engines as from NASA studies and the FAA CLEEN programs.

Milestone(s)

Milestones accomplished during this period of performance include the following.

1. Database development for nvPM mass, number emission data for fuels, engine thrust across field campaigns.
2. Compared GE Aviation cycle deck calculations at ground and cruise conditions, matching test point conditions in the NASA field campaigns.
3. Evaluation of current predictive methods to ground and cruise measurements using accurate engine operating conditions.
4. Formulated new predictive relationships for nvPM with engine thrust level.
5. Developed a universal relation as a predictive tool for estimating nvPM from Jet-A and alternative fuels.

Major Accomplishments

(as excepted from ES&T 2016 submission)

IMPROVED METHOD (ImFOX)

1. Improved Engine Condition Relations. In this section engine conditions required as inputs for the improved FOX (ImFOX) expression are more accurately provided in the form of predictive relations based on proprietary cycle deck calculations for a common RQL combustor. Aerosol emissions from the NASA campaigns: Aircraft Particle Emissions eXperiments (APEX-I)^{28,29}, Alternative Aviation Fuel Experiments I and II (AAFEX-1, AAFEX-II)^{30,31}, Alternative-Fuel Effects on Contrails & Cruise EmiSSions I and II (ACCESS-I, ACCESS-II)⁹ are from a Douglas DC-8 aircraft equipped with four CFM56-2C turbo fan engines. Although, this engine is an older design it is a high-bypass engine and serves as the basis for the whole engine family employed by thousands of commercial and military aircraft worldwide. The EI_{bc} curves from five of the six RQL style combustors tested during APEX-III³²⁻³⁴ followed a common curve³⁵, with upturns both at low (idle) and high (take-off) thrust levels. (The exception was the Rolls-Royce engine RB211-535E4-B with 40,100 lbs. maximum thrust, which has a BC emission profile peaking at 65% of the maximum thrust and decreased emissions thereafter.) Therefore, it appears the relationships developed here are considered applicable for a majority of rich-burn, quick-quench, lean-burn (RQL) style combustors. Only a select few engine conditions are addressed in this section. This is intentional as the goal is to simplify the calculations needed to predict EI_{bc} . For the relations developed here, the only needed input is the fuel flow rate from which all other engine conditions as input for the ImFOX expression can be calculated. For an extended study on conditions especially at cruise altitude the interested reader is referred to reference 1.



Air-to-Fuel Ratio, AFR. The first condition investigated is AFR, it should be mentioned that AFRs found here are those at the back of the combustor, typically referred to as plane-4, and are not the AFRs in the primary zone or the quench zone. The current method, equation 5, has been widely accepted. This is partially because an engine manufacturer had released nominal AFR values at 7, 30, 85, and 100 thrust settings.¹⁵ Those values were linearly fit to derive the current predictive AFR expression. However, after comparing values using this relation to engine cycle deck data it was evident that the current method results in over prediction of AFR. Two separate equations are needed to accurately calculate AFR. One for ground and another for cruise, equations 10 and 11 respectively.

$$AFR_{grd} = 71 - 35.8 \left(\frac{\dot{m}_f}{\dot{m}_{f,max}} \right)$$

[10]

$$AFR_{cru} = 55.4 - 30.8 \left(\frac{\dot{m}_f}{\dot{m}_{f,max}} \right)$$

[11]

As seen from the two AFR equations, at a matching thrust level AFR will be lower at cruise than at ground. This is sensible considering the decreased air density at altitude.

Flame Temperature, T_{fl} . Flame temperature is arguably the most important variable as it appears in both exponential terms in both the FOX and the Döpelheuer and Lecht scaling relation. Several T_{fl} predictive methods have been developed in addition to the one currently used in the FOX expression, equation 7. The common practice is to predict a T_{fl} using a linear relationship to T_3 . Whereas equation 7 assumes that 90 % of the incoming sensible heat from the hot air leaving the compressor, T_3 , adds to a stoichiometric adiabatic flame temperature of 2120 K. A common alternative flame temperature predictor for an RQL style combustor based on T_3 is given in equation 12.³⁶

$$T_{fl}[K] = 0.6T_3 + 1800$$

[12]

This method assumes that 60 % of the initial air temperature is converted to flame temperature and that the flame temperature without this addition is that of a fuel rich flame at 1800 K. Considering that the primary zone of an RQL combustor runs fuel rich for flame stabilization, equation 12 is a more realistic flame temperature predictor to determine the primary zone flame temperature. However, the only variable in either flame temperature predictor is T_3 and since the AFR is a function of thrust the second term should also be variable with relation to AFR, and hence thrust (given flame temperature dependence upon stoichiometry, or AFR). However, since this localized AFR as a function of thrust is proprietary and not readily determined we have elected to use the temperature at the back of the combustor (T_4) in place of primary zone flame temperature. Using T_4 for the flame temperature is logical considering that the AFR being used is also from the back of the combustor as a global average of the processes occurring in the formation and oxidation regions of the combustor. Additionally, T_4 is readily calculated by the engine cycle deck, yielding equation 13.

$$T_4[K] = 490 + 42,266FAR$$

[13]

There is a strong correlation between T_3 and T_4 , the Pearson r correlation value is 0.966. However, as seen in equation 13 it was not selected in the T_4 relation because there is a much stronger correlation between T_4 and fuel-air-ratio (FAR), Pearson r value of 0.995, but more importantly for the fact that an explicit AFR dependence accounts for the expected dependence of T_{fl} upon stoichiometry. Additionally, T_3 is an engine specific parameter that may not be readily available in all cases. Equation 13 accurately predicts T_4 at both ground and cruise. Given the success of this semi-empirical T_4 calculation based on FAR, a thermodynamic basis was evaluated for rationalization of this empirical result. The thermodynamic Air Standard Brayton Cycle is applied to a jet engine in the SI. The thermodynamic Brayton Cycle equates T_4 to exhaust gas temperature (EGT) squared divided by temperature ambient. The NASA campaigns (APEX I-III, AAFEX I & II, and ACCESS I & II) documented both EGT and ambient temperature. Values of T_4 found using the thermodynamic Brayton Cycle compared to values predicted using equation 13 were slightly higher (~10%), likely because the Brayton Cycle is treated as an idealized adiabatic system. While either relation can be used to find T_4 , the benefit of equation 13 is that only the FAR is needed and equations 10 and 11 provide accurate FAR relations for both ground and cruise respectively.



2. Improved El_{bc} Predictive Relations.

The model we have developed uses the FOX¹⁹ as the starting point. The FOX is a kinetically balanced relation predicting El_{bc} by subtracting the rate of soot formation from the rate of soot oxidation. Each global process is represented by a single-step Arrhenius rate. The activation energy (E_a) value in the oxidation step is the well accepted value first proposed by Lee et al.³⁷ Given the success of this value, no modification to the oxidation step was made, outside of correcting AFR and substituting T_{fl} with T_4 . The formation activation energy is that reported by Hall et al.³⁹ and is their inception E_a based on the formation of polyaromatic hydrocarbons (PAHs). The pre-exponential frequency factor (also referred to as formation constant) is a function of two and three member PAH concentrations, reflecting their role as BC building block molecules. Using a formation constant value of 356 Settler et al.¹⁹ achieve a coefficient of determination, R^2 , value of 0.8 when fitting to the APEX campaign data. The limitation of this approach is that it does not account for alternative fuels. A different formation constant would be necessary for each fuel composition. By combining the ImFOX with the ASAF relation developed by Speth et al.²⁰ determination of BC emissions from alternative fuels is possible. However, ASAF does not consider cycloalkanes known to have a higher sooting index^{26,39} than that of paraffinic compounds found predominantly in alternative fuels. Therefore, an alternative approach was developed using hydrogen content. Formulation and results from pairing the ImFOX with ASAF are given in the SI.

H-ImFOX. As previously mentioned, the pre-exponential frequency factor is a function of two and three member PAH concentration, which in turn is a function of PAH building block molecule concentrations; acetylene, benzene, phenyl radical, and hydrogen. Since there is no practical way to determine these molecular concentrations this pre-exponential factor (also referred to as a formation constant) is fit to C_{bc} data and given in equation 14.

$$A_{form} = 1013 - 4802\left(\frac{\dot{m}_f}{\dot{m}_{f,max}}\right) + 7730\left(\frac{\dot{m}_f}{\dot{m}_{f,max}}\right)^2 - 3776\left(\frac{\dot{m}_f}{\dot{m}_{f,max}}\right)^3 \quad [14]$$

There is a complex dependence, 3rd order, between thrust and the formation constant. This is sensible considering that PAH building block molecule concentrations will vary with thrust. High-resolution transmission electron microscopy and X-ray photoelectron spectroscopy have been used to demonstrate how the macro, micro, and nano-structure of BC from commercial aircraft vary across thrust settings.^{35,40} Black carbon nanostructure can reflect the formation conditions, i.e. species and temperature, of BC.³⁵ As reported by Vander Wal et al.³⁵ BC emissions vary from amorphous at low power (idle) to graphitic at high power (take off). This observation supports the need for the formation constant to have a complex dependence on thrust. Black carbon is not an equilibrium product of combustion.³⁶ Thus, it is difficult to predict its rate of formation and final concentration from kinetics or thermodynamics alone. In practice, the rate of soot formation is strongly impacted by the physical processes of atomization and fuel-air mixing as these processes control the equivalence ratio and resulting flame temperature.³⁶ This fuel air mixing is captured by the thrust dependent A_{form} term given in equation 14. This mixing effect is the same across all fuels: conventional, blended, and neat SPK. Therefore, equation 14 developed here for conventional fuel can be used to represent the mixing (combustor) effect across all fuels and a separate fuel term can be added to account for fuel effects, specifically decreasing El_{bc} with increasing hydrogen mass content. The new predictive expression is accordingly termed the H-ImFOX, and given in eqn. 15.

$$C_{bc}\left[\frac{mg}{m^3}\right] = \dot{m}_f \times e^{(13.6-H)} (A_{form} \times e^{(-6390/T_4)} - A_{ox} \times AFR \times e^{(-19778/T_4)}) \quad [15]$$

The H in equation 15 represents hydrogen mass percent and as seen in equation 15 BC emission decays exponentially with increasing hydrogen content. This trend was observed across the previously mentioned NASA campaigns.⁹ The H-ImFOX will hereafter be referred to as just the ImFOX as the new hydrogen fuel term is universally applied across all fuels and therefore, equation 15 is the ImFOX. A strong correlation between hydrogen content and BC reduction was recently observed during the Aircraft Particulate Regulatory Instrumentation Demonstration Experiment (A-PRIDE) 7. It was demonstrated by Brem et al.⁴¹ that BC emissions from conventional fuels vary due to a range of aromatic content and concluded that emissions are best predicted based on hydrogen mass content. Additionally, Lobo et al.⁴² recently reported similar findings by varying the ratio of SPK blending components with conventional fuel.

The hydrogen dependent fuel effect developed here based on ground data applies equally well at cruise as the BC emission trend with hydrogen content is the same at both ground and cruise altitude. However, El_{bc} measured at cruise during the recent ACCESS-II campaign was 264 % higher than ground based measurements when averaged across all observed powers. This is likely due to the decreased AFR at cruise brought on by the reduced air density. The lower AFR or higher equivalence ratio at cruise will give rise to more fuel rich pockets and higher concentrations of BC precursor molecular species. Accordingly, different A_{form} relations are necessary for ground and cruise. During cruise operation thrust settings are typically higher than 30 %, therefore, cruise El_{bc} emission profiles do not possess the commonly observed emission



curve with upturns both at low (idle) and high (take-off) thrust levels as measured from ground campaigns. From the limited cruise altitude BC measurements, the El_{BC} increases linearly with thrust, hence complex formation constants, like derived for ground based emissions, are not necessary. A complex expression for cruise A_{form} may ultimately be needed, however, the limited range of thrust values at cruise do not provide justification for such, instead the simplest expression (a constant) was chosen and found adequate by quality of fit. A constant A_{form} cruise value of 295 captures the observed linear trend of increasing El_{BC} with increased thrust at cruise.

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Publications & Presentations

1. Publications

1. Abrahamson, J. P., Zelina, J., Andac, G., and Vander Wal, R. L., Aviation black carbon mass predictive model for alternative and traditional fuels at ground and cruise.

FAA Hartman paper (Best paper of the year award). 2016.

Available at: <https://ascent.aero/competition/>

and

https://ascent.aero/wp-content/uploads/sites/192/2015/12/Hartman_CH_7-20-16IPA.pdf

2. Abrahamson, J. P., Zelina, J., Andac, M. G., & Vander Wal, R. L. (2016). Predictive Model Development for Aviation Black Carbon Mass Emissions from Alternative and Conventional Fuels at Ground and Cruise. *Environmental Science & Technology*, (submitted).

2. Presentations

Invited

1. Vander Wal, R. L., Abrahamson, J. P., Jet Engine nvPM Emissions: Status of Predictive Relations. Session 10: Fuel Composition Effects Upon Emissions. Aviation Emissions Characterization Roadmap. 14th Annual Meeting, National Academy of Sciences, Washington, D.C. May 24th – 26th, 2016.

Invited – Student of The Year Award

2. Abrahamson, J. P., and Vander Wal, R. L., nvPM Emissions Database Compilation, Analysis and Predictive Assessment. Project 24B. FAA ASCENT 5th Advisory Board Meeting. FAA Center of Excellence for Alternative Jet Fuels & Environment (FAA COE AJFE). Alexandria, VA April 26th-27th, 2016.

3. Vander Wal, R. L., Abrahamson, J. P., PM Database Compilation, Analysis and Predictive Assessments. Project 24B Report. 5th Advisory Board Meeting. FAA Center of Excellence for Alternative Jet Fuels & Environment (FAA COE AJFE). Alexandria, VA April 26th-27th, 2016.



4. Abrahamson, J. P., Vander Wal, R. L., (2016). Gas turbine nvPM formation and oxidation semi-empirical model for commercial aviation. Paper # 138IC-0025. Topic: Internal Combustion and Gas Turbine Engines. 2016 Spring Technical Meeting, Eastern States Section of the Combustion Institute, Princeton University, Princeton, NJ March 13-16th, 2016.
5. Abrahamson, J. P., and Vander Wal, R. L., Retooling Predictive Relations for non-volatile PM by Comparison to Measurements. Session: Quantifying Aviation Impacts on Air Quality and Climate. The annual American Geophysical Union (AGU) Annual Fall Meeting, Dec. 14th – 18th, 2015. San Francisco, CA.
6. Abrahamson, J. P., and Vander Wal, R. L., nvPM Emissions Database Compilation, Analysis and Predictive Assessment. Project 25B. FAA ASCENT Contractor's Meeting. Seattle WA, Oct. 13-15th, 2015.
7. Abrahamson, J. P., and Vander Wal, R. L., nvPM Emissions Database Compilation, Analysis and Predictive Assessment. Project 25B. FAA External Tools Meeting, Seattle WA, Oct. 20th, 2015.

Outreach Efforts

Informal discussions with GE US Aviation regarding the nature of nvPM from next generation lean-burn engines and potential differences relative to nvPM from RQL combustor designs.

Awards

Joseph P. Abrahamson – Energy and Mineral Engineering Dept. Penn State University

Joseph P. Abrahamson has received the FAA Center of Excellence Student of the Year (SOY) Award. Nationally competed, it is sponsored by the Department of Transportation, Council of University Transportation Centers and corporate affiliates. Joseph has also won the FAA ASCENT Joseph A. Hartman Student Paper Competition – a peer-reviewed process to select the best paper with focus on the environmental impact of the aviation industry. Joseph is presently a graduate student in The John and Willie Leone Family Department of Energy and Mineral Engineering at Penn State, pursuing his Ph.D. under the guidance of Professor Randy L. Vander Wal.

Student Involvement

The current graduate student, Joseph P. Abrahamson, is conducting data assembly, analysis and predictive relation assessment, towards partial fulfillment of his Ph.D. program in EME, with Fuel Science option.

Plans for Next Period

The tasks and milestones for this project were completed July 31st, 2016.