Project 024(B) PM Emission Database Compilation, Analysis and Predictive Assessment

The Pennsylvania State University, GE U.S. Aviation

Project Lead Investigator

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- P.I.(s): Randy L. Vander Wal, Professor, Energy and Mineral Engineering, Materials Science and Engineering
- FAA Award Number: Grant 12148585, Amendment No. 13-C-AJFE-PSU-019
- Period of Performance: Aug. 1st, 2016, July 31st, 2017
- Task(s):
    1. Test for improved accuracy by separating the temperatures associated with nvPM formation and oxidation. Presently the ImFOX kinetic expression uses one temperature at the exit of the combustor as representing the global temperature. The accuracy of T4 is confirmed by GE cycle deck calculations and consistent with the Brayton thermodynamic cycle for the engine. Yet for RQL style combustors soot formation necessarily occurs near an estimated $\varphi \sim 2$ while oxidation occurs under lean conditions, $\varphi \sim 0.9$. Such differences suggest different temperatures as better representing nvPM formation and oxidation regions.
    2. Assess ACCESS II test procedure upon engine conditions at cruise. A key difference between ground and cruise altitude is the ram effect at cruise and lower (external) pressure. These conditions alter the air-to- fuel ratio and hence while the form of the ImFOX relation is uniform between ground and cruise, different AFR relations may be necessary to capture these effects. With guidance from GE Aviation and their cycle calculations one can assess whether two separate or one unified AFR relations is sufficient – the latter then simplifying ImFOX use.
    3. Evaluate ASAF as the global scaling factor in the ImFOX relation. The ASAF relation was formulated by MIT as an empirical correlation of nvPM across all available engine emissions data. It is based upon aromatic content as the driving parameter for carbon aerosol emission. The MIT consensus is that the ASAF serve as global scaling factor for the ImFOX relation. This will be evaluated by comparison to measured nvPM from JP-8 and blends between conventional and alternative fuels.
    4. Investigate alternative representations to capture fuel composition effects for alternative fuels. Given the limitation of the present ASAF relation a more encompassing metric to capture fuel compositional effects is required. Alternative fuels do not have aromatic content but do have considerable and varying proportions of cyclic and normal paraffins. This introduces a hydrogen variation as well as C/H variation. Blended fuels will contain aromatics as carry-over from the original petroleum component. However, naphthalene is currently considered to contribute disproportionately to soot formation with current FAA interest being to remove it from fuels. Such twists necessitate a more encompassing relation than ASAF to represent the different and varying fuel component classes. The fuels used in AAFEX I: JP-8, coal and natural gas based FT fuels and 50:50 blends with JP-8 encompass a range of aromatic and hydrogen contents for which EI(BC) plots are linear in semi-log format. Such data suggests that either or both of these fuel factors may be incorporated into the ImFOX relation in the formation pre-factor. These alternative fuel dependencies will be tested against the field campaign data and compared to the ASAF relation across engine thrusts.
    5. Evaluate the ImFOX relation against the ACCESS II flight data from NASA for nvPM. Presently ground based emission levels are scaled by the Doppelheuer and Lecht (DL) relation to estimate cruise EI(BC). This approach imposes redundancy as the DL relation is a kinetic based expression that then duplicates the kinetic rates

explicit in the ImFOX relation. Our remedy is to avoid this scaling step by developing a direct predictive relation that does not require scaling or correction factors between ground and cruise. Using cycle deck data from GE Aviation, accurate engine conditions of AFR and Tfl are identified and relationships with thrust can be developed. This then permits true evaluation of the ImFOX relation – without skew by inaccuracies in engine operating conditions – an aspect that has plagued and limited prior such efforts.

6. Validate the ImFOX for other engines in the CFM class. As shown by our prior work, with guidance from cycle deck calculations, engine conditions may be accurately modeled known and hence comparison of ImFOX to measured nvPM provides a true assessment of the ImFOX predictive ability. Comparison to the CFM56-3B engine is planned given presently available test data for this engine and with cycle deck calculations provided by our GE partners.

Project Funding Level

FAA funding: $75,000

GE Aviation is the Industrial Partner supplying matching funds, level $75,000, from an original commitment of $1,724895 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

The recently developed FOX method removes the need for and hence uncertainty associated with (SNs), instead relying upon engine conditions in order to predict BC mass. Using the true engine operating conditions an improved FOX (ImFOX) predictive relation was developed. Necessary for its implementation are its development and validation to estimate cruise emissions and account for the use of alternative jet fuels with reduced aromatic content. Refinement by incorporating separate, independent temperatures for fuel-rich and fuel-lean regions of the combustor will be evaluated against another CFM engine. Comparison to measured nvPM at cruise, to EI(BC) from conventional and alternative fuels across thrust will critically test the ImFOX tool predictive ability with positive results then aiding its adoption for EI(BC) estimates at ground and cruise with varied fuel compositions.

Tasks

1. Test for Improved Accuracy by Separating the Temperatures Associated with nvPM Formation and Oxidation
2. Assess ACCESS II Test Procedure Upon Engine Conditions at Cruise
3. Evaluate ASAF as the Global Scaling Factor in the ImFOX Relation
4. Investigate Alternative Representations to Capture Fuel Composition Effects for Alternative Fuels
5. Evaluate the ImFOX Relation Against the ACCESS II Flight Data from NASA for nvPM
6. Validate the ImFOX for Other Engines in the CFM Class

Objective(s)

1. Develop a predictive relation for nvPM at ground.
2. Develop a predictive relation for nvPM at cruise.
3. Include fuel composition effects for alternative fuels (absent aromatics and naphthalenic compounds) and their

blends with conventional fuels.
4. Incorporate thrust dependence into the predictive tool.

Research Approach

Jet engine aircraft exhaust contains combustion byproducts and particulate matter in the form of non-volatile particulate matter (nvPM). Black carbon (BC) is used synonymously for nvPM throughout this paper. Aircraft cruise emissions are the only direct source of anthropogenic BC particles at altitudes above the tropopause.[1] Black carbon aerosols are strong solar radiation absorbers and have long atmospheric lifetimes.[2] Therefore, BC results in positive radiative forcing and is believed to be the second largest contributor to climate change.[3] Additionally, upper troposphere and lower stratosphere BC particles contribute to climate forcing indirectly by acting as ice nucleation sites and cloud activators.[4-6] With regard to human health, a link between cardiopulmonary diseases and carbonaceous black particulate matter has recently been suggested.[7] As concern for human health risks and environmental impacts caused by aviation BC emissions increases, emission reduction strategies will need to be implemented. Predictive tools capable of accurately estimating BC emissions from the current in-service fleet will be needed for the next decades to quantify atmospheric BC inventory from aviation.

Current models do not accurately predict BC emissions. The First Oder Approximation-3 (FOA3) methodology is used worldwide for estimating BC emissions within the vicinity of airports.[8] The FOA3 was endorsed by the (ICAO)[9] in February 2007 and relies on a measured SN to predict BC emission. Black carbon is most often reported as an emission index of black carbon (EI_{BC}), reported as milligrams of BC emitted per kilogram of fuel combusted. Due to inaccuracies in measuring low SNs produced by modern high bypass ratio engines, the FOA3 and its modifications are unreliable. Recently a kinetic model based on formation and oxidation rates termed the FOX method was reported.[10] The FOX does not require input of a SN, instead the input variables are engine conditions. Hence, the FOX avoids the measurement error built into the FOA3. However, the FOX is fuel independent and cannot be applied to predict EI_{BC} from alternative fuels and alternative fuels blended with conventional jet fuels. Recently, a relation, the Approximation for Soot from Alternative Fuels (ASAF) has been developed to predict BC from alternative fuels relative to conventional fuel BC emissions.[11] Both the FOA3 and the FOX methods are designed to predict EI_{BC} at ground level, which is important for assessing human health concerns at and in the vicinity of airports, however, it is the cruise EI_{BC} that is of the most importance in determining the role aviation BC plays on the Earth's radiative balance. The current practice to arrive at a predicted cruise EI_{BC} is to scale ground values with an additional kinetic type expression, the Dopelheuer and Lecht relation.[12] At the time the Döpelheuer and Lecht relation was developed there were limited cruise BC emission measurements. The available data was not representative of real aviation emissions because the aircraft operated at reduced weight and velocities compared to regular operation.[13]

In our prior work, current predictive methods were evaluated for accuracy by comparison to over a decade's worth of field campaign data collected by the National Aeronautics and Space Administration's (NASA) Langley Aerosol Research Group with inclusion of cruise data.[14] An improved semi-empirical method was developed. Accurate engine condition relations were developed based on proprietary engine cycle data for a common rich-quench-lean (RQL) style combustor. In the forthcoming work predictive relations will be developed for alternative fuels and fuel blends as well as a direct cruise prediction. The intent is to provide an improved method to calculate EI_{BC} reductions from the use of alternative fuels.

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Milestone(s)

Milestone	Planned Due Date
1. Comparison of ImFOX predictions for nvPM at cruise altitude and engine operating conditions to measured values from ACCESS II.	Sept. 30th, 2016
2. Develop a predictive relation for nvPM at cruise.	Dec. 30th, 2016
3. Include fuel composition effects for alternative fuels (absent aromatics and naphthalenic compounds) and their blends with conventional fuels.	March 30th, 2017
4. Incorporate thrust dependence into the predictive tool.	June 30th, 2017
5. Final report	July 30th, 2017

Major Accomplishments

Overview
Aviation black carbon (BC) emissions impact climate and health. Inventory estimates are essential to quantify these effects. These in turn require a means of estimating BC emission indices from jet aircraft. The first order approximation (FOA3) currently employed to estimate BC mass emissions under predicts BC emissions due to inaccuracies in measuring low smoke numbers (SNs) produced by modern high bypass ratio engines. The recently developed Formation and Oxidation (FOX) method removes the need for and hence uncertainty associated with (SNs), instead relying upon engine conditions in order to predict BC mass. Using the true engine operating conditions from proprietary engine cycle data an improved FOX (ImFOX) predictive relation is developed. Still, the current methods are not optimized to estimate cruise emissions or account for the use of alternative jet fuels with reduced aromatic content. Here improved correlations are developed to predict engine conditions and BC mass emissions at ground and cruise altitude. This new ImFOX is paired with a newly developed hydrogen relation to predict emissions from alternative fuels and fuel blends. The ImFOX is designed for rich-quench-lean style combustor technologies employed predominately in the current aviation fleet.

Preface to Task Progress
Given the dependence of task 5 upon the combustor temperature (task 1), AFR, (task 2), evaluation of the ASAF as a global factor for fuel effects (task 3) and evaluation of alternative measures of fuel composition, e.g. C/H ratio (task 4), tasks are reported in order as initial tasks represent key engine condition whose values must be determined prior to assessing the ASAF and C/H ratio methods for incorporating fuel dependence. Last, task 6 is then reported for comparison of ImFOX predictions to nvPM (EI_{BC}) from another RQL style combustor to evaluate the transferability and applicability of the predictive tool for other combustors in the current fleet.

Rationale for a Singular Predictive Tool for EI_{BC} from RQL style combustors – 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)[1,2]. Alternative Aviation Fuel Experiments I and II (AAFEX-1, AAFEX-II)[3,4]. Alternative-Fuel Effects on Contrails & Cruise EmiSSions I and II (ACCESS-I, ACCESS-II)[5], 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 curves from five of the six RQL style combustors tested during APEX-III [6-8] followed a common distorted U-shaped curve[9], 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 deceased 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.

Task 1- Test for Improved Accuracy by Separating the Temperatures Associated with nvPM Formation and Oxidation

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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 for 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-1.[10]

$$T_{fl}[K] = 0.6T_3 + 1800 \quad [1]$$

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-1 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 flame 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-2.

$$T_4[K] = 490 + 42{,}266FAR \quad [2]$$

There is a strong correlation between T_3 and T_4, the Pearson r correlation value is 0.966. However, 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-2 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. The thermodynamic Air Standard Brayton Cycle is applied to a jet engine in the SI. Two equations are required to define this cycle. The first is the definition of the polytropic compressor efficiency that is currently used to find combustor inlet temperature, T_3, and the second equation reveals that T_4 is equivalent 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 Brayton Cycle compared to values predicted using Equation-2 were slightly higher (~5%), likely because the Brayton Cycle is treated as an idealized adiabatic system. Either relation can be used to find T_4, the benefit of Equation-2 is that only the FAR is needed and Equations-3 and 4 below provide accurate FAR relations.

Task 2- Assess ACCESS II Test Procedure upon Engine Conditions at Cruise

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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 manufacture had released nominal AFR values at 7, 30, 85, and 100 thrust settings.11 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 3 and 4 respectively.

$$AFR_{grd} = 71 - 35.8\left(\frac{\dot{m}_f}{\dot{m}_{f,max}}\right) \quad [3]$$

$$AFR_{cru} = 55.4 - 30.8\left(\frac{\dot{m}_f}{\dot{m}_{f,max}}\right) \quad [4]$$

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. However, the cruise cycle deck calculations were case matched to the ACCESS-II campaign and ACCESS-II conditions do not exactly match real conditions. During ACCESS-II the outboard engines were significantly throttled back to maintain an aircraft Mach number of 0.6. This was done so the chase plane could keep up. Therefore, the inboard engines from which the emissions were measured, were burning fuel at a rate typical of a Mach speed of 0.75, the DC-8's nominal cruising speed. It is likely that the AFR would be increased from the ram effect at a higher Mach number, therefore, it is possible that a singular relation (Equation-3) may adequately predict AFR at both ground and cruise.

Task 3- Evaluate ASAF as the gGlobal Scaling Factor in the ImFOX Relation

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ASAF inclusion. Black carbon emissions from turbo fan jet engines are significantly reduced when conventionally produced (i.e., from petroleum) Jet-A or JP-8 are blended with low aromatic content synthetic blending components as demonstrated in recent measurement campaigns.[5,12-14] Efforts to relate BC emissions from gas turbines to fuel chemistry is a research focus of long-standing interest. A prime motivator is that a decrease in aromatic content results in reduced BC emissions. The ASAF is the first analytical approximation to estimate the BC emission reduction associated with using alternative fuels as compared to conventional jet fuel BC emissions.[15]

$$B = 1 - \left(1 - \lambda\frac{\dot{m}_f}{\dot{m}_{f,max}}\right)(1 - \hat{A}) \quad [5]$$

Where B is the relative BC emission reduction, λ is a fitting parameter, and Â is the normalized aromatic content and equal to aromatic content of the fuel over aromatic content of a reference conventional fuel.

The model we have developed uses the FOX16 as the starting point. The FOX is a kinetically balanced relation predicting EI_{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.[17] 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.[18] and is their inception E_a based on the formation of polyaromatic hydrocarbons (PAHs). The pre-exponential frequency factor is a function of two and three member PAHs concentration, which in turn is a function of PAH building block molecules; acetylene and benzene. 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. Using a formation constant value of 356 Settler et al.[16] 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. A solution encompassing alternative fuels follows.

By combining the ImFOX with the ASAF relation developed by Speth et al.[15] determination of BC emissions from alternative fuels is possible.

$$C_{BC}[\frac{mg}{m^3}] = \dot{m}_f \times B\,(A_{form} \times e^{(-6390/T_4)} - A_{ox} \times AFR \times e^{(-19778/T_4)}) \quad [6]$$

Where B in Equation-6 is the ASAF value found using Equation-5. The fitting parameter λ was found to vary between neat (i.e., 100%) alternative fuel blend components ($\lambda_{alt\text{-}neat}$) and alternative fuel blends ($\lambda_{alt\text{-}blend}$) as follows:

$$\lambda_{alt\text{-}neat} = -0.058 + 0.105(\frac{\dot{m}f}{\dot{m}f,max}) \quad [7]$$

$$\lambda_{alt\text{-}blend} = -5.3 + 9.6(\frac{\dot{m}f}{\dot{m}f,max}) - 4.7(\frac{\dot{m}f}{\dot{m}f,max})^2 \quad [8]$$

Since the ASAF provides the relative EI_{BC} reduction due to decreased aromatic content, it is ideal as a global correction factor located outside of the ImFOX expression. However, ASAF does not consider naphthenic compounds known to have a higher sooting index[19,20] than that of paraffinic compounds found predominantly in alternative fuels and fuel composition effects more logically belong in the formation constant, rather than as a global correction factor for the ImFOX. Therefore, an alternative approach was developed using hydrogen content in the form of fuel carbon-to-hydrogen (C/H) ratios to determine the formation constants for alternative fuels.

The current version of the FOX over predicts measured values, as displayed in Figure-1. However, the method is promising considering the clear trend between EI_{BC} and thrust.

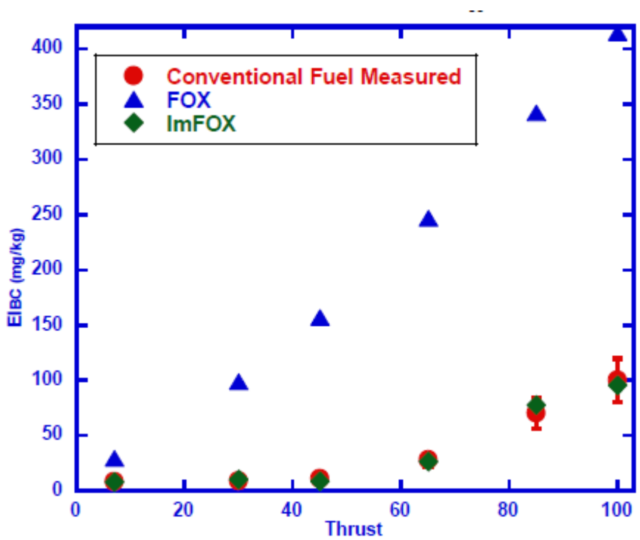

Figure 1. Measured conventional fuel black carbon emission from AAFEX-I (red circles) Shown for comparison are predicted EI_{BC} values from the FOX (blue triangles) and the ImFOX (green diamonds).

As seen in Figure-1 the ImFOX method accurately captures the emissions trend across a full range of thrust settings. The ImFOX method developed subsequently utilizes improved engine condition relations and a thrust dependent formation constant to accurately predict BC emissions from petroleum-based fuel combustion. The agreement represents a vast improvement from the current FOX method given the mean variance is reduced from 400% to less than 10%.

Task 4- Investigate Alternative Representations to Capture Fuel Composition Effects for Alternative Fuels

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C/H-ImFOX. An alternative approach was developed using hydrogen content in the form of fuel carbon-to-hydrogen (C/H) ratios to determine the formation constants for alternative fuels. This revised expression is Equation 6 without the ASAF correction (B) and the addition of a variable A_{from} constant. The formation constants have units of (mg×s/kg-fuel×m[3]). The formation constant relation, analogous to the ASAF fitting factor (λ), needs to vary between neat alternative fuels ($A_{form,alt\text{-}neat}$) and alternative fuel blends ($A_{form,alt\text{-}blend}$) as given here:

$$A_{form,alt-neat} = \left(\frac{C}{H} - 0.342\right)T \quad [9]$$
$$A_{form,alt-blend} = \left(\frac{C}{H} - 0.212\right)T \quad [10]$$

Equations 9 and 10 go a step beyond just correcting for C/H ratio, as they relate the formation constant to thrust. The term T, a third order expression, captures the thrust dependent relation and is equal to:

$$T = 1013 - 4802\left(\frac{\dot{m}f}{\dot{m}f,max}\right) + 7730\left(\frac{\dot{m}f}{\dot{m}f,max}\right)^2 - 3776\left(\frac{\dot{m}f}{\dot{m}f,max}\right)^3 \quad [11]$$

For conventional fuels T is the formation constant, without a C/H correction. EI_{BC} was not found to vary between conventional fuels with varying aromatic contents tested during APEX-I, however, the hydrogen content of the fuels tested were nearly equivalent. As part of the Aircraft Particulate Regulatory Instrumentation Demonstration Experiment (A-PRIDE) 7, it was demonstrated by Brem et al.[21] that BC emissions from conventional fuels may vary due to a range of aromatic content and emissions are best predicted based on hydrogen mass content. Therefore, the addition of a C/H term in equation 11 to account for the varying hydrogen content in available conventional fuels may prove to make the relation applicable to a wider range of conventional fuels. However, Equation 11 based on the available NASA data should capture EI_{BC} from the majority of conventional jet fuels. The complex relation between thrust and the formation constant is also evident in the ASAF-ImFOX relation as the λ values already contain thrust terms and are multiplied by an additional thrust term in the ASAF relation, Equation 9. 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.[9, 22] Black carbon nanostructure can reflect the species concentrations available for BC formation and growth.[9] As reported by Vander Wal et al.[9] 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.

The C/H dependent fuel effect developed here based on ground data applies equally well at cruise as the emission trend with C/H ratio is the same at both ground and cruise altitude. However, EI_{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. Therefore, the A_{form} needs to be unique between ground and cruise to account for this. During cruise operation thrust settings are typically higher than 30 %, therefore, cruise EI_{BC} emission profiles do not possess the common 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 EI_{BC} increases linearly with thrust, hence complex formation constants, like derived for ground based emissions, are not necessary. A constant formation constant of 295 captures the observed linear trend of increasing EI_{BC} with increased thrust at cruise.

To capture the emission reductions from the use of alternative fuels two variations of the ImFOX were compared: the ASAF-ImFOX and the C/H-ImFOX. Black carbon emissions from a FT fuel measured during AAFEX-I are plotted in Figure 2 with the calculated values from the two versions of the ImFOX expression.

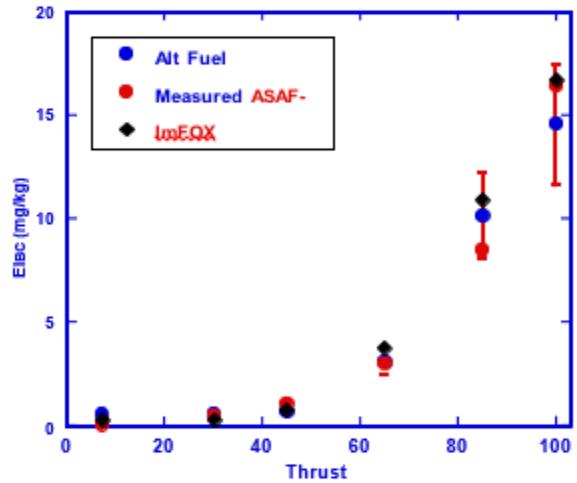

Figure 2. Neat Fischer-Tropsch blend component BC emissions measured during the AAFEX-I campaign. Comparison of the ASAF-ImFOX and C/H-ImFOX methods used for EI_{BC} predictions.

As displayed in Figure 3 both the ASAF-ImFOX and C/H-ImFOX methods capture the emission reductions from the use of a neat Fischer-Tropsch synthetic paraffinic kerosene (SPK) blend component. Due to fuel performance requirements including mass density and wetted-material compatibility SPKs such as the Fischer-Tropsch depicted in this work are approved as alternative fuels only when blended up to a maximum of 50% blend ratio with conventional fuel. Regardless, the SPKs blended up to this limit are still an attractive solution for reducing BC emissions. The ASAF-ImFOX and C/H-ImFOX calculated values are compared to measured BC in Figure 3 for a FT-JP-8 50/50 blend that is within the alternative fuel specification requirements.

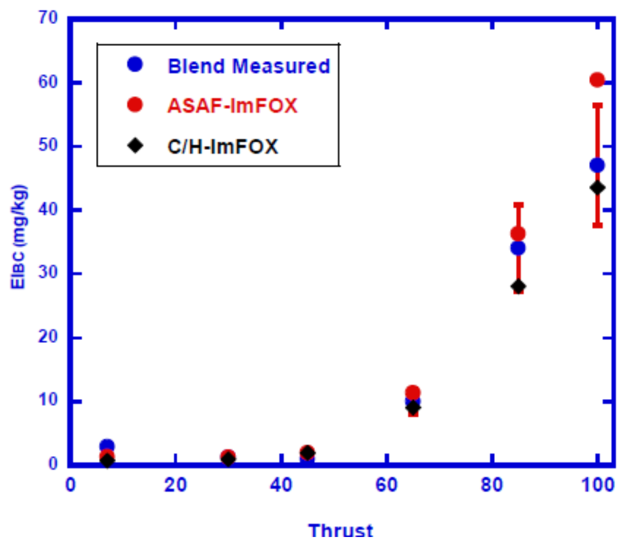

Figure 3. EI_{BC} from a 50/50 blend of Fischer-Tropsch and JP-8 measured during the AAFEX-I campaign. Also shown is a comparison of the ASAF-ImFOX and C/H-ImFOX methods for EI_{BC} predictions of the alternative fuel blend.

As demonstrated in Figure 3 alternative fuel blend emissions are accurately calculated with both expressions except for the ASAF-ImFOX slightly over predicting EI_{BC} at 100% thrust level. This demonstrates that EI_{BC} reductions from alternative fuels can be predicted by correlating the ImFOX with an aromatic or C/H reduction term.

Task 5- Evaluate the ImFOX Relation Against the ACCESS II Flight Data from NASA for nvPM

The Pennsylvania State University

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 data and given in equation 12.

$$A_{form} = 1013 - 4802\left(\frac{\dot{m}f}{\dot{m}f,max}\right) + 7730\left(\frac{\dot{m}f}{\dot{m}f,max}\right)^2 - 3776\left(\frac{\dot{m}f}{\dot{m}f,max}\right)^3 \quad [12]$$

This 3[rd] order dependence of the formation constant upon thrust 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.[9, 22] Black carbon nanostructure can reflect the formation conditions, i.e. species and temperature, of BC.[9] 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.[10] 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.[10] This variable, thrust dependent fuel air mixing may be the origin of the complex dependence of A_{from} upon thrust, as expressed in equation 12. This mixing effect would apply across all fuels: conventional, blended, and neat SPK. Therefore, equation 12 developed here for conventional fuel can be used to represent the mixing (combustor) effect across all fuels with a separate fuel term then added explicitly for fuel composition, specifically decreasing EI_{BC} with increasing hydrogen mass content. The new predictive expression is accordingly termed the H-ImFOX, and given in equation 13.

$$C_{BC}\left[\frac{mg}{m^3}\right] = \dot{m}_f \times e^{(13.6-H)} \left(A_{form} \times e^{(-6390/T_4)} - A_{ox} \times AFR \times e^{(-19778/T_4)}\right) \quad [13]$$

The "H" in equation 13 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 13 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. Brem et al.21 found BC emissions from conventional fuels to vary due to a range of aromatic content and concluded that emissions are best predicted based on hydrogen mass content. Additionally, Lobo et al.23 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, EI_{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 to account for these differences in mixing. During cruise operation thrust settings are typically higher than 30%, therefore, cruise EI_{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 in ground campaigns. From the limited cruise altitude BC measurements, the EI_{BC} increases approximately linearly with thrust, hence complex formation constants, like derived for ground based emissions, are not necessary. Although a complex expression for cruise A_{form} may ultimately be needed, however, the limited range of thrust values at cruise presently do not provide justification for such, instead the simplest expression (a constant) was chosen and found adequate by quality of fit. A A_{form} increased cruise value of 295 captures the observed linear trend of increasing EI_{BC} with increased thrust at cruise.

ImFOX Direct Cruise Prediction.

The litmus test of the ImFOX formalism is whether it captures the range of cruise EI_{BC} values. The ImFOX predictive tool only requires the combustor conditions, AFR and T_4, as input values. If these can be known or otherwise accurately predicted at cruise, then the ImFOX should accurately predict EI_{BC}. Predicted values are compared to measurements made at cruise altitudes during the ACCESS-II campaign for both conventional fuel and an alternative fuel blend, displayed in Figure-4.

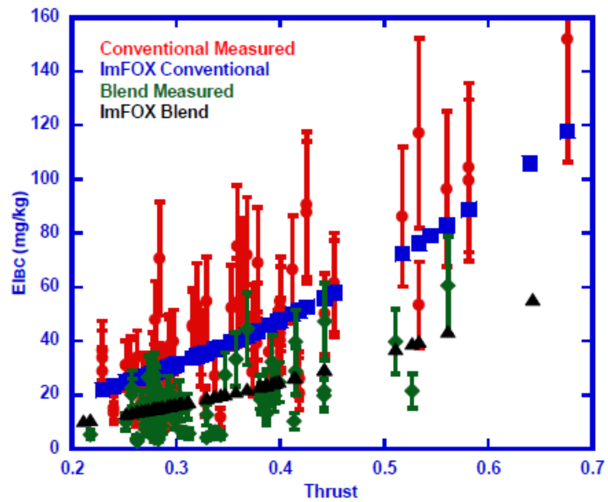

Figure 4. Measured EI_{BC} at cruise altitude burning Jet-A (red circles) and 50/50 blend of Hydrotreated Esters and Fatty Acids (HEFA-SPK) and Jet-A (green diamonds). Shown for comparison are ImFOX predicted values for conventional (blue squares) and blended alternative (black triangles) fuels.

This demonstrates that the ImFOX can be applied to directly predict EI_{BC} values at cruise and will yield accurate results if combustor conditions are known. Predicted values were found using a constant formation constant of 295 and the hydrogen dependent fuel term as described above.

Task 6- Validate the ImFOX for Other Engines in the CFM Class

The Pennsylvania State University

CFM56-3B. If the form of the ImFOX is correct, it should accurately estimate nvPM emissions from other RQL style combustors. When engine cycle data is not available, the above AFR and T_4 relations can be used. Comparison of the 2C to the 3B is interesting as both are RQL technology and have the same maximum fuel flow rate. Thus, predicted AFR will be the same as dependence is on fuel flow rate with respect to maximum ground fuel flow rate. Predicated T_4 will also be the same as it is dependent on AFR. The ImFOX therefore predicts equivalent emission from the two engines. Evaluating the ImFOX against the 3B is essentially boiled down to comparing emission from the 2C with the expectation of equivalent emissions. Measured nvPM emissions from the NASA APEX campaigns for both engines are provided in Fig. 5. As seen the emission profiles are within the measurement standard deviation. Although within measurement uncertainty, the average emission from three repeated measurements is higher from the 3B as compared to the 2C at higher fuel flow rates. The key difference between these engines is the shape, the 3B has a less rounded bottom by design so it could readily fit under the 737. In doing so, it cut 8 inches off of the front fan blade. Since this was a design restriction and not an engine optimization it may have resulted in a less efficient engine as compared to the 2C. The 2C has a higher pressure ratio and higher maximum thrust. This subtle difference between these two similar engines and the potentially higher emissions from the 3B shows how sensitive emissions are to engine design.

Emission trends from newer combustor technology like the dual staged CFM56-5 and lean burn CFM56-7 are of interest. This is a potential area of collaboration between Penn State and Georgia Institute of Technology as Georgia can provide engine calculations for these engines.

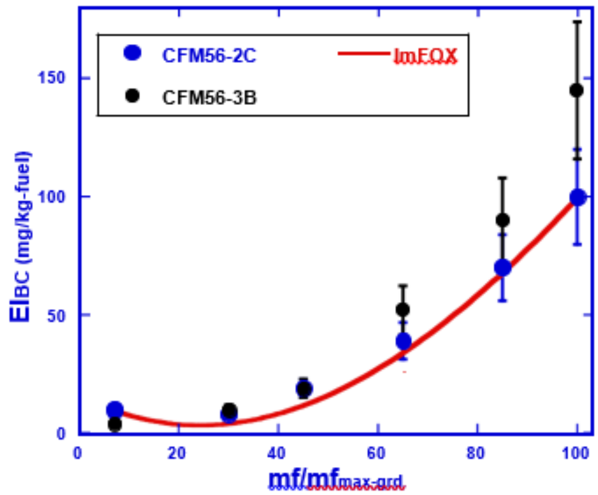

Figure 5. EI_{BC} curves for CFM56- 2C and 3B. Predicted ImFOX values shown for comparison.

Publications and Presentations

Publication

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, 50(21), 12048-12055.

Presentations

Vander Wal, R. L. Abrahamson, J. P., ASCENT Project No. 24B, Emissions data analysis for CLEEN, ACCESS and other tests. FAA Center of excellence for alternative jet fuels and environment. Contractor's workshop. Alexandria, VA. Sept. 27th–28th, 2016.

Abrahamson, J. P., Vander Wal, R. L., PM Emissions Analysis and Predictive Assessment: Update on nvPM predictive modeling from conventional and alternative jet fuels. Aviation Emissions Council (AEC) WEBEX seminar. Feb. 23rd, 2017.

Vander Wal, R. L., Abrahamson, J. P., nvPM Emissions Analysis and Predictive Summary. Poster Presentation. Project 24B Report. FAA Center of Excellence for Alternative Jet Fuels & Environment (FAA COE AJFE). Alexandria, VA April 18th - 19th, 2017.

Abrahamson, J. P., Vander Wal, R. L., (2017). Gas turbine nvPM formation and oxidation semi-empirical model for commercial aviation. Paper 2E19. Topic: Gas Turbine Combustion. 10th US National Meeting of the Combustion Institute, The University of Maryland, College Park, MD April 23rd - 26th, 2017.

Conference Paper

Abrahamson, J. P., Vander Wal, R. L., (2017). Gas turbine nvPM formation and oxidation semi-empirical model for commercial aviation. Paper 2E19. Topic: Gas Turbine Combustion. 10th US National Meeting of the Combustion Institute, The University of Maryland, College Pak, MD April 23rd - 26th, 2017.

Outreach Efforts
Informal discussions with the US EPA regarding variations in nvPM structure and composition dependent upon source.

Awards
None

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
Options offered:

Possible tasks for this coming year could include,

1. Evaluation of the ImFOX against newer, lean burn engines.
2. Formulation and evaluation of T3, P3 scaling relationships for nvPM (EIbc) between ground and cruise.
3. Testing for correlation between YSI (a lab-based measurement for fuel sooting tendency) and measured EIbc (from jet engines) for JP-8, synthetic fuels and their blends.
4. Develop a number-based predictive relation, including fuel dependence, given forthcoming regulations.

These are described in more detail in the white paper, which was shared with James Hileman and Ralph Iovinelli in April of 2017.

Based on the AEC Roadmap meeting of June 13-15 2017, other needs may be:

1. In our petroleum engineering program, and fuel science courses, we use HYSYS. Aspen HYSYS is the energy industry's leading process simulation software that's used by top oil and gas producers, refineries and engineering companies for process optimization in design and operations. Aspen HYSYS is a process simulation software for the optimization of conceptual design and operations including multiphase flow modeling, gas processing, refining and distillation. We could evaluate necessary refinery operations.
2. Based on Dr. Bruce Anderson's overview of their upcoming contrail/plume measurements this coming year, he stated that extra sampling ports were available on the NASA DC-8, and that other measurements could be accommodated. This would truly be a unique opportunity to collect in situ particulate samples for microscopic analyses, SEM, TEM to benchmark what other aerosol instrumentation is actually measuring, (and insights into the aerosol processing within the plume.)

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