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 3rd 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.

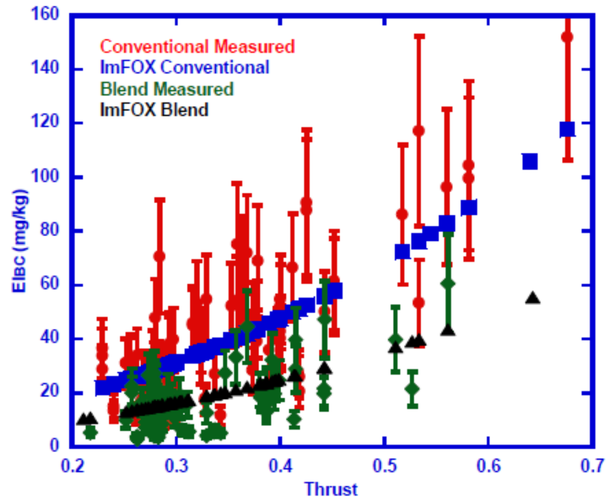

Figure 4. Measured EI_{BC} at cruise altitude burning Jet-A (red circles) and 50/50 blend of Hydrotreated Esters and Fatty Acids (HEFA-SPK) and Jet-A (green diamonds). Shown for comparison are ImFOX predicted values for conventional (blue squares) and blended alternative (black triangles) fuels.

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.

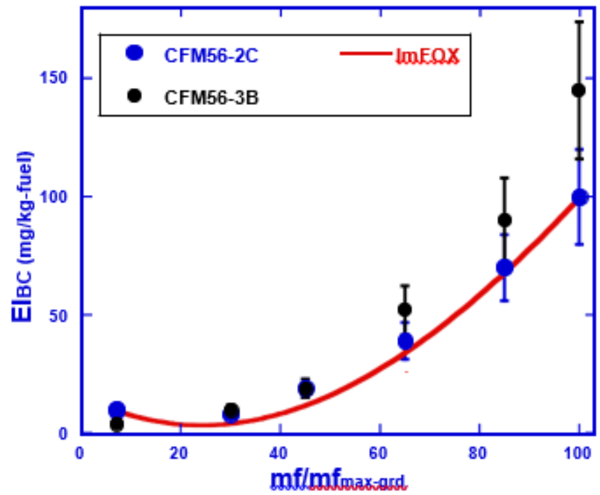

Figure 5. EI_{BC} curves for CFM56- 2C and 3B. Predicted ImFOX values shown for comparison.

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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