# Aviation Black Carbon Mass Predictive Model for Alternative and Conventional Fuels at Ground and Cruise

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ABSTRACT: 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 the recently developed Approximation for Soot from Alternative Fuels (ASAF) and a newly developed C/H 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.



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# 1. INTRODUCTION

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.<sup>1</sup> Black carbon aerosols are strong solar radiation absorbers and have long atmospheric lifetimes.<sup>2</sup> Therefore, BC results in positive radiative forcing and is believed to be the second largest contributor to climate change.<sup>3</sup> Additionally, upper troposphere and lower stratosphere BC particles contribute to climate forcing indirectly by acting as ice nucleation sites and cloud activators.<sup>4-6</sup> With regards to human health, a link between cardiopulmonary diseases and carbonaceous black particulate matter has recently been suggested.<sup>7</sup> As concern for human health risks and environmental impacts caused by aviation BC emissions increases, emission reduction strategies will need to be implemented. An ambitious carbon, solid and gaseous, emission reduction goal of 50 % reduction by 2050 as compared to 2000-2005 levels has already been defined by the International Air Transport Association and Advisory Council for Aviation Research and Innovation in Europe.<sup>8</sup> Meeting these goals will require significant engineering advancements requiring a long implementation period. However, in the near term, alternative jet fuels with reduced aromatic content are an attractive solution for reducing BC emissions.<sup>9-12</sup> Alternative aviation fuels containing synthetic blend components with near zero aromatic content (synthetic paraffinic kerosenes, SPKs) such as those synthesized via the Fischer-Tropsch (FT-SPK) process and hydrotreated esters and fatty acids (HEFA-SPK) overall contain

highly reduced aromatic content compared to conventional fuel and thus significantly reduce aircraft engine BC emissions.<sup>9-12</sup>

Currently there is not a direct regulation on BC emissions from jet engines. Rather, BC emissions during the landing and take-off (LTO) cycle are limited by the International Civil Aviation Organization (ICAO) through regulations on smoke number (SN).<sup>13</sup> The smoke number regulation introduced in 1981 was put in place with the purpose of reducing plume visibility and no engines have failed this regulation since 1990.<sup>14</sup> With increasing concern on both human health and environmental impacts caused by jet engine BC emissions the EPA is expected to place regulations on such emissions.<sup>15</sup> The ICAO's Committee on Aviation Environmental Protection is currently developing a regulatory standard for BC emissions. The pending regulation will require BC emissions from new jet engines to be measured by a standard procedure. A standardized measurement methodology was defined in the Aerospace Information Report 6241<sup>16</sup>, with much of the research effort led by Missouri University of Science and Technology<sup>17</sup>. Such a regulation would likely apply to new engines with the existing fleet grandfathered in. However, in-service engine lifetimes can be in excess of 20 years and current engine designs will continue to be manufactured for several more years. Therefore, predictive tools capable of accurately estimating BC emissions from the current in-service fleet will be needed for the next couple 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.<sup>15</sup> The FOA3 was endorsed by the (ICAO)<sup>18</sup> 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 (EIBC), in 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.<sup>19</sup> 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.<sup>20</sup> Both the FOA3 and the FOX methods are designed to predict EI<sub>BC</sub> at ground level, which is important for assessing human health concerns at and in the vicinity of airports, however, it is the cruise EI<sub>BC</sub> 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<sub>BC</sub> is to scale ground values with a kinetic ratio, the Döpelheuer and Lecht relation.<sup>21</sup> At the time the Döpelheuer and Lecht relation was developed limited cruise BC emission measurements were available. The available data was not representative of real aviation emissions because the aircraft operated at reduced weight and velocities compared to regular operation.<sup>22</sup>

In this work current predictive methods are 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.<sup>9</sup> An improved semi-empirical method is developed. Accurate engine condition relations are developed based on proprietary engine cycle data for a common rich-quench-lean (RQL) style combustor. Alternative fuels and fuel blend predictive relations are developed as well as a direct cruise

prediction. The intent is to provide an improved method to calculate  $EI_{BC}$  from in-service aircraft and account for  $EI_{BC}$  reductions from the use of alternative fuels.

## 2. CURRENT METHODS

## 2.1 FOA3.

Since SN regulation took effect the ICAO has compiled a large database containing SNs from certified engines at the four characteristic ICAO certification thrust settings (LTO cycle): idle (7%), approach (30%), climb out (85%), and takeoff (100%).<sup>15</sup> Several researchers have sought out an accurate correlation between SN and mass concentration in milligrams of BC per  $m^3$  of exhaust volume (C<sub>BC</sub>). The most widely accepted method is the FOA3 as given in equation 1.

$$C_{\rm BC}[\frac{mg}{m^3}] = 0.0694({\rm SN})^{1.24}$$
 [1]

Both Wayson et al.<sup>15</sup> and Stettler et al.<sup>23</sup> have suggested modifications to equation 1 that result in higher predicted concentrations; shown in equations 2 and 3 respectively.

$$C_{\rm BC}[\frac{mg}{m^3}] = 0.0012({\rm SN})^2 + 0.1312({\rm SN}) + 0.2255$$
[2]

$$C_{\rm BC}[\frac{mg}{m^3}] = 0.236({\rm SN})^{1.126}$$
 [3]

All three SN to  $C_{BC}$  relations are recommended when measured SN is less than 30, which is almost a certainty today. To convert a  $C_{BC}$  (mg/m<sup>3</sup>) to an EI<sub>BC</sub> the  $C_{BC}$  is multiplied by the volume of exhaust gas per kg of fuel combusted, Q (m<sup>3</sup>/kg). Where Q is found based on a relation between air-fuel ratio (AFR) and exhaust volume.<sup>15</sup>

$$Q_{\text{core}}[\frac{m^3}{kg}] = [0.776(\text{AFR}) + 0.887]$$
[4]

Where the core subscript designates the volumetric flow rate from the core and does not account for bypass flow. The bypass flow, air drawn in from the fan but directed around the core is sometimes mixed with the core exhaust prior to the exit plane and the bypass ratio ( $\beta$ ) needs to be included when calculating Q for these engines, see references 15 and 19. The AFR is proprietary, however, representative values have been reported<sup>15</sup> and extrapolated into the following relation.<sup>19</sup>

$$AFR_{core} = (0.0121(\frac{F}{F_{oo}}) + 0.008)^{-1}$$
[5]

Where  $\frac{F}{F_{oo}}$  is thrust over the maximum rated thrust, it has been demonstrated that  $\frac{\dot{m}_f}{\dot{m}_{f,max}}$  can be used interchangeably for  $\frac{F}{F_{oo}}$ .<sup>24</sup> Where  $\frac{\dot{m}_f}{\dot{m}_{f,max}}$  is fuel flow rate over maximum fuel flow rate.

## 2.2 FOX.

Due to uncertainties in using SN to estimate  $C_{BC}$  and potential error in SN measurement, Settler et al.<sup>19</sup> developed a new method to predict  $C_{BC}$  independent of SN. The proposed method predicts BC emissions based on formation and oxidation rates, therefore, it is termed the FOX approximation and is given in equation 6.

$$C_{BC}[\frac{mg}{m^{3}}] = \dot{m}_{f} \times (A_{form} \times e^{(-6390/T_{fl})} - A_{ox} \times AFR \times e^{(-19778/T_{fl})})$$
[6]

The pre-exponential factors  $A_{form}$  and  $A_{ox}$  are constants, 356 and 608 respectively. Without input of a measured SN the FOX requires engine condition inputs including: fuel flow rate ( $\dot{m}_f$ ), flame temperature ( $T_{fl}$ ), and AFR. Where flame temperature is predicted based on linear dependence to combustor inlet temperature  $T_3$ . Combustor inlet temperature  $T_3$  is found by the definition of the polytropic compressor efficiency, see reference 19.

$$T_{\rm fl}[K] = 0.9 \times T_3 + 2120$$
<sup>[7]</sup>

Combustor inlet pressure ( $P_3$ ) which is needed to determine  $T_3$ , is identified based on thrust dependence, see reference 19. The FOX utilizes the same AFR and Q relations developed for the FOA3 method, given in equations 5 and 4 respectively.

#### 2.3 Döpelheuer and Lecht Cruise Scaling Relation.

The Döpelheuer and Lecht approximation is used to scale up ground  $C_{BC}$  ( $C_{BC,ref}$ ) to an estimated cruise value and is given in equation 8. Where the subscript "ref" refers to ground values and non-subscripted terms are cruise values.

$$C_{BC}\left[\frac{mg}{m^{3}}\right] = C_{BC,ref}\left(\frac{AFR_{ref}}{AFR}\right)^{2.5} \times \left(\frac{P_{3}}{P_{3,ref}}\right)^{1.35} \times \frac{e^{-20,000/Tfl}}{e^{-20,000/Tfl,ref}}$$
[8]

Input engine conditions include  $T_{fl}$ , AFR, and  $P_3$ , both at ground and cruise. The engine conditions are found by the previously mentioned relations.

### 2.4 ASAF.

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.<sup>9-12</sup> 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, as demonstrated.<sup>25-27</sup> 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.<sup>20</sup>

$$B = 1 - (1 - \lambda \frac{\dot{m}_f}{\dot{m}_{f,max}})(1 - \hat{A})$$
[9]

Where B is the relative BC emission reduction,  $\lambda$  is a fitting parameter, and  $\hat{A}$  is the normalized aromatic content and equal to aromatic content of the fuel over aromatic content of a reference conventional fuel.

#### 3. IMPROVED METHOD

#### **3.1 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)<sup>28,29</sup>, Alternative Aviation Fuel Experiments I and II (AAFEX-1, AAFEX-II)<sup>30,31</sup>, Alternative-Fuel Effects on Contrails & Cruise EmiSSions I and II (ACCESS-I, ACCESS-II)<sup>9</sup>, 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<sub>BC</sub> curves from five of the six RQL style combustors tested during APEX-III<sup>32-</sup> <sup>34</sup> followed a common curve<sup>35</sup>, 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<sub>BC</sub>. 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, 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 with supporting validation by nominal AFR values at 7, 30, 85, and 100 thrust settings, released by an engine manufactuerer.<sup>15</sup> Those values were linearly fit to derive the current predictive AFR expression. This relation results in an over prediction as compared to engine cycle deck data. Additionally, there is currently no cruise AFR predictor. Therein two new and 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 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 12.<sup>36</sup>

$$T_{\rm fl}[K] = 0.6T_3 + 1800$$
[12]

This relation 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. Yet both approaches possess an inherent limitation. As the only variable in either flame temperature predictor is T<sub>3</sub> 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<sub>4</sub>) in place of primary zone flame temperature. Using T<sub>4</sub> for the flame temperature is consistent with the AFR value being used in that it is at the back of the combustor. Thus both values represent a global average of the combustion processes occurring in the fuel-rich and fuel-lean zones of the combustor, corresponding to the soot formation and oxidation regions respectively. Additionally, T<sub>4</sub> is readily calculated by the engine cycle deck, yielding equation 13.

 $T_4[K] = 490 + 42,266(AFR^{-1})$ [13]

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 air-fuel-ratio (AFR), 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 altitude.

Given the success of this semi-empirical T<sub>4</sub> calculation based on FAR, a thermodynamic basis was evaluated. 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<sub>3</sub>, and the second equation reveals that T<sub>4</sub> 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<sub>4</sub> found using the 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. Either relation can be used to find T<sub>4</sub>, the benefit of equation 13 is that only the FAR is needed and equations 10 and 11 provide accurate AFR relations for both ground and cruise respectively.

# **3.2 Improved EIBC Predictive Relations.**

The model we have developed uses the FOX<sup>19</sup> 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<sub>a</sub>) value in the oxidation step is the well accepted value first proposed by Lee et al.<sup>37</sup> Given the success of this value, no modification to the oxidation step was made, outside of correcting AFR and substituting T<sub>fl</sub> with T<sub>4</sub>. The formation activation energy is that reported by Hall et al.<sup>39</sup> and is their inception E<sub>a</sub> based on the formation of polyaromatic hydrocarbons (PAHs). The pre-exponential frequency factor (also referred to as formation of PAH building block molecule concentrations; 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.<sup>19</sup> achieve a coefficient of determination, R<sup>2</sup>, 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.

*ASAF-ImFOX*. By combining the ImFOX with the ASAF relation developed by Speth et al.<sup>20</sup> determination of BC emissions from alternative fuels is possible.

$$C_{BC}\left[\frac{mg}{m^{3}}\right] = \dot{m}_{f} \times B \left(A_{form} \times e^{(-6390/T_{4})} - A_{ox} \times AFR \times e^{(-19778/T_{4})}\right)$$
[14]

Where B in equation 14 is the ASAF value found using equation 9. The fitting parameter  $\lambda$  was found to vary between neat (i.e., 100%) alternative fuel blend components ( $\lambda_{alt-neat}$ ) and alternative fuel blends ( $\lambda_{alt-blend}$ ) as follows:

$$\lambda_{\text{alt-neat}} = -0.058 + 0.105 \left(\frac{\dot{\text{m}}f}{\dot{\text{m}}f, max}\right)$$
[15]

$$\lambda_{\text{alt-blend}} = -5.3 + 9.6(\frac{\text{m}f}{\text{m}f,\text{max}}) - 4.7(\frac{\text{m}f}{\text{m}f,\text{max}})^2$$
[16]

Since the ASAF provides the relative  $EI_{BC}$  reduction due to decreased aromatic content, it is best suited as a global correction factor located outside of the ImFOX expression. However, ASAF does not consider cycloalkanes known to have a higher sooting index<sup>26,39</sup> than that of paraffinic compounds found predominantly in alternative fuels.

*C/H-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. This revised expression is equation 14 without the ASAF correction (B) and the addition of a variable  $A_{\text{from}}$  constant. The formation constants have units of (mg×s/kg-fuel×m<sup>3</sup>). The formation constant relation, analogous to the ASAF fitting factor ( $\lambda$ ), needs to vary between neat alternative fuels ( $A_{\text{form,alt-neat}}$ ) and alternative fuel blends ( $A_{\text{form,alt-blend}}$ ) as given here:

$$A_{form,alt-neat} = \left(\frac{c}{H} - 0.342\right)T$$
[17]

$$A_{form,alt-blend} = \left(\frac{C}{H} - 0.212\right)T$$
[18]

Equations 17 and 18 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:

$$T = 1013 - 4802(\frac{\dot{m}f}{\dot{m}f,max}) + 7730(\frac{\dot{m}f}{\dot{m}f,max})^2 - 3776(\frac{\dot{m}f}{\dot{m}f,max})^3$$
[19]

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.<sup>40</sup> 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 19 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 19 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  $\lambda$  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.<sup>35,41</sup> Black carbon nanostructure can reflect the species concentrations 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<sub>BC</sub> 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<sub>form</sub> 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<sub>BC</sub> 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<sub>BC</sub> 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<sub>BC</sub> with increased thrust at cruise.

# 4. RESULTS AND DISCUSSION

# 4.1 EI<sub>BC</sub> from Conventional Fuel.

The FOA3 and its modifications estimate  $EI_{BC}$  based on a correlation to SN. These methods are most accurate when SN is measured during BC mass measurements. The SN based methods are compared to AAFEX-I values because SNs were accurately measured during this campaign.<sup>42</sup> Certification SNs in the ICAO database can vary greatly from SNs measured from deteriorated engines. Estimates of  $EI_{BC}$  predicted using FOA3 and the modified versions, equations 1-3, are displayed against measured  $EI_{BC}$  values from the AAFEX-I campaign in Figure 1.



**Figure 1.** Predicted  $EI_{BC}$  values using FOA3 and modified versions, equations 1-3 as compared to measured values from the AAFEX-I campaign. Black squares represent correlation between SNs measured during the AAFEX-I campaign and  $EI_{BC}$ .

As seen in Figure 1 the FOA3 method under predicts BC emissions, however, the FOA3 is still a highly valued tool because it can be applied universally across all combustor technologies as long as SNs can be accurately measured. The two modified versions result in higher predicted  $EI_{BC}$  values, however, the accuracy is limited. This likely reflects the difficulties in measuring an accurate SN and assumptions regarding soot particle size, filtration efficiency, etc., as noted elsewhere.<sup>23,43</sup> For this reason, a kinetic approach dependent on thrust is favored. One such model already available is the FOX. The current version of the FOX over predicts measured values, as displayed in Figure 2. However, the method is promising considering the clear trend between  $EI_{BC}$  and thrust.



**Figure 2.** Measured conventional fuel black carbon emission from AAFEX-I (red circles) Shown for comparison are calculated  $EI_{BC}$  values from the FOX (blue triangles) and the ImFOX (green diamonds).

As seen in Figure 2 the ImFOX method accurately captures the emissions trend across a full range of thrust settings. The ImFOX ground method developed in Section 3.2 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 %.

# 4.2 Alternative Fuels EIBC.

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 3 with the calculated values from the two versions of the ImFOX expression.



**Figure 3.** 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<sub>BC</sub> 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 4 for a FT-JP-8 50/50 blend that is within the alternative fuel specification requirements.



**Figure 4.**  $EI_{BC}$  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 4 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.

# 4.3 Cruise EIBC.

# Döpelheuer and Lecht Cruise Scaling.

The current method to predict BC cruise emissions requires the use of a reference ground value that is scaled to a cruise value with the Döpelheuer and Lecht approximation. The direct test of this relation is comparison of actual measured ground and cruise values from the same plane, engine, fuel, thrust level, and even time frame. Such data is rare, but recently made possible because both ground and cruise emissions were recorded during ACCESS-II. A measured ground  $EI_{BC}$  from JP-8 at 45 % thrust was scaled with the Döpelheuer and Lecht approximation and compared to a measured cruise value from JP-8 at 45 % thrust. Results are shown in Figure 5.



**Figure 5.**  $EI_{BC}$  measured at ground operating at 45 % thrust scaled to a cruise value with the Döpelheuer and Lecht approximation (blue bar) with comparison to measured  $EI_{BC}$  at cruise from the same plane (DC-8), thrust (45%), and fuel (Jet A) (red bar).

The scaling under predicts the measured cruise value even with the large potential error from the cruise measurement. 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 (Airbus A310-300 and Boeing B737-300) operated at reduced weight and velocities compared to regular operation.<sup>22</sup> The ImFOX directly predicts EI<sub>BC</sub> and with use of the recent ACCESS-II data the ImFOX could be formulated to directly predict BC cruise emissions using the measurements as a benchmark. Previous approaches to predict cruise BC, without the benefit of the ACCESS-II data, were constrained to rely upon measured ground based emissions followed by scaling with the Döpelheuer and Lecht relation.

#### ImFOX Direct Cruise Prediction.

The litmus test of the ImFOX method is whether it is capable of directly predicting cruise  $EI_{BC}$  values. The ImFOX predictive tool only requires the combustor conditions, AFR and T<sub>4</sub>, as input values. If these can be known or otherwise accurately predicted at cruise, then the ImFOX should accurately predict  $EI_{BC}$ . Calculated 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 6.



**Figure 6.** 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 calculated 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. Calculated values were found using a constant formation constant of 295 and the C/H dependent fuel term as described in Section 3.2.

In conclusion, with use of newly developed engine condition relations the ImFOX is optimized to accurately predict BC emission form the current in-service aviation fleet, RQL style combustors. This model can be applied to conventional and alternative jet fuels at ground and cruise. This model can be used to improve BC inventory estimates from the current fleet and will aid in climate models in assessing aviation's BC impact on the environment. Mass emission of BC was the sole focus of this work, however, number based BC emission ( $EI_n$ ) is an important research topic for both health and atmospheric impacts. If the BC particle size distribution can be determined by means on transmission electron microscopy than mass emission can readily be converted to number based emission.

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