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Uncertainty quantification of an Aviation Environmental Toolsuite

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ABSTRACT

This paper describes uncertainty quantification (UQ) of a complex system computational tool that supports policy-making for aviation environmental impact. The paper presents the methods needed to create a tool that is "UQ-enabled" with a particular focus on how to manage the complexity of long run times and massive input/output datasets. These methods include a process to quantify parameter uncertainties via data, documentation and expert opinion, creating certified surrogate models to accelerate run-times while maintaining confidence in results, and executing a range of mathematical UQ techniques such as uncertainty propagation and global sensitivity analysis. The results and discussion address aircraft performance, aircraft noise, and aircraft emissions modeling.

1. Introduction

Uncertainty quantification (UQ) broadly entails quantitative characterization, management, and reduction of uncertainty in applications, and encompasses many different elements (e.g., uncertainty analysis, sensitivity analysis, optimization under uncertainty, design validation, and model calibration). UQ is becoming an essential aspect of the development and use of computational simulation and modeling tools. For example, the National Academy of Sciences has recognized the "ubiquity of uncertainty in computational estimates of reality and the necessity for its quantification" [28] while NASA established a formal standard setting requirements and recommendations for uncertainty assessment in the use of modeling and simulation to support critical decisions [27]. This paper describes how state-of-the-art UQ methods together with surrogate models are combined to achieve UQ of a real-world complex system modeling tool that supports policy-making for aviation environmental impact.

The FAA Office of Environment and Energy, in collaboration with Transport Canada and NASA, is developing a suite of computational tools to support decision and policy-making for aviation environmental impact. This Environmental Toolsuite includes integrated models of airline economics, environmental economics, aircraft operations, aircraft performance, aircraft emissions, noise, local air quality, and global climate. The main goal of the effort is to develop a new critically needed capability to characterize and quantify the interdependencies among aviation-related noise and emissions, impacts on health and welfare, and industry and consumer costs, under different policy, technology, operational, and market scenarios. A comprehensive UQ effort is an important component of this tool development, with the following specific goals: (1) provide sensitivity analyses of the outputs to uncertainties in the inputs and assumptions, establishing procedures for future assessment efforts; (2) identify gaps in functionality within the tools, leading to the identification of high-priority areas for further development; (3) assess confidence in the evaluation of various analysis scenarios such as oxides of nitrogen (NOx) stringency and future aircraft technologies; and (4) continue to contribute to the development of external understanding of the FAA Toolsuite capabilities. A critical aspect of a comprehensive UQ effort is the ability to make the behavior of a tool both transparent and comprehensible to decision makers while incorporating a variety of uncertainties in the tool. To ensure this, the overall UQ process for the Environmental Toolsuite includes tasks related to expert review, verification, validation, capability demonstration, and parametric uncertainty/sensitivity analysis [17]. We focus here on the UQ challenges related to enabling parametric uncertainty and sensitivity analyses.

The scale and complexity of the problem make UQ for this toolset a daunting task that challenges state-of-the-art in UQ methods. Many of the component computational models have long run times. There is a large amount of data even for a single deterministic analysis (e.g., an analysis of one year involves over two million flight operations with 350 aircraft types). Several of the component computational models are built on legacy tools that were designed with a firmly deterministic mindset; thus, there are few opportunities for intrusive UQ methods. And while

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there is a recognition of a need to quantify and account for uncertainties, formal characterizations of parameter uncertainties (e.g., via probabilistic distributions) are not typically available for any of the component models.

In this paper, we present methodology and results for UQ of the Aviation Environmental Design Tool (AEDT), one component of the overall Environmental Toolsuite, but in itself a complex system model embodying all of these challenges. Section 2 provides background on AEDT and its constituent models. Section 3 describes the methods developed to achieve UQ of AEDT, including development of a tool that is "UQ-enabled"; establishing a process to quantify parameter uncertainties via data, documentation and expert opinion; creating certified surrogate models to accelerate run-times while maintaining confidence in results; and executing a range of mathematical techniques such as uncertainty propagation and sensitivity analyses. Section 4 presents UQ results and Section 5 discusses overall findings. Finally, Section 6 discusses conclusions.

2. Aviation Environmental Toolsuite

In this section we first describe the Aviation Environmental Toolsuite and the relationships among its components. We then provide background on AEDT.

2.1. Overview of Aviation Environmental Toolsuite

The Environmental Toolsuite, which is depicted in Fig. 1, has three main functional components: the Environmental Design Space (EDS), which estimates source noise, exhaust emissions, performance and economic parameters for future aircraft designs under different technological, operational, policy and market scenarios; the Aviation Environmental Design Tool (AEDT), which takes as input detailed fleet descriptions and flight schedules, produces estimates of noise, fuel burn and emissions at global, regional, and local levels; and the Aviation environmental Portfolio Management Tool (APMT), which provides an economic model of the aviation industry and performs comprehensive environmental impacts analyses following inputs from AEDT and EDS. Evaluating a scenario with the Toolsuite consists of an integrated analysis of EDS, AEDT, and APMT. The analysis requires the definition of aircraft properties, such as weight, thrust specific fuel consumption, and drag coefficients that define an AEDT aircraft. Economic and market scenarios in APMT Economics are required in the analysis to provide fleet composition and flight route information to AEDT to determine which aircraft to fly and where to fly them. Once AEDT simulates the operation of the fleet, noise and emission estimates from AEDT are passed to APMT impacts, where the information is used to estimate quantities such as global temperature change and the number of people exposed to certain decibel levels around airports.

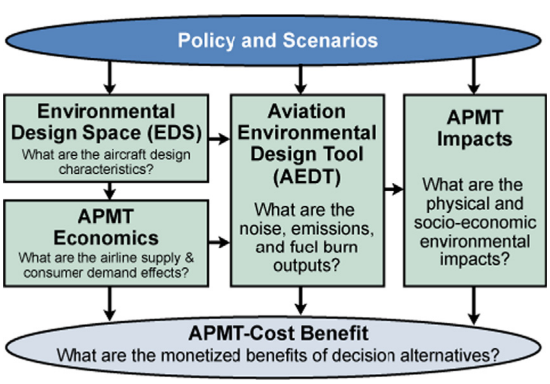

Fig. 1. Aviation Environmental Toolsuite.

In this paper, we focus on UQ of the AEDT system component. Similar approaches to creating UQ-enabled tools are required for the other components of the system. The actual UQ tasks, such as uncertainty analysis, can be integrated at the Toolsuite level following the approach of Amaral et al. [3] once the individual component level analyses have been completed. We also note here that more complex evaluation scenarios within AEDT, which could involve more airports and larger datasets, can be assembled from airport or regional level analyses via the approach of Amaral et al. [3].

2.2. AEDT

AEDT consists of an integrated set of common models and databases used for conducting noise, emissions, and fuel burn analyses on a local (analyzed at the flight level), national, regional, and global scale. A typical forward run of AEDT involves simulation of a "representative day" of operations, which involves analyzing approximately 10^5 individual aircraft operations. This translates into hours of CPU time for a global analysis, and involves processing gigabytes of data.

AEDT is a completely redesigned, integrated tool, building upon the requirements of the Integrated Noise Model (INM) [6], the Emissions and Dispersion Modeling System (EDMS) [12], the Noise Integrated Routing System (NIRS) [35], the Model for Assessing Global Exposure from Noise of Transport Airplanes (MAGENTA) and the System for assessing Aviation's Global Emissions (SAGE) [24]. AEDT is an integrated model that is approved by the FAA to be used to conduct environmental analysis for FAA federal actions and NEPA analyses. In addition, it is used by the FAA to conduct analysis to help inform policy decisions. The tool is used to dynamically model aircraft performance in space and time, using system data and user inputs, to produce fuel burn, emissions and noise estimates. Interdependencies among fuel burn, emissions, and noise can be studied

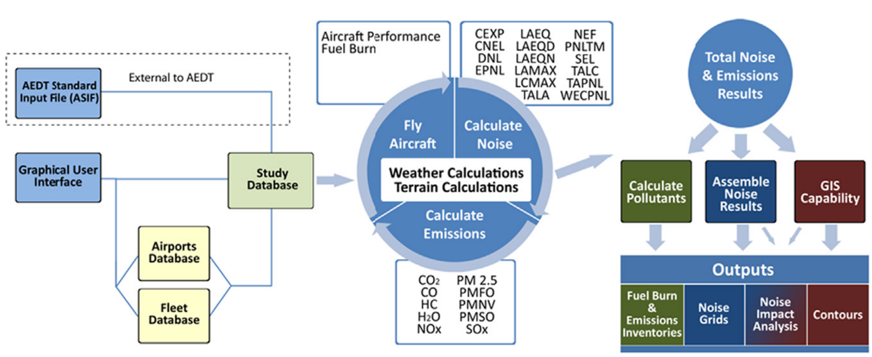

Fig. 2. System structure of AEDT2a. Figure from "Aviation Environmental Design Tool (AEDT) 2a User Guide" [16].

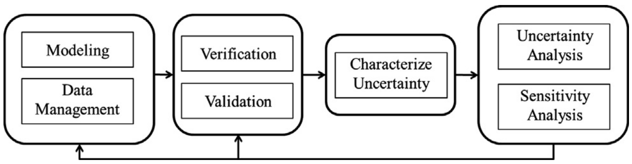

Fig. 3. Uncertainty quantification process.

by AEDT from a single flight at an airport to scenarios at the regional, national, and global levels [16].

The structure of AEDT is shown in Fig. 2. The analysis relies upon two large databases: the Airports Database, which contains specific information about each airport analyzed (e.g., information about airport flight patterns and runway parameters, average monthly values for airport relative humidity, pressure and temperature, diurnal and seasonal variation of the local mixing height for pollutant atmospheric mixing, etc.) and the Fleet Database, which contains information associated with aircraft airframe and engine characteristics. These databases embody an enormous number of AEDT input parameters, all of which are potentially uncertain. In this paper, we present UQ results for the AEDT Alpha version, a pre-release version of the tool. However, the tool structure and underlying models are very similar to the released AEDT 2a version [16].

3. Uncertainty quantification methodology

This section presents the methods developed to achieve UQ of AEDT. We first provide background on UQ for complex systems. We then discuss the modeling and tool development considerations needed to build a tool that is UQ-enabled. Following that, we describe the mathematical UQ methodologies that contribute to achieving our UQ objectives in providing sensitivity analyses, identifying high-priority areas for further development, and assessing confidence in scenario analyses.

3.1. *Uncertainty quantification background*

Uncertainty quantification is a field that has received a lot of recent attention. State-of-the-art structure-exploiting methods for uncertainty analysis such as polynomial chaos expansions (PCE) [37,30], stochastic collocation [4], and reduced-order modeling techniques [7] have been developed. However, these methods are either intrusive (projection-based reduced models) or build on underlying smoothness of the models (PCE, stochastic collocation), and can thus not be applied to tools such as AEDT that contain black-box models and legacy codes. State-of-the-art sensitivity analysis methods, such as global sensitivity analysis [32] have been applied to complex application cases such as nuclear waste repositories [19], ice sheet modeling [5], and for the design of nuclear turbosets [38]. In these applications, many challenges to perform sensitivity analysis exist, such as computational expense and the large number of desired scenarios to be analyzed. Techniques such as surrogate modeling, surrogate sensitivity analysis procedures, and sample reuse have been employed to help overcome these challenges. In general, developing a UQ enabled tool such as AEDT requires overcoming these same challenges, as well as additional challenges related to data storage requirements, the black-box nature of the models, and the required integration of analyses from many components. Our contribution is in bringing existing methods together in a way that enables UQ at the large scale for such real world tools.

3.2. *Uncertainty quantification process: building a tool that is UQ-enabled*

Creating a toolset of the complexity of AEDT encompasses significant challenges in modeling, data management, software development, and user interfaces. Carrying out UQ concurrently with the tool development is essential for guiding allocation of development resources and for providing support to the tool validation and verification process. The overall process is presented in Fig. 3.

3.2.1. *Modeling*

Modeling considerations for UQ must address the question of computational cost, as well as appropriate probabilistic characterizations of uncertain model parameters and model inputs. Computational cost becomes of significant concern in the UQ-enabled tool, since most UQ analysis methods require many simulation runs (e.g., a Monte Carlo simulation to propagate input uncertainties may require many thousands of analysis runs). A detailed component model that is suitable for a single analysis may be inappropriate for use in the UQ setting, since run times can quickly become prohibitive even when parallel computations are employed.

To address this challenge, we use surrogate models—simplified approximate models that are fast to execute but retain the essential features of the system input–output behavior. In general, surrogate models can take many forms: data-fit models (e.g., response surfaces and Kriging models), hierarchical models (e.g., simplified physics models or coarse discretizations), or reduced-order models (e.g., projection-based proper orthogonal decomposition models). Data-fit surrogate approaches are most appropriate in the case that the model is a black box with unknown and/or unexploitable structure, although these techniques cannot deal with high-dimensional parameter spaces, as is the case for AEDT [18]. If the problem structure admits a projection-based approach, as is often the case for systems described by partial differential equations, then a reduced-order model can provide dramatic speedups for UQ sampling while retaining high levels of accuracy in estimated statistics [7]. In the case of AEDT, we can exploit model structure to build a hierarchical surrogate model that estimates outputs based on sampling a small subset of flight operations from the “representative day” used in a typical AEDT analysis run [1]. As described in detail in Allaire and Willcox [1], this approach yields significant speedups in computational simulation time and also provides quantified confidence intervals on the statistics estimated using the surrogate model.

3.2.2. *Data management*

As already shown in Fig. 2, a single AEDT analysis run involves managing a large amount of data, both in terms of interacting with large input databases and in terms of the analysis data generated. Both the software implementation and the UQ task formulation must be architected carefully to make the data management task tractable in the UQ setting. We achieve an efficient scalable implementation via a distributed processing configuration that permits flexibility in database management. The databases can reside on the AEDT client itself, or on a separate database server. With regard to the UQ task formulation, our UQ approach emphasizes the importance of conducting UQ analyses with a particular goal in mind. By this, we mean that it is not practical to assess the effects of uncertainty in every AEDT input parameter with respect to every AEDT output parameter; nor is it useful, since an assessment of the uncertainties in AEDT should relate to a particular analysis context. Rather, we focus on a specific set of scenarios and use cases. Through these scenarios we define quantities of interest, often integrated quantities (e.g., total fuel burn or total emissions for a given airport). In this way, the amount of output data for a given UQ analysis becomes tractable, and our conclusions from that UQ analysis relate directly to the fidelity of the tool in a particular specified context.

3.2.3. Verification and validation

Verification and validation efforts are essential to the confirmation of a tool's functionality and credibility for conducting the analyses for which it was designed. UQ tasks of parametric uncertainty and sensitivity analysis provide critical support for identifying gaps in functionality as part of the verification process, as well as results that can be compared with gold standard data as part of the validation effort.

3.2.4. Characterizing uncertainty

Quantification of input uncertainties is a critical step in the overall uncertainty quantification process. However, often only limited information, which may be in the form of historical data or expert opinion, exists for a given input. We use the Principle of Maximum Entropy to estimate probability distributions describing input uncertainties [22]. These maximum-entropy distributions are consistent with known constraints arising from the available information, but are maximally noncommittal, in an information theory sense, to information we do not have pertaining to a given input.

The entropy we wish to maximize is defined as

$$H(X) = -\sum_{i=1}^{n} \mathbb{P}_X(x_i) \log \mathbb{P}_X(x_i), \tag{1}$$

for the case of discrete random variables, where X is some discrete random variable, $\mathbb{P}_X(x_i)$ is the probability that $X = x_i$, and there are n possible values x can take. For the continuous case, the entropy is defined as

$$h(X) = -\int_{\mathbb{X}} p_X(x) \log p_X(x)\, \mathrm{d}x, \tag{2}$$

where now X is some continuous random variable, $p_X(x)$ is the probability density function of X, and $\mathbb{X}$ is the support of $p_X(x)$. The information we may have regarding a given factor typically consists of bounds for the input and/or moments (e.g., mean and variance). This information is used to constrain the set of possible probability distributions in a formal entropy maximization optimization problem [11]. Distributions that result from typical available information are a discrete uniform distribution, if our information consists only of a set of discrete values; a continuous uniform distribution, if our information consists of upper and lower bounds for the input; a Gaussian distribution, if we have information regarding only the first two moments of the input; and a beta distribution, if we have information regarding the first two moments as well as bounds for the input.

3.3. Uncertainty and sensitivity analysis

Uncertainty analysis encompasses the task of propagating uncertainty associated with inputs to a tool to the outputs of the tool [8]. Typically when performing uncertainty analysis for decision-making, statistical quantities of interest, such as the mean and variance of a given output are reported. Consider a general model $y = f(\mathbf{x})$, where $\mathbf{x} = [x_1, x_2, \ldots, x_k]^T$ is a vector of k inputs to the model. If the inputs are random variables with associated probability distributions, then the mean and variance of the model output are given as

$$\mathbb{E}[Y] = \int_{\mathbb{X}} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x})\, \mathrm{d}\mathbf{x}, \tag{3}$$

$$\mathrm{var}(Y) = \int_{\mathbb{X}} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x})^2 \mathrm{d}\mathbf{x} - \left(\int_{\mathbb{X}} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x})\, \mathrm{d}\mathbf{x} \right)^2, \tag{4}$$

where $p_{\mathbf{X}}(\mathbf{x})$ is the joint probability density function of the random inputs $\mathbf{X}$ and $\mathbb{X}$ is the support of the joint density $p_{\mathbf{X}}(\mathbf{x})$. By the law of large numbers we can estimate the mean and variance of the model output using Monte Carlo simulation as

$$\mathbb{E}[Y] \approx \overline{y}_N = \frac{1}{N} \sum_{m=1}^{N} f(\mathbf{x}^m), \tag{5}$$

$$\mathrm{var}(Y) \approx \frac{1}{N-1} \sum_{m=1}^{N} (f(\mathbf{x}^m) - \overline{y}_N)^2, \tag{6}$$

where N is the number of model evaluations in the simulation, $\overline{y}_N$ is the sample mean of the output y using the N model evaluations, and $\mathbf{x}^m = [x_1^m, x_2^m, \ldots, x_k^m]^T$ denotes the mth sample realization of the random vector $\mathbf{X}$.

Sensitivity analyses are conducted to determine the key inputs that contribute to output variability. Quantification of system sensitivities lends understanding of which factors contribute to uncertainty in the outcome of a particular scenario analysis. For example, sensitivity analysis reveals which modeling assumptions, uncertain model inputs and/or uncertain scenario parameters are most important. In addition to supporting better decision-making through an understanding of uncertainties, sensitivity analysis is critical for directing future research efforts aimed at reducing output variability. This is particularly important in situations where the variability is so large that model results are useless for supporting decision-making (e.g., when the difference between the outcomes of two policy alternatives is not statistically significant due to large uncertainty). The recommended method for the apportionment of output variance across model factors is global sensitivity analysis [32], which is a quantitatively rigorous method for determining key contributors to output variability [9]. For models with a large number of inputs, such as AEDT, the Monte Carlo based Sobol′ method [20] is the most appropriate approach for conducting a global sensitivity analysis.

Variance-based global sensitivity analysis is based on the fact that the variance of the generic random model output Y can be decomposed according to $\mathrm{var}(Y) = \mathbb{E}[\mathrm{var}(Y|X_i)] + \mathrm{var}(\mathbb{E}[Y|X_i])$, for any X_i, where $i \in \{1, \ldots, k\}$. Global sensitivity indices of Y may be written as

$$S_i = \frac{\mathrm{var}(\mathbb{E}[Y|X_i])}{\mathrm{var}(Y)}, \tag{7}$$

$$\tau_i = 1 - \frac{\mathrm{var}(\mathbb{E}[Y|X_{i^c}])}{\mathrm{var}(Y)}, \tag{8}$$

where S_i is the main effect sensitivity index of the random input X_i, τ_i is the total effect sensitivity index of X_i, and X_i^c denotes all random inputs except X_i. The main effect sensitivity indices represent the expected reduction in output variance that would occur if a given factor was to be known precisely. These indices can be used to direct resource allocation aimed at reducing output variance. The total effect sensitivity indices represent the expected amount of output variance that is attributable to a given factor and all interactions in which that factor is involved. These indices can be used to determine which factors may be fixed to some value of their domain without significantly impacting the output.

Following Sobol′ [34] and Homma and Saltelli [20], the main effect sensitivity indices can be written as

$$S_i = \frac{\int_{\mathbb{X}} \int_{\mathbb{X}_i} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x}) p_{\mathbf{V}}(\mathbf{v}) p_{X_i'}(x_i') f(\mathbf{v}, x_i')\, \mathrm{d}\mathbf{x}\, \mathrm{d}x_i' - \mathbb{E}[Y]^2}{\mathrm{var}(Y)}, \tag{9}$$

where $\mathbf{v} = (x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_k)$ and X_i' represents a second independent identically distributed version of the input X_i.

Similarly, the total effect sensitivity indices can be written as

$$\tau_i = 1 - \frac{\int_{\mathbb{X}}\int_{\mathbb{V}} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x}) p_{\mathbf{V}'}(\mathbf{v}') p_{X_i}(x_i) f(\mathbf{v}', x_i)\, d\mathbf{x}\, d\mathbf{v} - \mathbb{E}[Y]^2}{\mathrm{var}(Y)}. \tag{10}$$

The sensitivity indices defined by Eqs. (9) and (10) can be computed using Monte Carlo simulation to estimate the integrals.

The AEDT system analyzed here has millions of inputs. Obtaining main and total effect sensitivity indices for each input is a computationally intractable task and would also overwhelm the analysis with data containing little useful information. From a practical standpoint, we are more interested in determining the sensitivity of model outputs to *groups of inputs of interest*. For example, while each aircraft operation could in theory have an uncertain parameter that varies independently, it is practically more useful for us to assess the impact of uncertainty in the parameter over aircraft operations as a group. For example, rather than considering uncertainty due the reference emissions index specific to each engine on each operation (which would result in ~ 7.5 million uncertain parameters to be analyzed), we might consider uncertainty due to the entire group of parameters corresponding to reference emissions indices over all operations of a given aircraft type. Estimating sensitivity indices of groups of inputs has been discussed in Sobol′ [34], Saltelli et al. [32], Allaire and Willcox [1]. Following Sobol′ [34], consider an arbitrary group of m inputs for which we would like to estimate the main and total effect sensitivities. Let $\mathcal{G} = \{g_1, \ldots, g_m\}$, where $1 \le g_1 < \cdots < g_m \le k$ and $g_i \in \mathbb{N}$ for $i = 1, 2, \ldots, m$, $\mathcal{X} = \{1, 2, \ldots, k\}$, and $\mathcal{G}_c = \mathcal{X} \setminus \mathcal{G}$. Also, let $\mathbf{X}_{\mathcal{X}} = (X_1, \ldots, X_k) = \mathbf{X}$, $\mathbf{X}_{\mathcal{G}} = (X_{g_1}, \ldots, X_{g_m})$, and $\mathbf{X}_{\mathcal{G}_c} = (X_{l_1}, \ldots, X_{l_j})$, where $m + j = k$, $l_1, \ldots, l_j \in \mathcal{G}_c$, $1 \le l_1 < \cdots < l_j \le k$, and $l_i \in \mathbb{N}$ for $i = 1, 2, \ldots, j$. Then we may write the main effect index, $S_{\mathcal{G}}$, of the group of inputs $X_{\mathcal{G}}$ as

$$S_{\mathcal{G}} = \frac{\int_{\mathbb{X}}\int_{\mathbb{G}} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x}) p_{\mathbf{X}_{\mathcal{G}_c}}(\mathbf{x}_{\mathcal{G}_c}) p_{\mathbf{X}'_{\mathcal{G}}}(\mathbf{x}'_{\mathcal{G}}) f(\mathbf{x}_{\mathcal{G}_c}, \mathbf{x}'_{\mathcal{G}})\, d\mathbf{x}\, d\mathbf{x}'_{\mathcal{G}} - \mathbb{E}[Y]^2}{\mathrm{var}(Y)}, \tag{11}$$

where $\mathbb{G}$ is the support set of the joint density $p_{\mathbf{X}_{\mathcal{G}}}(\mathbf{x}_{\mathcal{G}})$. Similarly, we may write the total effect sensitivity index, $\tau_{\mathcal{G}}$, of the group of inputs $\mathbf{x}_{\mathcal{G}}$ as

$$\tau_{\mathcal{G}} = 1 - \frac{\int_{\mathbb{X}}\int_{\mathbb{G}_c} p_{\mathbf{X}}(\mathbf{x}) f(\mathbf{x}) p_{\mathbf{X}'_{\mathcal{G}_c}}(\mathbf{x}'_{\mathcal{G}_c}) p_{\mathbf{X}_{\mathcal{G}}}(\mathbf{x}_{\mathcal{G}}) f(\mathbf{x}'_{\mathcal{G}_c}, \mathbf{x}_{\mathcal{G}})\, d\mathbf{x}\, d\mathbf{x}_{\mathcal{G}_c} - \mathbb{E}[Y]^2}{\mathrm{var}(Y)} \tag{12}$$

The group sensitivity indices defined by Eqs. (11) and (12) can be computed using Monte Carlo simulation to estimate the integrals.

4. Uncertainty quantification results

This section first presents the UQ problem setup, then describes the uncertainty sources considered and their assumed maximum entropy probability distributions. In some cases we employ triangular distributions, since often the triangular distribution is used as a proxy for the beta distribution for policy-level analyses, given the transparency of the roles of the parameters of the triangular distribution as compared to those of the beta distribution [36,23]. We then present AEDT UQ results for several output quantities of interest. The numerical results presented in this section are a selection intended to highlight some of the analysis results; in the next section, we present a comprehensive discussion of the insights gained from the full UQ study. We note here that if a decision-maker wishes to study the impact of different input distributions on a particular scenario, a sample reuse strategy developed in Allaire and Willcox [2] can be incorporated into the UQ process, which does not require further tool evaluations. Here, however, we focus on the maximum entropy distributions determined by the available information regarding the inputs.

4.1. Problem setup

Due to the computational requirements of the UQ analysis, surrogate models were required. A single day of operations from October 18th, 2006 at John F. Kennedy Airport (JFK), Hartsfield–Jackson Atlanta International Airport (ATL), and Teterboro, Airport (TEB) was used as a surrogate model to approximately represent a year′s worth of flights at each airport. The selection of these three airports was made to compare the possible differences in UQ results for emissions and fuel burn that could be caused by different aircraft fleet mixes. From previous UQ studies on individual components of AEDT it was determined that the sensitivity of certain input factors can vary by aircraft type. JFK was chosen because it is a large international hub airport, comprising 1145 total operations (567 departures and 578 arrivals) on the day analyzed, and utilizing a wide mix of narrow-body, wide-body, and regional-jet aircraft types. The ATL study comprises 2650 operations (1333 departures and 1317 arrivals). ATL is a hub airport for Delta Airlines and Airtran Airways in which the 2006 fleets for these airlines consisted of a large mix of Boeing aircraft types. The mix of Boeing aircraft types and other non-Boeing aircraft types can affect how thrust specific fuel consumption factors are ranked. The TEB study comprises 497 operations (246 departures and 251 arrivals) and was chosen because it is a commercial airport dominated by private jets and general aviation which utilize different input factors than jet aircraft when calculating aircraft performance.

A single airport was utilized in conducting the noise analysis which consisted of a single day of operations at JFK. A single airport was modeled due to the more intensive computational run time required for conducting a noise analysis versus conducting an emissions and fuel consumption analysis. The computational run time differences for the noise analysis are attributed to the use of individual aircraft trajectories for each aircraft operation and noise receptor grid points. The emissions and fuel burn analysis models flights as if they fly straight in and straight out trajectories with no geospatial importance of where the emissions and fuel burn occurs with exception to altitude. The noise analysis calculates the noise intensity at each receptor grid point based upon the geospatial location of the aircraft in reference to each grid point. The noise intensity for each grid point is adjusted as the aircraft flies on different segments along its assigned track.

Also, while the emissions and fuel burn analysis used operations from October 18th, 2006, the noise analyses utilized an Average Annual Day (AAD) for JFK. The AAD represents an average days worth of aircraft operations with representative flight trajectories. Throughout an entire year an airport might have tens of thousands of individual flight tracks. The AAD utilizes a back boning process that groups flight operations on representative flight tracks to represent an average day. The AAD of operations at JFK consisted of 599 departures and 677 arrivals.

4.2. Characterization of uncertainty

AEDT has three core modules that conduct the fuel consumption, emissions and noise calculations. These are the Aircraft Performance Module (APM), Aircraft Emissions Module (AEM) and Aircraft Acoustic Module (AAM). The uncertain input parameters described in this subsection are binned by high level groups: Airport Atmospherics; Aircraft Performance; Aircraft Emissions; and Aircraft Noise. For many of these parameters, engineering judgement is cited as the source of the probability distributions listed. These judgements were performed by engineers on the tool development team with substantial experience in working with the models and their inputs. However, a formal elicitation process, such as that discussed in Cooke and Goosens

Table 1
Inputs and distribution parameters for airport atmospherics. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the airport database.

Input	Distribution min, max	Explanation of distribution	Source
Airport temperature	± 10%	Diurnal variation	Engineering judgment
Airport pressure relative to mean sea level	± 3%	Diurnal variation	Engineering judgment
Average headwind value	+100%, −125%	Variation of the wind speed vector applied to the aircraft during terminal area operations	Engineering judgment
Average relative humidity	± 15%	Diurnal variation	Engineering judgment

[10] was not conducted. Such a process is desirable for establishing the uncertainties associated with the inputs to the tool when being used in a decision making context. Here, however, we are focused on the data management and computational challenges of developing a UQ-enabled tool.

4.2.1. Airport atmospherics

Airport atmospherics parameters are utilized in all three AEDT modules. Temperature, pressure, and headwind are used to calculate aircraft performance. Temperature, pressure, and relative humidity are used to calculate noise and emissions. Average temperature, pressure, relative humidity and headwind information for each airport are stored in the Airports Database and retrieved for a specific aircraft operation. For UQ purposes, temperature, pressure and relative humidity data from the Airports Database are assumed to be representative of all temperature, pressure, and relative humidity values that occur in the month corresponding to the flight being modeled. An average headwind value is assumed for all segments of all operations at an airport. The airport atmospherics input parameters and their probability distributions are listed in Table 1.

4.2.2. Aircraft performance

The input parameters associated with calculating aircraft performance can be categorized into three categories: flaps, thrust, and fuel consumption. There are two methodologies implemented in AEDT to calculate aircraft performance: the Society of Automotive Engineers Aerospace Information Report 1845 (SAE-AIR-1845) Procedure for the Calculation of Airplane Noise in the Vicinity of Airports [31] and Eurocontrol's Base of Aircraft Data (BADA) [29]. SAE-AIR-1845 estimates the altitude profile, including net corrected thrust for terminal area operations below 10,000 ft in altitude. BADA calculates the fuel consumption based on net corrected thrust output from the SAE-AIR-1845 algorithms. BADA also calculates aircraft performance based on airframe (versus the use of aircraft airframe and engine in SAE-AIR-1845), and applied to aircraft operations greater than 10,000 ft in altitude.

The flap input parameters and probability distributions are shown in Table 2. These parameters are stored in AEDT's Fleet Database and retrieved for computations. The assumptions associated with these parameters are specific to terminal area operations. These data are empirically derived from proprietary information provided by aircraft manufacturers.

The thrust input parameters and their associated probability distributions are listed in Table 3. The thrust input parameters are stored in AEDT's Fleet Database and are retrieved for a specific aircraft operation. The assumptions associated with these parameters are representative of the aircraft engine conditions that determine the power required at particular operating modes such as take-off or arrival. These data are empirically derived from proprietary information provided by aircraft manufacturers. Thrust coefficients E, F, Ga, Gb and H are input parameters used for jet aircraft operations; the efficiency and power parameters are used for propeller aircraft operations. The weight parameter

Table 2
Inputs and distribution parameters for flap settings for the aircraft performance module. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the fleet database.

Input	Distribution min, max	Explanation of distribution	Source
Takeoff distance coefficient (Flaps Coefficient B)	± 14%	Estimation of variation of take off distance coefficient	Engineering judgment
Takeoff and landing calibrated airspeed coefficient (Flaps Coefficient CD)	± 14%	Estimation of variation of takeoff and landing calibrated airspeed coefficient	Engineering judgment
Drag-over-lift ratio (Flaps Coefficient R)	± 14%	Estimation of drag-over-lift ratio	Based upon a validation analysis which compared coefficient R values in AEDT to computer flight data recorder data

Table 3
Inputs and distribution parameters for thrust settings for the aircraft performance module. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the fleet database.

Input	Distribution min, max	Explanation of distribution	Source
Corrected net thrust per engine coefficient (Coefficient E)	± 15%	Variation of takeoff thrust	Validation analysis using computer flight data recorder data
Speed adjustment coefficient (Coefficient F)	± 15%	Variation of speed adjustment coefficient	Engineering judgment
Altitude adjustment coefficient (Coefficient Ga)	± 2.5%	Variation of altitude adjustment coefficient	Engineering judgment
Altitude-squared adjustment coefficient (Coefficient Gb)	± 2.5%	Variation of altitude squared adjustment coefficient	Engineering judgment
Temperature adjustment coefficient (Coefficient H)	± 2%	Variation of temperature coefficient	Engineering judgment
Propeller efficiency ratio	± 10%	Variation of propeller efficiency ratio	Engineering judgment
Net propulsive power per engine	± 10%	Variation of net propulsive power	Engineering judgment
Aircraft weight during current operation (starting weight)	± 10%	Variation of aircraft takeoff weight	Engineering judgment

Table 4
Inputs and distribution parameters for thrust specific fuel consumption settings for the aircraft performance module. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the fleet database.

Input	Distribution min, max	Explanation of distribution	Source
Thrust specific fuel consumption Coeff1 (Boeing) -Constant	±10%	Estimation of variation of TSFC	Engineering judgment
Thrust specific fuel consumption Coeff2 (Boeing) -Mach	±10%	Estimation of variation of TSFC	Engineering judgment
Thrust specific fuel consumption Coeff3 (Boeing) -Altitude	±10%	Estimation of variation of TSFC	Engineering judgment
Thrust specific fuel consumption Coeff4 (Boeing) -Thrust	±10%	Estimation of variation of TSFC	Engineering judgment
1st thrust specific fuel consumption coefficient (TSFC BADA 1)	±10%	Estimation of variation of TSFC	Engineering judgment
2nd thrust specific fuel consumption coefficient (TSFC BADA 2)	±10%	Estimation of variation of TSFC	Engineering judgment
1st descent fuel flow coefficient (TSFC BADA 3)	±10%	Estimation of variation of TSFC	Engineering judgment
2nd descent fuel flow coefficient (TSFC BADA 4)	±10%	Estimation of variation of TSFC	Engineering judgment

Table 5
Inputs and distribution parameters for emission indices for the aircraft emissions module. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the fleet database.

Input	Distribution min, max	Explanation of distribution	Source
ICAO reference fuel flow	±5%	Variation of ICAO fuel flow	Engineering judgment
ICAO reference emissions index for CO (CO EI)	±26%	Variation of ICAO carbon monoxide emissions indices	Validation analysis while establishing ICAO certification procedure
ICAO reference emissions index for HC (HC EI)	±55%	Variation of ICAO hydrocarbon emissions indices	Validation analysis while establishing ICAO certification procedure
ICAO reference emissions index for NO_x (NO_x EI)	±24%	Variation of ICAO nitrogen oxides emissions indices	Validation analysis while establishing ICAO certification procedure
ICAO reference smoke number (SN)	±3	Estimation of variation of ICAO smoke number	Validation analysis while establishing ICAO certification procedure

Table 6
Inputs and distribution parameters for the aircraft noise module. Each distribution is triangular and the distribution minimum and maximum values are relative to the nominal values in the fleet database.

Input	Distribution min, max	Explanation of distribution	Source
Noise-power distance (NPD) curves	±1.5 dB	Variation of noise certification data	Noise certification guidelines

represents the weight of the aircraft. This value is determined by the distance between the origin and destination airports referred to as the "stage length" of the aircraft operation.

Fuel consumption is calculated in AEDT by determining the required thrust for a flight operation and assigning the appropriate thrust specific fuel consumption (TSFC) coefficients. To estimate fuel consumption, the SAE-AIR-1845 methodology calculates the thrust that corresponds to specific TSFC coefficients for an operating mode such as departure or approach. The TSFC input parameters and their probability distributions are listed in Table 4. The TSFC input parameters are stored in AEDT's Fleet Database and are retrieved for a specific aircraft operation.

4.2.3. Aircraft emissions

Aircraft emissions are calculated by AEDT's Aviation Emissions Module (AEM) using the fuel consumption computed by the APM and the engine-specific emissions index stored in the Fleet Database. The input parameters and their probability distributions are listed in Table 5. Aircraft emission parameters are specific to aircraft operation mode, namely take-off, climb-out, approach and idle. The data are derived empirically from aircraft certification tests required by the International Civil Aviation Authority (ICAO). ICAO maintains a database of the certification data which includes data for fuel flow, carbon monoxide (CO), hydrocarbons (HCs), oxides of nitrogen (NOx), and smoke number (SN) (used for determining non-volatile particulate matter) measured at the four landing and take-off cycle (LTO) power settings noted above.

The use of LTO cycle values of the ICAO emission indices calculated at sea level static conditions introduces uncertainty in emissions inventory calculations because emissions must be calculated with the Boeing Fuel Flow Method 2 (BFFM2) [13] at non-reference conditions and power settings other than the four ICAO settings. The ICAO Committee on Aviation Environmental Protection (CAEP) Working Group 3 has shown that BFFM2 computations of NOx, CO, and HCs at non-reference conditions and non-LTO-cycle power settings have an uncertainty of 10% [21]. Also, the published literature indicates that engine-to-engine emission index variability can be estimated to be 16% for NOx, 23% for CO, and 54% for HC at the 90% confidence interval for a representative sample of new, uninstalled engines [25]. The emission indices in the ICAO emissions database do not include changes in emission characteristics due to engine deterioration over time. The effects of engine deterioration on NOx emissions are estimated to be −1% to +4% [26]. Engine deterioration effects are applied to the final input distribution for NOx. These effects were not applied to the final input distributions for CO and HC.

4.2.4. Aircraft noise

The probability distributions for each input parameter for calculating the aircraft noise are listed in Table 6. Aircraft noise parameters are located within AEDT's Fleet Database and are retrieved for a specific aircraft operation on the geospatial location of the aircraft in reference to a grid point. Noise-power-distance (NPD) curves are a function of engine power and distance from a particular grid point and are developed according to SAE-AIR-1845. They are used to determine noise level values by interpolating and/or extrapolating by the net corrected thrust and slant distance between an aircraft and grid point. The interpolation/extrapolation process is a piecewise linear one between the engine power setting and the base-10

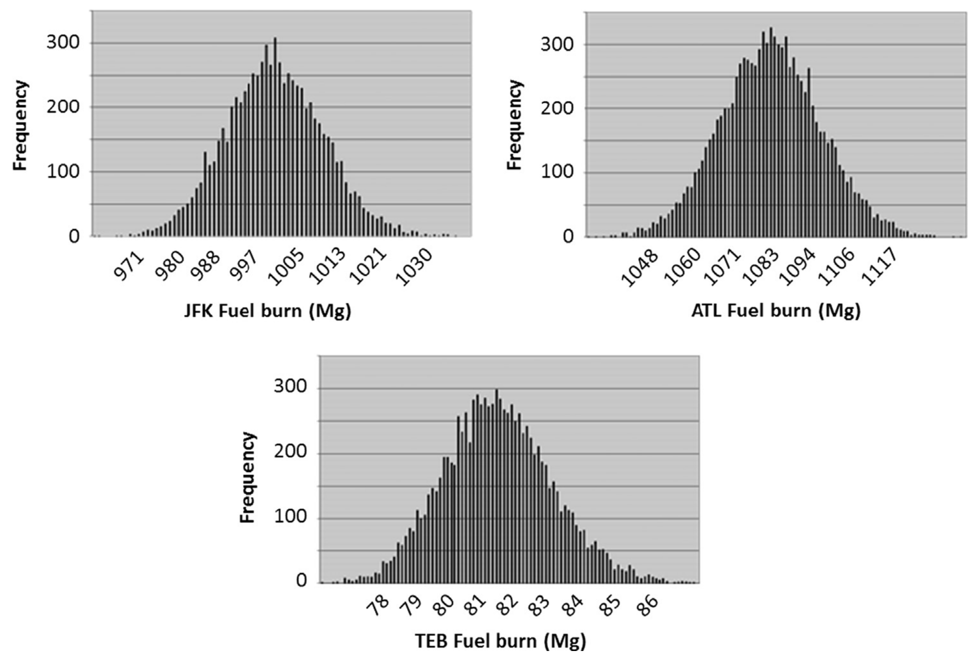

Fig. 4. Fuel burn output distributions for JFK (upper left), ATL (upper right), and TEB (lower).

Table 7
Fuel burn and emissions statistics for JFK, ATL and TEB.

Output	Airport	JFK	ATL	TEB
Fuel burn	Mean (Mg)	1005	1081	83
	Standard deviation (Mg)	9	12	1.5
	Coefficient of variation (%)	0.9	1.2	1.8
NOx	Mean (kg)	14,116	14,777	883
	Standard deviation (kg)	362	470	41
	Coefficient of variation (%)	2.6	3.2	4.6
CO	Mean (kg)	12,368	12,513	1720
	Standard deviation (kg)	316	366	52
	Coefficient of variation (%)	2.6	2.9	3.0
HC	Mean (kg)	1655	1838	653
	Standard deviation (kg)	77	122	74
	Coefficient of variation (%)	4.6	6.6	11.3
PM	Mean (kg)	304	397	37
	Standard deviation (kg)	5.6	9.0	1.2
	Coefficient of variation (%)	1.8	2.3	3.3

logarithm of distance. Noise certification values are reported within an error of +/− 1.5 decibels (dB) [14].

4.3. UQ results: fuel burn and emissions

Fig. 4 shows the output histograms of fuel burn for JFK, ATL and TEB, respectively. Table 7 lists the mean, standard deviation, and coefficient of variation for the fuel burn distributions in each case. Even accounting for the many uncertain input parameters described in the previous section, AEDT estimates of fuel burn have relatively low uncertainty, with standard deviations of less than 2% of the mean values for all airports analyzed. Fig. 5 shows the total sensitivity indices (TSIs) for those input parameters that contributed the most to the fuel burn output variance for each airport analyzed. The biggest contributor to the variance for fuel burn across all airports is aircraft weight. The ranking of the TSI values for the other parameters vary for each of the airports analyzed. The TSFC BADA 1 coefficient was the second highest contributor to the variance for JFK and TEB; however, for ATL it was the fifth highest contributor. This difference is due to fleet mix differences between the three airports. The fleet mix for JFK consists of many aircraft that utilized the BADA TSFC coefficients.

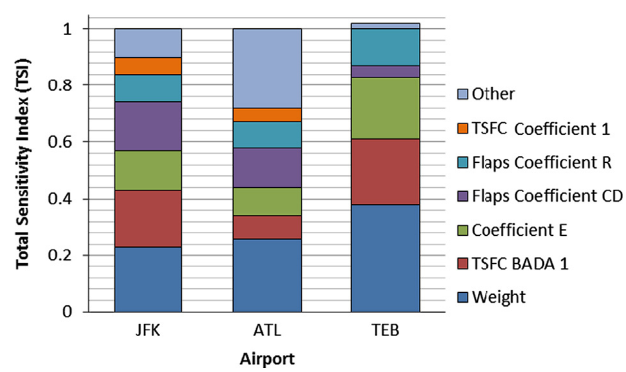

Fig. 5. Fuel burn TSI values for JFK, ATL and TEB.

ATL has a large portion of Boeing aircraft within its fleet, which utilize the Terminal TSFC coefficients.

Table 7 also shows the mean, standard deviation, and coefficient of variation for the distributions of NOx, CO, HC, and particulate matter (PM) emissions. It can be seen that uncertainty in emission estimates is generally higher than for fuel burn estimates. This is because emission estimates are subject to the additional uncertainty stemming from the emissions indices. HC emissions show the largest coefficient of variation results. Fig. 6 shows the TSI values for the most significant contributors to output variance in HC emissions. We see that uncertainty in HC emissions is dominated by the HC Emissions Index (EI). For JFK, temperature and pressure also contribute a small amount to the HC emissions variance. Fig. 7 shows sensitivity indices for PM emissions. In this case, there is not a single dominating input parameter. Aircraft weight is important, as there are various coefficients in the models of aircraft and engine performance.

4.4. UQ results: noise

We present noise uncertainty analysis and sensitivity analysis results for JFK airport only. The output of interest in this case is the Sound Exposure Level (SEL), which is a measure of the total noise energy produced by a noise event. The noise analysis was conducted using an 81-point evenly spaced receptor grid that

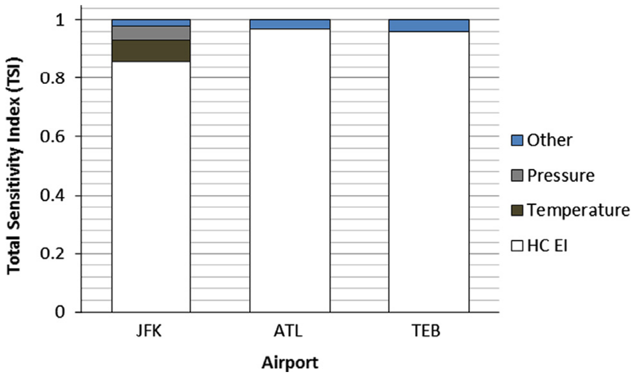

Fig. 6. Hydrocarbon emission TSI Values for JFK, ATL and TEB.

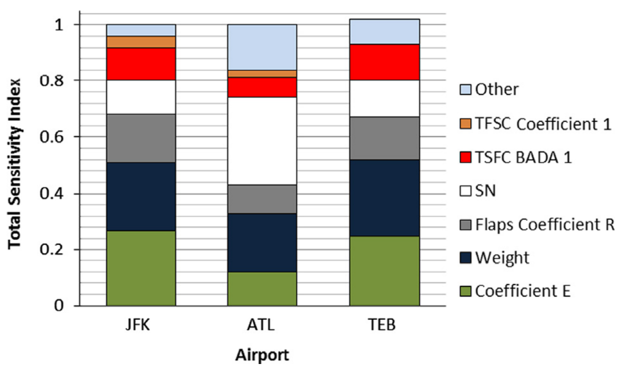

Fig. 7. Particulate matter emission TSI Values for JFK, ATL and TEB.

covers a 20×20 nautical mile area around JFK airport. Fig. 8 depicts a noise contour plot of the mean SEL values resulting from the uncertainty analysis, conducted via Monte Carlo simulation. Sensitivity analysis computes TSI values for each grid point. The numerical values of the sensitivity indices are not shown here due to the large number of grid points. Fig. 9 presents the total sensitivity indices for a grid point near JFK (point A in Fig. 8) and a grid point farther away from JFK (point B in Fig. 8). The sensitivity analysis for these grid points is typical for all grid points and reveals that the uncertainty surrounding the noise-power-distance (NPD) curves is the most significant contributor to SEL variance. TSI values for NPD curves were typically above 0.95 for each grid point analyzed. Thrust Coefficient E was the second highest contributor to the output variance, with TSI values around 0.05 at each grid point. The analysis also showed small contributions ($<1\%$) to SEL variance from aircraft weight and atmospheric temperature parameters.

5. Discussion

The sensitivity and uncertainty analyses conducted for AEDT have identified input parameters that contribute the most to output variance and uncertainty for emissions, fuel burn, and noise. Even though the scope of these analyses was limited to the use of the AEDT Alpha version, the results are generally applicable to more advanced versions of AEDT, because the core algorithms and associated assumptions are carried forward in those releases of AEDT. In total, 29 individual input parameters contributed significantly to the output variances across all emissions and noise output metrics. Only 12 of those input parameters are significant contributors to the output variances of all the emission metrics at the airport level within the terminal area. Only two parameters contributed to the output variance for noise. While the discussion below focuses on the technical details of AEDT models, it demonstrates more generally how the UQ analyses support the specific goals described in Section 1. In particular, the uncertainty analysis and sensitivity analysis results highlight the most important assumptions within the models, identify gaps in the models, and indicate important areas for future tool development.

5.1. Emissions Indices (EIs)

The ICAO engine EI uncertainties were found to be the main contributors to output variance for NOx, HC and CO emissions. As shown in Table 5, the distributions assumed for the EIs were triangular with upper/lower bounds of 24% of the mean value for NOx, 26% for CO, and 55% for HC. These EI uncertainties include engine-to-engine variations as well as the uncertainty in Boeing Fuel Flow Method 2 (BFFM2) calculations. These values were derived from published data based on the fuel venting and exhaust emissions requirements associated with the engine certification process [15]. In the context of engine emissions certification, the Dp/Foo value represents the mass of any gaseous pollutant emitted during the LTO cycle divided by an engines rated thrust output. The minimum requirement for engine certification is that a single engine is tested three times; the mean Dp/Foo values are calculated from those three tests. To determine if the engine type meets the certification emission requirements, the mean Dp/Foo values are adjusted upward by 16% for NOx, 23% for CO, and 54% for HC to calculate the characteristic Dp/Foo. This value is then compared to certification emission standards. The characteristic Dp/Foo value accounts for the uncertainty associated with engine-to-engine EI variability; if the characteristic Dp/Foo for the engine does not meet the certification emission standards then additional engines of that same model number are tested to reduce the overall uncertainty in calculating the characteristic Dp/Foo values. These adjustment factors are based on certification-like studies that were conducted in the 1970s [25]. They may be considered conservative due to how modern aircraft engines have evolved. Also, all EI and SN values have four certification points for take-off (100% power), climb-out (85% power), approach (30% power), and idle (7% power). For this analysis, the same probability distribution was used for each power setting, although in reality the EI uncertainty associated with each power setting may vary. A better understanding for which power setting the EI uncertainty is most important may provide valuable guidance to mitigating the effects of this uncertainty.

5.2. Aircraft weight

Aircraft weight was found to be a significant contributor to the output variance for CO_2, fuel burn, NOx, and particulate matter. AEDT determines aircraft weight based upon origin-to-destination stage length distance. Each aircraft can have multiple stage length distances based upon range and purpose. Our analysis used a triangular distribution to represent weight uncertainty, with upper and lower bounds of 10% of the mean value. Because the aircraft weight was observed to be such a large contributor to the output variance of multiple output metrics, this is a valuable area in which to invest resources to better understand the associated uncertainties. For example, computational fight recorder data could be analyzed to better characterize stage length weight and its variations.

5.3. Terminal and BADA TSFC coefficients

The Terminal and BADA TSFC 1 coefficients are significant contributors to the output variance of CO_2, fuel burn, NOx, and particulate matter. The Terminal coefficients were developed by

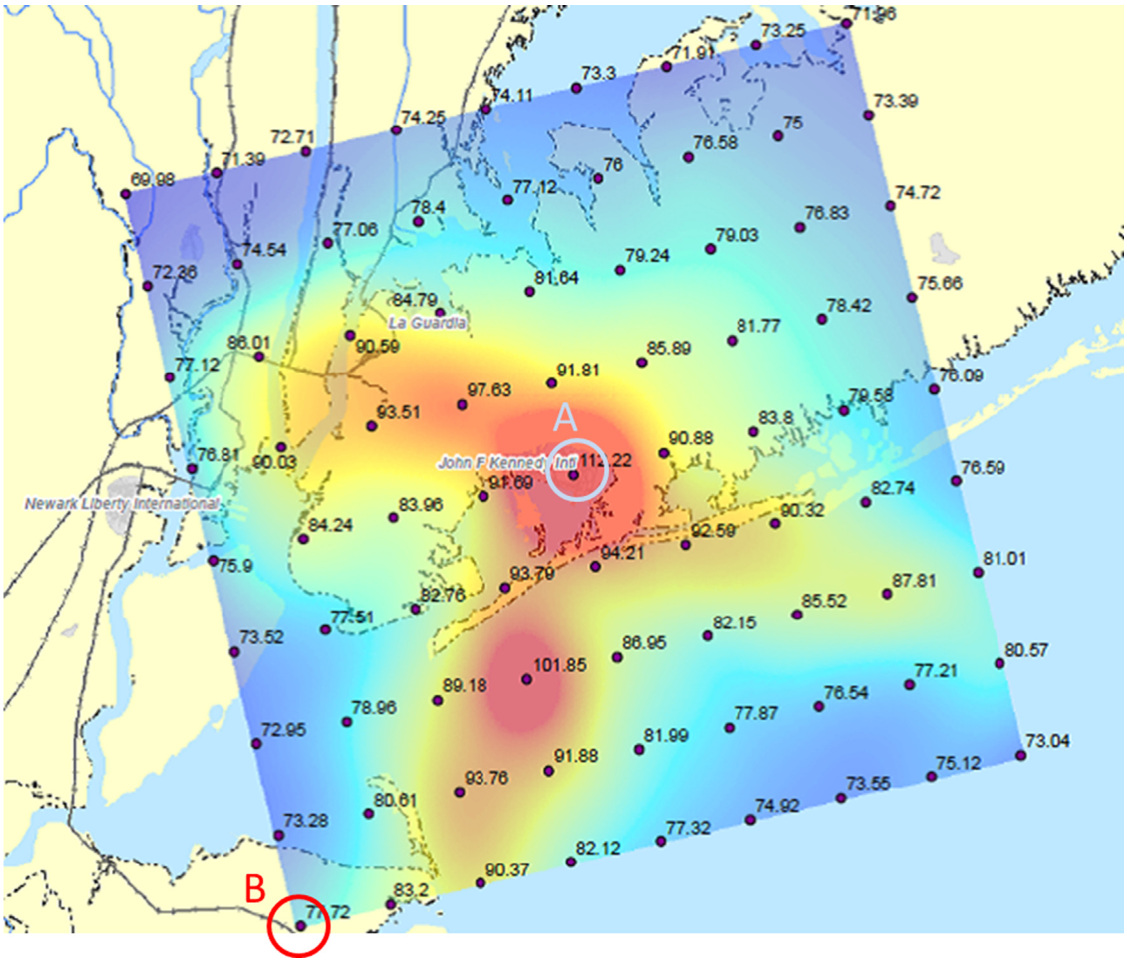

Fig. 8. JFK Sound Exposure Level (SEL) contour plot with two representative grid points highlighted; point A is close to JFK and point B is farther away. The total sensitivity indices for SEL at these two grid points are presented in Fig. 9.

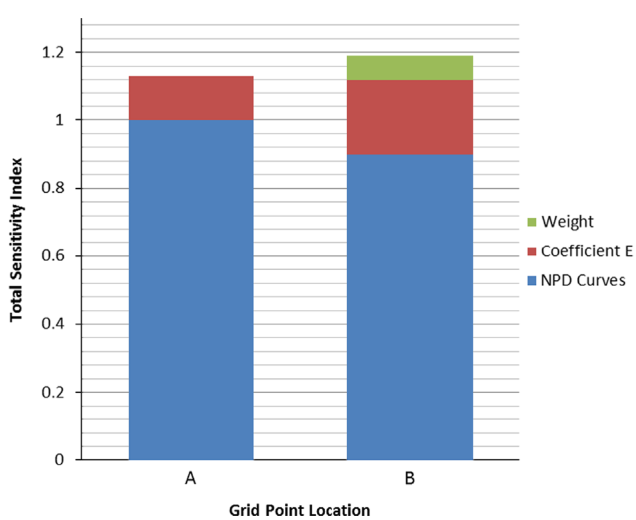

Fig. 9. Sound exposure level TSI values for grid points A and B in Fig. 8 for JFK.

the Volpe Center using proprietary aircraft performance models and computational flight recorder data [33]. The BADA coefficients are provided by Eurocontrol. The Terminal TSFC coefficients used in AEDT currently apply to newer Boeing aircraft models, while the BADA coefficients apply to all other aircraft. The BADA TSFC 1 typically ranked higher than the Terminal TSFC 1 in the sensitivity analysis; however, this is most likely due to the number of aircrafts to which these coefficients are assigned. Because the Terminal and BADA TSFC coefficients are significant contributors to the output variance of multiple output metrics, further verification and validation efforts should continue in this area. Past verification and validation has led to the creation of the Terminal TSFC coefficients, which replaced BADA coefficients for newer Boeing aircraft types. The Terminal TSFC coefficients have been shown to be more accurate in predicting fuel burn, especially during the departure.

5.4. SAE-AIR-1845 performance coefficients

Thrust Coefficient E (corrected net thrust per engine) is a significant contributor to the output variance for CO_2, fuel burn, NOx, and particulate matter. This input parameter is also a contributor to the output variance associated with SEL for noise. Other SAE-AIR-1845 coefficients are also contributors to the output variance for CO_2, fuel burn, NOx, and particulate matter, including Flaps Coefficient R (drag-over-lift ratio) and Flaps Coefficient CD (takeoff and landing calibrated airspeed). However, these input parameters are typically outranked by weight, NOx EI, and the TSFC coefficients. The range of probabilistic distributions were mostly determined by the percent reduction in take-off thrust observed while analyzing computational flight recorder data. Currently, AEDT does not model reduced thrust take-offs. However, because Thrust Coefficient E was identified as a key contributor to the output variance for multiple output metrics, it is suggested that further research efforts be conducted to investigate the potential impact of AEDT not having this capability.

5.5. NPD curves

The NPD curves are the most significant contributor to the variability of SEL noise output. Atmospheric parameters, such as temperature, pressure, and relative humidity, do not significantly contribute to the output variance. Like the ICAO EI values, which are based upon the emissions certification process, the current NPD generation process is unlikely to change. For this analysis, each point along an NPD curve was varied independently. An alternate approach would be to shift all of the points along the NPD curve in unison. Future analysis should determine the appropriateness of each approach. Items that were not addressed with this analysis include the variation of type of profile or track. Since both items affect the location of the aircraft, their variation (reflecting day-to-day variation at a given airport) would likely contribute further to SEL variance. In addition, our analysis used 81-points in the receptor grid. Future analyses will assess whether output variance contributions change when more grid points closer to the airport are considered.

6. Conclusions and future work

This paper has presented methodology and results for uncertainty quantification of a real-world complex system modeling tool. The approaches described in the paper overcome the complexities of long run times and massive input/output datasets, using a combination of surrogate modeling and grouped sensitivity analysis. Several general conclusions can be drawn from the UQ effort presented here. First, sensitivity analysis on a black-box code is a systematic and effective means of identifying high priority areas for future research as well as insignificant factors that can be fixed to nominal values. For models with high-dimensional input factors, the latter is an essential part of managing database and analysis complexity. Second, surrogate models are essential for achieving UQ at scale in complex tools. Third, the overall AEDT development process benefited from conducting UQ concurrently with the tool development. Developers were able to include in the toolset the necessary software and database attributes to create a UQ-enabled tool. In return, the concurrent UQ analysis was able to identify and feed back analysis limitations, in time to have impact on the tool development. Although challenging to manage, concurrent development and UQ assessment processes bring significant benefit.

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