ARTICLE IN PRESS

Transport Policy ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

Transport Policy

journal homepage: www.elsevier.com/locate/tranpol

Uncertainty assessment of complex models with application to aviation environmental policy-making

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ARTICLE INFO

Keywords:
Uncertainty assessment
Uncertainty analysis
Sensitivity analysis
Aviation
Environment

ABSTRACT

Numerical simulation models that support decision-making and policy-making processes are often complex and involve many disciplines. These models typically have many factors of different character, such as operational, design-based, technological, and economics-based. Such factors generally contain uncertainty, which leads to uncertainty in model outputs. For such models, it is critical to both the application of model results and the future development of the model that a formal approach to the assessment of uncertainty in the model be established and carried out. In this paper, a comprehensive approach to the uncertainty assessment of complex models intended to support decision-making and policy-making processes is presented. The approach consists of seven steps, which are establishing assessment goals, documenting assumptions and limitations, documenting model factors and outputs, classifying and characterizing factor uncertainty, conducting uncertainty analysis, conducting sensitivity analysis, and presenting results. Highlights of the approach are demonstrated on a real-world model intended to estimate the impacts of aviation on climate change.

1. Introduction

The growing use of numerical simulation models in decision-making and policy-making processes, and the presence of uncertainty in all aspects of modeling, has naturally led to questions such as: What confidence does one have in model results? What can be done to improve confidence in model results? What are the limits in terms of applicability of model results? (Cacuci, 2003; Saltelli et al., 2008). *Uncertainty analysis*, which can be defined as the determination of the uncertainty in model results that derives from uncertainty in model factors (Helton et al., 2006), and *sensitivity analysis*, which can be defined as the study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in model factors (Saltelli et al., 2008), provide the answers to these questions. The process of conducting both uncertainty and sensitivity analyses is referred to as *uncertainty assessment*.

For complex models intended to support decision-making and policy-making processes, there are many techniques and approaches that can be used to direct an uncertainty assessment. This paper presents a step-by-step sampling-based probabilistic approach to uncertainty assessment that builds off the general guidelines to uncertainty assessment presented by Morgan and Henrion (1990). The focus is on the impacts of factor uncertainty, where a factor is defined here as an external input to a model and thus, model form uncertainty is not considered. Section 2 presents the step-by-step approach to uncertainty assessment recommended in this work. Section 3 demonstrates the approach on a real-world model intended to estimate the impacts of aviation on climate change, and Section 4 discusses general conclusions of this work.

2. Step-by-step approach to uncertainty assessment

Depending on the objectives of an uncertainty assessment (e.g. studying the sensitivity of model outputs in local regions of interest, determining which factors are responsible for most of the output variability, etc.), certain techniques of uncertainty and sensitivity analyses may be more relevant than others. Further, prior to engaging in an uncertainty or sensitivity analysis, it is necessary to establish the types of uncertainties present and how they should be characterized, which requires careful consideration of model factors and model outputs. Finally, once uncertainty and sensitivity analyses have been carried out, results of the analyses must be presented in a meaningful manner. Thus, a formal assessment of uncertainty should include the following steps: *Step 1:* establish the objectives of the uncertainty assessment; *Step 2:* document assumptions and limitations of

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http://dx.doi.org/10.1016/j.tranpol.2014.02.022
0967-070X © 2014 Published by Elsevier Ltd.

Please cite this article as: Allaire, D., Willcox, K., Uncertainty assessment of complex models with application to aviation environmental policy-making. Transport Policy (2014), http://dx.doi.org/10.1016/j.tranpol.2014.02.022

the model; *Step 3:* document factors and outputs of the model; *Step 4:* classify and characterize factor uncertainty; *Step 5:* conduct uncertainty analysis; *Step 6:* conduct sensitivity analysis; *Step 7:* present results. Each step, as it relates to the uncertainty assessment of models intended to support policy-making processes, is discussed in the following paragraphs.

Approach Step 1: Establish objectives. For complex models intended to support decision-making and policy-making processes, uncertainty assessment objectives should include goals based on decision-making and model development.

Typical decision-making objectives for an uncertainty assessment are such things as providing quantitative evaluation of the performance of the model relative to fidelity requirements for various analysis scenarios, and providing quantitative comparisons of various policy scenarios, taking into account uncertainty in model outputs. Typical development oriented objectives are such things as identifying gaps in functionality that significantly impact the achievement of model requirements, leading to the identification of high-priority areas for further development, and determining how factors contribute to output variability to inform future research, verification, and validation efforts.

Approach Step 2: Document assumptions. For complex models intended to support decision-making and policy-making processes, there will typically be many modeling assumptions employed, as well as inherent limitations to the model's capability. The transparent presentation of how each assumption impacts a model's performance, as well as limitations in terms of model applicability to certain classes of problems is critical to the proper application of the model.

Approach Step 3: Document factors and outputs. Given that many factors of a complex model will have some degree of variability associated with them, it is necessary to establish what is known regarding the uncertainty associated with each factor prior to determining how the uncertainty should be represented. It is also necessary to identify the outputs of the model, where here the term output refers to a model result of interest, as well as which factors influence each output. This information is necessary for determining the type of uncertainty associated with each output, which is required for the proper analysis and presentation of results.

Approach Step 4: Classify and characterize uncertainty. Uncertainty is generally classified as being either aleatory or epistemic, where aleatory uncertainties arise through natural randomness and epistemic uncertainties arise through imperfect knowledge. Some studies decompose the epistemic uncertainty into epistemic uncertainty due to modeling choices and epistemic uncertainty used in the characterization of quantities assumed to contain aleatory uncertainty (Helton, 2009). This decomposition of epistemic uncertainty leads to a hierarchical approach to uncertainty analysis, where epistemic modeling uncertainties are sampled in an outer loop, and aleatory and epistemic modeling uncertainties are sampled in an inner loop. Here however, a scenario-based approach is taken where specific realizations of epistemic modeling parameters of interest constitute a model that is used to support policy-making, and thus the models considered in this type of uncertainty assessment do not contain epistemic modeling uncertainties.

After uncertainties have been classified as either aleatory or epistemic, it is necessary to characterize the uncertainties probabilistically. This characterization should be done in a manner that is consistent, meaningful, and defensible; consistent, in that the same rules have been enforced in all uncertainty characterizations for a particular analysis; meaningful in the sense that the uncertainty characterizations allow for clear interpretation of results; and defensible in the sense that concrete reasons can be supplied for all decisions regarding the chosen uncertainty characterizations. In the context of decision-making and policy-making processes, models are typically used in ampliative reasoning, that is, problems involving drawing conclusions that are not entailed in the given premises (Ayyub and Klir, 2006). In the case of complex models, the premises are the uncertainty information associated with model factors, such as ranges and most-likely values, and the conclusions are the uncertainties associated with model outputs and any decisions made using that information. When characterizing uncertainty probabilistically, assigning a probability distribution to a given factor is in fact implying that more is known about the uncertainty associated with that factor than is known from the information at hand. The propagation of this uncertainty through a model to model outputs leads to estimates of output probability distributions, which gives the appearance of fully quantified uncertainty. Thus, it is essential that uncertainty be characterized via the *principle of maximum uncertainty*, which is used to maximize nonreliance on information not contained in premises (Ayyub and Klir, 2006).

The principle of maximum uncertainty is enforced by selecting probability distributions that maximize some measure of uncertainty. Here maximization of information entropy is recommended as it is a widely used method (Jaynes, 2003 and Ayyub and Klir, 2006), and produces consistent, meaningful, and defensible results (Allaire, 2009).

Approach Step 5: Conduct uncertainty analysis. The purpose of conducting uncertainty analysis is to determine how uncertainties in model factors propagate to uncertainties in model outputs. Such things as output means, variances, and histograms are typically the desired outcomes of this task. While there are a variety of methods available for achieving these outcomes, as noted in Section 1, the focus here is on sampling-based approaches. These methods proceed by considering a general model $f(\mathbf{x})$, where $\mathbf{x}=[X_1, X_2, \cdots, X_k]^T$ is a vector of k factors of a model. Given that model factors are viewed as random variables with associated probability distributions, the mean value of a model output can be computed from a Monte Carlo simulation as

$$\frac{1}{N}\sum_{m=1}^{N} f(\mathbf{x}^m) \to E[f(\mathbf{x})] \text{ as } N \to \infty, \tag{1}$$

where N is the number of model evaluations in the Monte Carlo simulation and $\mathbf{x}^m=[X_1^m, X_2^m, \cdots, X_k^m]^T$ denotes the mth sample realization of the random vector $\mathbf{x}$. Convergence of the sample mean in Eq. (1) to the expected value of $f(\mathbf{x})$ is guaranteed by the strong law of large numbers, and the convergence rate is $1/\sqrt{N}$, as given by the Central Limit Theorem (Grimmet and Stirzaker, 2006). Output variances and other distributional quantities can be similarly computed by Monte Carlo simulation.

Approach Step 6: Conduct sensitivity analysis. A sensitivity analysis is conducted to determine the key factors that contribute to output variability, which is critical for directing future research efforts aimed at reducing output variability in situations where the variability is so large that model results are useless for supporting decision-making. Further, knowledge of the key factors serves the purpose of a "sanity check" in terms of model verification and validation efforts. If certain anticipated key factors are not identified as major contributors to output variability, then future development efforts can focus on further model verification and validation exercises. If the identified key factors are as anticipated, further confidence in the model is gained.