Uncertainty Quantification In Predictive Modelling Of Heat Demand Using Reduced-order Grey Box Models

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Abstract

As building energy modelling becomes more sophisticated, the amount of user input and the number of parameters used to define the models continue to grow. There are numerous sources of uncertainty in these parameters especially when a modelling process is being performed before construction and commissioning. Therefore, uncertainty quantification is important in assessing and predicting the performance of complex energy systems, especially in absence of adequate experimental or real-world data.

The main aim of this research is to formulate an uncertainty framework to identify and quantify different types of uncertainties associated with reduced-order grey box energy models used in heat demand prediction of the building stock. The uncertainties are characterized and then propagated using the Monte-Carlo sampling technique. Results signify the importance of uncertainty identification and propagation within a system and thus, an integrated approach to uncertainty quantification is necessary to maintain the relevance of developed models.

Introduction

New building energy modeling tools and methodologies have been devised over the past few decades to support building professionals in their effort to optimize designs and to enhance energy performance. These tools for energy simulation have evolved into a suite of detailed physical relations, both differential and algebraic, that describe the way various disturbances (from weather, humans, control systems, etc.) influence the thermodynamic behaviour of the building itself (Eisenhower et al., 2012). The physical relationships are defined using numerous parameters, the details of which are often not available to modelers. Therefore, these parameters are either derived from the previous literature or set to default values and best educated guesses due to which the simulation results might differ significantly from the actual ones (de Wilde and Tian, 2009). Furthermore, building simulation often requires the introduction of simplifications and assumptions that adds to the differ-

ence between actual and predicted energy consumption and limits the confidence of simulation results. Hence, it is crucial to identify and quantify such uncertainties to effectively use the energy simulation results (Hopfe and Hensen, 2011).

Uncertainty analysis (UA) in building simulation is not a new concept. A common approach to conduct UA is to use a deterministic model but assign probability distributions to the uncertain input parameters. Several studies exist in literature that implement UA to quantify the uncertainties in parameters and further analyze the effect of these uncertainties on energy simulation results ((Eisenhower et al., 2012; Fu et al., 2017; Hopfe and Hensen, 2011). These studies use standard techniques of risk management in load forecasting models, for instance, the Monte Carlo (MC) technique (Fumo, 2014; Fouquier et al., 2013). Uncertainty quantification is performed by using the concepts from probability theory, for instance, assigning probability distribution functions (PDFs) to uncertain inputs. Numerical simulations are then done to identify the statistics associated with the desired outputs (Tian et al., 2018).

Uncertainty classification is often overlooked while performing UA although it is quite crucial to model each uncertainty category in a different manner. In terms of the inherent variability, the uncertainties are classified as aleatory and epistemic uncertainties (Helton et al., 2010). Aleatory uncertainty (type A uncertainty) arises due to the inherent or natural variation of the system under consideration whereas epistemic uncertainty (type B uncertainty) arises mainly due to lack of knowledge (Hayes, 2011). Differentiating between the type of uncertainty is important because they are mitigated in completely different ways. Epistemic risk is the relatively easier type to deal with as the existing gaps in knowledge can be addressed which will reduce the uncertainty. However, it is not possible to remove inherent randomness from a process. Aleatory uncertainties can be handled using past historical data with probabilistic models (Kiureghian and Ditlevsen, 2009). For instance, solar radiation data is considered as an aleatory uncertainty which can be better handled using additional obser-

vations, although it is fundamentally impossible to predict variations of future radiation patterns. An example of epistemic uncertainty would be lighting and appliance power densities. Although probabilistic frameworks are used to quantify aleatory uncertainties, epistemic uncertainties can be represented using probabilistic or non-probabilistic frameworks (Hayes, 2011). These epistemic uncertainties are modeled by defining the probability that the risk will occur, the time frame in which that probability is active, and the probability of an impact or consequence from the risk when it does occur (Dutta, 2013).

Based on the different characteristics of uncertainty, studies in the building simulation literature have proposed several classifications of uncertainty (Van Gelder et al., 2014). However, these classifications exist in a disintegrated manner without any concrete framework. A study by Silva and Ghisi (2014) classified uncertainty as model form and parametric uncertainty. Model form uncertainty incorporates all the numerical approximations, approximations due to underlying physics and other limitations of simulation software whereas parametric uncertainty includes the uncertainty associated with the values of model parameters. Another study by Huang et al. (2015) explored the different categories of parametric uncertainty. The study categorized the uncertain parameters in parametric uncertainty as design, inherent and scenario parameters. As evident from the literature, the frameworks are often disintegrated and focus on only limited aspects of uncertainty.

UA studies in the literature mostly follow a similar process of analyzing uncertainties (assigning PDFs and then performing numerical simulations using samples from the distribution) though these studies deploy different sampling algorithms to create samples from the distributions. For instance, several studies implement the random sampling method, also known as the Monte Carlo method, to select random samples from user defined PDFs (Prada et al., 2014; Kavgic et al., 2015). A study by Asadi et al. (2014) implemented the MC sampling method to generate 70,000 energy models with different input samples in order to analyse the effects of building shape on energy performance. Another sampling method, known as Latin Hypercube sampling (LHS), is a stratified sampling method that divides the range of every input variable into N segments (the specific sample size) with equal probability (Kim et al., 2014).

Most of the studies mentioned above focus on limited aspects of analyzing uncertainties. None of these uncertainty studies deal with an integrated analysis of different aspects in the quantification process of uncertainty. For instance, a majority of these studies focus on quantifying the uncertainties due to input parameters, like solar irradiation and do not take into account the uncertainty propagation amongst differ-

ent sub-models. Moreover, these studies lack an intensive classification of various uncertainties that are present in the energy models. For instance, none of the studies deal with handling aleatory and epistemic uncertainties separately.

As building energy modelling becomes more sophisticated, the amount of user input and number of parameters used to define the models continue to grow. There are numerous sources of uncertainty in these parameters. Therefore, this paper aims to systematically identify the various sources of uncertainty and develop the framework for including them in the overall uncertainty quantification. The paper addresses the uncertainty in building performance simulation using four aspects: basics of uncertainty classification, dealing with different uncertainty categories, quantifying uncertainty using appropriate metrics and analyzing the effects of uncertainty on overall simulation results.

The main aim of this research is to identify and quantify different types of uncertainties associated with reduced-order grey box energy models used in heat demand prediction of the building stock. Uncertainty analysis is performed through five major steps of probabilistic analysis that involve input uncertainty identification, uncertainty characterization, uncertainty quantification, uncertainty propagation analysis and probabilistic performance assessment.

The paper is structured as follows: Section II describes the devised methodology of uncertainty quantification in energy systems. A case study to implement the methodology is discussed in Section III. Section IV mentions the analysis of results and the subsequent discussions. Conclusions and future work are presented in Section V.

Background

Sources of Uncertainty

On the whole, the various sources and categories of uncertainty identified in the risk management literature can be classified into one of these four categories: epistemic uncertainty, aleatory uncertainty, linguistic uncertainty and decision uncertainty. As mentioned in the Introduction, epistemic uncertainty is the uncertainty associated with knowledge while aleatory uncertainty is the uncertainty associated with diversity or heterogeneity and cannot be eliminated with additional research or observation. Epistemic and aleatory uncertainties are quite prominent in the uncertainty analysis of building performance simulation (Titikpina et al., 2015). The other two categories mainly prevail at the pre and post simulation level and are disconnected from epistemic and aleatory uncertainties. Fig. 1 illustrates the four broad categories of uncertainty.

As aleatory and epistemic uncertainties are crucial in building simulation, we will only discuss in detail

Figure 1: Different categories of uncertainties. Out of the four, epistemic and aleatory uncertainties are relevant in building energy simulation.

the uncertainty categorization for these two uncertainties. The two categories can be further classified as follows:

Aleatory Uncertainty

Aleatory uncertainty is a direct result of randomness in any process or system variables. We identified and classified demographic variations and inherent randomness as the two main sources that may result in aleatory uncertainty. In building simulation, demographic variations largely relate with the user behavior as people respond to heat transfer mechanism differently. Occupancy profiles and weather data are linked to inherent randomness as there is never enough information to reliably make any future predictions (Regan et al., 2002).

The above mentioned categorizations can only be characterized and propagated using risk assessment techniques. These uncertainties can never be minimized. Furthermore, it is fairly important to correctly identify the data used to represent the randomness in the dynamics of the process.

Epistemic Uncertainty

As aptly stated by Hayes (2011), Epistemic uncertainty stems from the lack of data, understanding and knowledge about the world. We identified and classified the parametric, structural, algorithmic, experimental and interpolation uncertainties as the main sources that may result in epistemic uncertainty. Parametric uncertainty arises due to uncertain model parameters, for instance, material properties. Structural uncertainty results due to an inaccurate description of the underlying physics in the model. For instance, building heat transfer is usually considered as a 1D phenomenon when the buildings are modeled using grey-box networks. Algorithmic uncertainty results out of the trade-offs between accuracy and computational efficiency in building energy models. For instance, lumped parameter models introduce the algorithmic uncertainty in the simulation results. Experimental uncertainty is purely obser-

vational and arises due to variability in experimental measurements. For instance, the measured data used to calibrate grey-box networks will always possess some sort of experimental uncertainty. Interpolation uncertainty kicks in whenever there is a lack of data associated with simulation models. To predict the missing data, it is often necessary to interpolate or extrapolate using some assumptions or approximations that introduce the uncertainty in simulation results.

Treating Different Classes of Uncertainties

Numerous methods exist to characterize, treat and propagate epistemic and aleatory uncertainties. We have classified the methods based on the availability or non-availability of data.

Aleatory uncertainties can easily be represented in a probabilistic framework, for instance, using probability theory. The probability theory is defined as follows:

Let X be a random discrete variable. A probability mass function can be defined as:

$$f(x_i) \geq 0; \sum f(x_i) = 1; f(x_i) = p(x = x_i) \quad (1)$$

The cumulative distribution function of a discrete random variable X , denoted as $F(x)$, is

$$F(x) = P(X \leq x) = \sum_{x \leq x_i} f(x_i) \quad (2)$$

Let X be a continuous random variable. A probability distribution function is a non-negative function f , which satisfies

$$P(X \in B) = \int_B f(x) dx \quad (3)$$

for every subset B of the real line.

As X must assume some value, f must satisfy

$$P(X \in (-\infty, \infty)) = \int_{-\infty}^{\infty} f(x) dx = 1 \quad (4)$$

This means the entire area under the graph of the PDF must be equal to a unit. In particular, the probability that the value of X falls within an interval $[a, b]$ is

$$P(a \leq X \leq b) = \int_a^b f(x) dx \quad (5)$$

Epistemic uncertainty can be represented in many ways, including, probability theory, fuzzy sets, second-order probability, and imprecise probability. The problem of selecting an appropriate mathematical structure to represent epistemic uncertainties is usually challenging (Swiler et al., 2009).

Methodology

The performance assessment of a complex energy system involves the use of numerous analysis models,

Figure 2: Steps in the uncertainty analysis framework.

each with its own assumptions and approximations. Thus it is necessary to systematically identify the various sources of uncertainty and develop the framework for including these uncertainties in the overall uncertainty quantification. The research conducted in this paper deals with different aspects of uncertainty existing in a system and thus focuses on a novel integrated approach to uncertainty. The novelty lies in the classification and quantification of different classes of uncertainty sources. We conducted the uncertainty analysis using the five basic steps of constructing an uncertainty framework as detailed below (Fig. 2).

Uncertainty Analysis

Uncertainty Source Identification: This step involves the identification of the most prominent sources of uncertainty prevailing in a system under study. For instance, in a typical building simulation, uncertainties can arise due to weather data, building envelope, HVAC systems or occupant behavior.

Uncertainty Characterization: This step is the most crucial step in the entire uncertainty framework. All uncertainties in the simulation need to be characterized before any analysis is performed to quantify the uncertainties. This step includes the identification and subsequent classification of uncertainties in the system. Therefore, we separated the parameters that result in aleatory uncertainties from the ones causing epistemic uncertainties. For instance, weather data is put into the category of aleatory uncertainty while grey-box parameter values are put into the category of epistemic uncertainty. We also sorted out the uncertainties based on availability or non-availability of data.

Uncertainty Quantification: This step involves the quantification of the characterized uncertainties. We quantified the aleatory uncertainties using the probability distribution framework. Appropriate distributions for aleatory uncertainties are identified using an automated procedure (in Minitab® 18) that compares the available data with all possible distributions and gives the best fit PDF based on some criterion. Possible criteria include the negative log-likelihood (Eq. 6), Bayesian Information Criterion (BIC) (Eq. 7), Akaike Information Criterion (AIC) (Eq. 8) and AIC with a correction for finite sample size (AICc)

(Eq. 9).

$$-\log \mathcal{L}(\theta|x) = -\log \prod_{i=1}^{\infty} f(X_i|\theta) \quad (6)$$

$$BIC = -2\log \mathcal{L}(\theta|x) + k * \log(n) \quad (7)$$

$$AIC = -2\log \mathcal{L}(\theta|x) + 2k \quad (8)$$

$$AICc = AIC + \frac{2k(k+1)}{n-k-1} \quad (9)$$

θ denotes the parameters of the probability distribution and is determined using maximum likelihood estimation. $X_1, \dots, X_n$ denotes the observed data and are assumed to be independent and identically distributed. n is the number of observations and k is the number of parameters to be estimated. For instance, if the probability distribution under consideration is the normal distribution, then $k = 2$ and $\theta = (\mu, \sigma)$ since the normal distribution is defined by two parameters, mean (μ) and standard deviation (σ). Given $X_1, \dots, X_n$ maximum likelihood estimation maximizes $\mathcal{L}(\theta|x)$ over all possible θ .

For continuous parameters, we characterized the ranges of variation by PDFs bounded by upper 95th and lower 5th probability threshold values (Hayes, 2011). We characterized the discrete variables by minimum, maximum and base-case values. For this study, each set of observed data is fitted to 14 continuous PDFs or 2 discrete PDFs accordingly. The different PDFs for continuous variables used include normal, uniform, Cauchy, t, F, Chi-square, exponential, Weibull, log-normal, gamma, double-exponential, power normal, power log-normal and beta distributions. Binomial and Poisson distributions are used for discrete variables. The probability distribution that gives the minimum negative log-likelihood is selected and used to generate inputs to the building energy model.

We implemented the second-order probability approach to quantify and propagate the epistemic uncertainties. The advantage of this approach over the others is that it enables the separation of aleatory vs epistemic uncertainty. This approach implements an

outer and an inner loop. We specified the epistemic variables in the outer loop as intervals on parameter values (means or standard deviations of uncertain variables). A particular value is then selected from within the specified intervals and sent to the inner loop. In the inner loop, the values of the distribution parameters are set by particular realizations of the epistemic variables, and the inner loop performs sampling on the aleatory variables in the usual way. In this fashion, we generate families or ensembles of response distributions, where each distribution represents the uncertainty generated by sampling over the aleatory variables. Plotting an entire ensemble of cumulative distribution functions (CDFs) in a horsetail plot allows to visualize the upper and lower bounds on the family of distributions.

For instance, weather data is quantified using PDFs while the model parameters are quantified using second-order probability method.

Uncertainty Propagation: Simulations are performed in this step using a sampling based technique. This method of uncertainty propagation is termed as external uncertainty propagation and has the ability to maintain a well validated model. We implemented the MC-based simulation in this study as the method is very intuitive and offers easy implementation over the other methods.

Probabilistic Performance Assessment: This step concludes the uncertainty analysis framework and involves the presentation of probabilistic model predictions using numerical indicators, such as mean, median, standard deviation etc. or using typical graphical methods, for instance, histograms, box plots, density plots etc. We assessed the dynamic building behavior using time-series energy plots. We also used box plots to show the variations of time series energy data.

The workflow of the framework is depicted in Fig. 3 and can be summarised by the following steps:

1. Determine the source of uncertainty in the building simulation model.
2. For every source of uncertainty; Characterize and segregate based on inherent randomness (aleatory) or lack of knowledge (epistemic). Check whether observed data is available, if yes, assign best-fit PDFs to the sources of aleatory uncertainty and intervals to the sources of epistemic uncertainty. If observed data is unavailable, use previous literature and expert judgement to assign PDFs to aleatory uncertainties and intervals to epistemic uncertainties. Previous literature and expert judgement might include case studies, current standards, etc.
3. Generate random samples and perform simulations with these samples as inputs to the building energy model.
4. Analyze the results.

Figure 3: Workflow of the uncertainty analysis framework.

Case Study

To demonstrate the application of the devised framework, an administrative building connected to the district heating network at University College Dublin's (UCD) campus is analyzed for uncertainty in heat demand predictions. The building occupies an area of 3390 m². The outer walls of the building consist of brick blocks insulated according to Building Regulations 2000 (Office, 2000). The building rests on an insulated floor slab consisting of 30 mm insulation and 150 mm of cast concrete. Windows constitute of approximately 42% of the external wall area. The building interiors consist of a large office area with small cubicles on the ground floor while the first and second floors consist of individual offices and meeting rooms. The roof is flat and insulated according to Building Regulations 2000. The occupancy pattern follows a typical 9AM - 5PM office schedule. Measured energy consumption on 15 minute basis is available for this building. The building is modeled using a second order reduced grey-box RC network as shown in Fig. 4. We calibrated the RC network using CTSM-R to obtain the model parameters.

We initiated the uncertainty analysis according to the steps identified in the framework as follows:

Sources of Uncertainty: We first identified the different sources of uncertainty in our simulation model. Considering our simulation model, the sources of uncertainties include the solar radiation data, ambient temperature, grey-box model parameters (thermal resistances, R and heat capacities, C), infiltration rates, and lighting and equipment heat gains. There can be other sources of uncertainties such as building age-

Figure 4: Second order grey-box RC network used for energy simulations. C_i and C_e represent the internal and external heat capacities. ϕ_h and ϕ_s represent the radiator and solar radiation fluxes. R_{ea} and R_{ie} represent the thermal resistances. T_i and T_e represent the internal and external temperature states. A_w represents the effective window area.

ing etc. but these are considered to stay constant as these will require historical building data which is not available for the building. Moreover, while calibrating the grey-box network, these uncertainties are indirectly accounted for in the analysis.

Uncertainty Characterization: The next step involved the characterization of uncertainties identified in the previous step. Due to the inherent randomness in their nature, solar irradiation data and ambient temperatures are put into the aleatory uncertainty category. Uncertainties, such as, grey-box model parameters (thermal resistances, R and heat capacities, C), infiltration rates, lighting and equipment heat gains are characterized as epistemic uncertainties as these can be improved by collecting more information or taking detailed measurements.

Uncertainty Quantification: The uncertainties are then quantified using PDFs for aleatory uncertainties and second-order probability for epistemic uncertainties. We used the Minitab software to identify PDFs that closely relate to the uncertain parameter. The different PDFs for continuous variables used include normal, uniform, Cauchy, t , F , Chi-square, exponential, Weibull, log-normal, gamma, double-exponential, power normal, power log-normal and beta distributions. Binomial and Poisson distributions are used for discrete variables (de Wilde and Tian, 2009). We also assigned intervals to epistemic sources of uncertainties. The intervals are derived from relevant literature in the uncertainty analysis domain.

Uncertainty propagation: We implemented the MC sampling-based simulation to deal with different types of probability functions of input variables. The energy simulations are performed in Dymola to obtain the heat load demand for the administrative building at UCD using a second order RC network as shown in Fig. 4. The network is calibrated using building's heat demand, internal temperature profile, ambient temperature, and solar irradiance to obtain the values of C_i , C_e , R_{ea} and R_{ie} . The formulated network is then used to predict the heat demand. The heat

demand is analyzed for a particular working day in the month of February at an hourly level. We performed the MC simulations using the Design library in Dymola.

Probabilistic Performance Assessment: We obtained the time series and box plots for the heat load demand. The plots represent the variations in heat demand due to different uncertainty sources and are discussed in the Results and Discussion section.

Results and Discussion

Figure 5: Formulated PDF of ambient temperature for the month of February.

This section describes the results of uncertainty quantification and uncertainty propagation. The uncertainty quantification results (PDF and intervals identification) are listed in Table 1. The PDF of ambient temperature for the month of February is depicted in Fig. 5 and closely follows a Weibull 3-parameter distribution. It is crucial to note that wide monthly and yearly variations occur in the ambient temperature and as such, many years of observed data are required to make a reasonable conclusion about the associated PDF. To obtain the PDF in this study, we used 10 past years of weather data to obtain the PDFs. Similarly, we obtained PDFs for global solar radiation. For rest of the variables, intervals are assigned based on past literature and expert judgement.

The baseline simulated and measured hourly heat demand patterns are depicted in Fig. 6. The variations in the pattern (within $\pm 10\%$) arises due to several un-

Figure 6: Measured and simulated heat demand under uncertainty for the administrative building.

Table 1: Uncertainty quantification results for different sources of uncertainties. PDFs are listed with their associated distribution parameters. Intervals are listed with the confidence limits.

Uncertainty Source	PDFs with parameters	Intervals with limits	Method
Ambient temperature	Weibull (Shape: 23.77 K, Scale: 68.73 K, Threshold: 211.73 K)		PDF identification using data
Global Solar Radiation	Logistic (location: 37.83 Wh/m^2 , Scale: 48.06 Wh/m^2)		PDF identification using data
Thermal Resistance		R_{ea} : 11.153 ± 0.010 $^{\circ}C/kW$, R_{ie} : 49.81 ± 0.007 $^{\circ}C/kW$	Model Calibration
Thermal Capacitance		C_e : 1.048 ± 0.012 $kWh/^{\circ}C$, C_i : 17.57 ± 0.052 $kWh/^{\circ}C$	Model Calibration
Equipment and Lighting Heat Gain		14 - 24 W/m^2	Literature (de Wilde and Tian, 2009)
Infiltration		0.1 - 0.25 ACH	Literature (Tian et al., 2018)

Figure 7: Hourly heat demand PDFs of the simulated and measured consumption values.

certain parameters. We then performed several simulations using the MC based sampling technique to identify the distribution of hourly heat demand (Fig. 7). As clearly depicted in Fig. 7, the difference in the PDFs arises due to the combined effects of multiple operation parameters (aleatory and epistemic).

We used box plots to identify the effects of aleatory and epistemic uncertainties on the daily heat energy consumption values (Fig. 8).

Figure 8: Variations in the daily energy consumption data due to different uncertainty sources.

Epistemic uncertainties produce a larger proportion of variations in the predicted energy consumption when compared to aleatory uncertainties and hence, play a significant role in grey box model uncertainty quantification.

Conclusions and Future Work

As new design ideas push the envelope of building performance, their performance evaluation needs to be justified by building energy simulation. Studies in literature have established that deterministic model predictions only provide limited confidence in any building's energy performance reaching a certain level. It has become crucial to investigate the accuracy, validity and relevance of the developed models for building simulation. As these models involve several thousands of input parameters, the uncertainty introduced by each one of them can invalidate the entire simulation result. Therefore, the need for uncertainty analysis in building simulation is quite evident.

The research conducted in this study proposes an uncertainty analysis framework to effectively recognize, identify, characterize and quantify the different sources of uncertainty in building energy simulation. The proposed framework includes five major steps to perform uncertainty analysis, namely, uncertainty source identification, uncertainty characterization, uncertainty quantification, uncertainty propagation and probabilistic performance assessment. The framework stresses on the importance of uncertainty characterization as every uncertainty needs to be treated in a different manner. The devised framework will provide a firm foundation for performing different types of uncertainty analysis, and eventually enhance the quality of building energy simulations.

This study could be extended to include several other aspects of uncertainty in building energy simulation. Future work to this study could include the compar-

ison of different sampling techniques to generate the uncertainty results. Also, the different approaches to quantify epistemic uncertainties could be compared to investigate their effectiveness in representing the underlying uncertainties in parameters.

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