Characterizing Material Emissivity Uncertainty in Fire Environments for Computational Simulation

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Abstract

As the mathematical basis and implementation of uncertainty quantification methods for forward propagation have continued to be developed and refined, their use in physics-based simulations has increased. In order to increase the value of the information generated from uncertainty quantification studies, we now consider the quality of the uncertainty characterizations that are propagated forward. This work focuses on developing a defensible, physics-based uncertainty characterization approach for material surface emissivities of engineered systems in fire environments. The characterization approach is meant to act as an analyst’s fallback standard for situations with minimal available information. Within the fire environments of interest, material surfaces may be within the system or facing away from the fire, and experience relatively lower temperatures. In those cases the uncertainty in the emissivity of a material surfaces may be primary driven by aleatory uncertainty from processes used to generate the material or different sources of the material, as well as measurement uncertainty. Other surfaces on the system may be directly exposed to the fire, and experience high temperatures and physical phenomena including oxidation and sooting that can drastically change emissivity. While such phenomena would ideally be captured with a physics model, this is often not the case due to the simulations’ fidelity and thus must be captured as an epistemic uncertainty source. In order to capture these independent sources of uncertainty, a multi-piece uncertainty model with temperature dependence was developed. The impact of this uncertainty characterization approach is demonstrated on a simple example, and the implications on large system models in complex fire environments will be discussed. Confidence in information gained from uncertainty quantification studies can only be as high as the confidence placed on the input uncertainty characterizations utilized.

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Outline

High Level Motivation

Thermal Modeling Application
  • Uncertainty Characterization Challenge

Proposed Methodology
  • Two Possible Forms Provided

Compare Methodology with Challenge

Apply Methodology to Representative Finite Element Problem

Conclusions
ModSim Generating Evidence to Support Decision Making

- Application Driver
- Planning
- Experiment Design, Execution & Analysis
- Code Verification
- Solution Verification
- Metrics
- Validation Assessment
- Model Prediction & Credibility
- Document and Communicate

Analysis Execution and V&V Activities
High Level Motivation

Common V&V Activities:
- Select Quantities of Interest (QoI)
- **Characterize model input uncertainty sources**
- Propagate uncertainty sources (UQ)
- Determine validation metrics
- Assess validation comparison
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Challenges:
- Large number of uncertain parameters
- Limited resources (time, budget)
  - Literature search
  - Experiments
- Surprisingly limited availability of this type of information
Motivating Thermal Modeling Application

Abnormal Thermal Environments – Fires
- Common thermal analysis at Sandia is assessing safety of engineered system in accident scenarios that may include fire.
  - *Collaborators for this work are from a range of projects.*
- Fires bring high heat fluxes, can significantly change the local atmosphere, and cause significant damage.
- Dominant heat transfer modes can change throughout the event.

Model Input Uncertainties
- Thermal properties changing as function of temperature.
- Emissivity may changes due to alterations to the surface.
  - Soot deposition
  - Oxidation
  - Organic films

Fig. Example of fire impacting engineered system. [1]
Emissivity can drastically change in fire environments. Yet, analysts often have minimal information about how the surface changes.

- Common to have single value for room temperature;
- Or measurement pre- and post-test.
- Accident scenarios are often stochastic leading to variability in effects such as sooting.
  - *We don’t want to just capture an experiment, but the full range of possibilities.*
- Evolution of emissivity will impact system’s internal thermal conditions.

Fig. Compilation of Inconel 600 emissivity values for a range of temperatures. [2-5]
Proposed Methodology

\[ \tilde{\varepsilon} = \varepsilon + X_\alpha \alpha + X_\beta \beta \]

- **\( \tilde{\varepsilon} \)** - Perturbed emissivity value
- **\( \varepsilon \)** - Nominal emissivity definition
  - Constant or \( f(T) \)
- **\( \alpha \)** - Nominal uncertainty term for non-fire related uncertainty sources
  - Surface finish, material variability, measurement uncertainties (aleatory)
  - Constant or \( f(T) \)
- **\( \beta \)** - Nominal uncertainty term for fire related uncertainty sources
  - \( f(T) \), sooting, oxidation (epistemic)
  - Functional form depends on application, 2 possible forms suggested
- **\( X_\alpha, X_\beta \)** - Multiplicative standardized uncertainty terms
  - Sampled for UQ/validation/sensitivity studies
Physics-Inspired Beta

\[ \beta_\varepsilon (T) = 1 - \frac{\overline{T}^4 - T^4}{\overline{T}^4} \]

Inspired by radiation transport

- User specified Dirichlet boundary condition
  - e.g., 1000°C for a fully engulfing hydrocarbon fuel fire

Fig. Functional behavior of physics-inspired β form over a temperature range relevant to fire environments.
Sigmoidal Beta

Designed to allow greater functional flexibility, but requires additional parameter assignments.

\[ \beta_S = \frac{\gamma}{1 + e^{-k(T - T_0)}} \]

\( \gamma \) - Asymptote value

\( k \) - Rate of transition

\( T_0 \) - Transition point

Fig. Illustrating range of functional behaviors of sigmoidal Beta form over temperature range relevant to fire environments. Impacts of a) Varying \( \gamma \), b) varying \( k \) and c) varying \( T_0 \).
Stainless steel is a common material encountered in engineered systems of interest.

Emissivity is clearly a function of oxidation state, surface finish, and any machining.

Even if initial emissivity is known, a wide/evolving range of potential values could occur in oxidizing fire environments.
Applied proposed uncertainty characterization method to stainless steel example dataset.

\[ \tilde{\varepsilon} = \varepsilon + X_\alpha \alpha + X_\beta \beta \]

\[ \beta_\varepsilon (T = 1283K) \]
\[ \beta_S (T_0 = 900K, \gamma = 0.6, k = 0.01) \]
\[ \alpha = 0.07 \]
\[ X_\alpha = [-1, 1] \]
\[ X_\beta = [0, 1] \]

Analyst subject matter expertise applied.

- Increased oxidation of SS deemed unlikely to reduce emissivity; lower bound set based on \( \alpha \)
- Upper bound set to physical bound (1)

Fig. Comparing proposed emissivity uncertainty ranges with values for stainless steel of various surface conditions. [6]
Application Example

Metal box inside fully-engulfing, oxidizing fire environment (1000°C) for 600 seconds.

Quantity of interest will be thermocouple reading at location on inside surface of box face.

Analyst provided single room temperature emissivity value of 0.3.

Apply proposed methodology with both forms of $\beta$.

Fig. a) Cube geometry in fully engulfing fire environment, b) quantity of interest
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Fig. Emissivity as a function of temperature using $\beta_\varepsilon$ with $T_o=1000^\circ$C and $\beta_S$ with $\gamma=0.44$, $k=0.01$ and $T_o=600^\circ$C. $\alpha_{X_\varepsilon}=\pm 0.06$ and $X_\beta=\pm 20\%$ for both versions.
Applications Example

80 incremental Latin hypercube samples used to propagate $X_\alpha$ and $X_\beta$ uncertainties.

Proposed methodology compared with simple multiplicative uncertainty of $\pm 20\%$.

Results demonstrate that neglecting epistemic uncertainty due to fire’s impact on the surface can cause underprediction of both the mean and uncertainty.

- Decision makers could be misinformed.
- Analyst judgment on selection of $\beta$ form will impact outcome.

Fig. Comparing 95% confidence bounds predicted over time using proposed methodology, with different forms of $\beta$, against a simple multiplicative uncertainty approach.
Conclusions

Characterizing uncertainty sources is an important step of the V&V process that is often neglected.

We proposed a means of characterizing emissivity uncertainty in fire environments.

\[ \tilde{\varepsilon} = \varepsilon + X_\alpha \alpha + X_\beta \beta \]

Approach separates and addresses both measurement and fire related uncertainty sources

- Two versions of beta were proposed, but analyst should select what best represents their application
- Analyst modification of equation to best fit application is advocated

Approach is physics informed, but could eventually be replaced by including the additional (expensive) physics currently missing

- Meant for sparse data situations; use data if available.


Questions?

Feel free to email comments / questions:
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