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Systematic validation of non-equilibrium thermochemical models using Bayesian inference

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ABSTRACT

The validation process proposed by Babuška et al. [1] is applied to thermochemical models describing post-shock flow conditions. In this validation approach, experimental data is involved only in the calibration of the models, and the decision process is based on quantities of interest (QoIs) predicted on scenarios that are not necessarily amenable experimentally. Moreover, uncertainties present in the experimental data, as well as those resulting from an incomplete physical model description, are propagated to the QoIs. We investigate four commonly used thermochemical models: a one-temperature model (which assumes thermal equilibrium among all inner modes), and two-temperature models developed by Macheret et al. [2], Marrone and Treanor [3], and Park [4]. Up to 16 uncertain parameters are estimated using Bayesian updating based on the latest absolute volumetric radiance data collected at the Electric Arc Shock Tube (EAST) installed inside the NASA Ames Research Center. Following the solution of the *inverse* problems, the *forward* problems are solved in order to predict the radiative heat flux, QoI, and examine the validity of these models. Our results show that all four models are invalid, but for different reasons: the one-temperature model simply fails to reproduce the data while the two-temperature models exhibit unacceptably large uncertainties in the QoI predictions.

1. Introduction

The National Aeronautics and Space Administration (NASA) is presently in the midst of an extensive experimental testing program to support development of the next generation of space vehicles. While the essential elements of the evolving design are based on Apollo-era concepts, the Multi Purpose Crew Vehicle (MPCV) – commonly known as the Crew Exploration Vehicle (CEV) – will be substantially larger than the Apollo capsule. The heating environment experienced during atmospheric entry will therefore be significantly different. In particular, the radiative component of heating will become more significant.

One critical issue that needs to be addressed during the design of an atmospheric entry vehicle is the accurate prediction of the recession rate of the thermal protection system (TPS), which is strongly dependent on the wall heating. In particular, at high reentry speeds, a significant portion of the heating experienced by the spacecraft can be due to radiation. Radiation

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is highly sensitive to the concentration of the gas species and distribution of their internal energy level populations. Hence, accurate prediction of the radiative heating is strongly influenced by thermal and chemical relaxation models. A number of physical models describing the evolution of concentration of gas species and the distribution of their internal energy level populations can be found in the literature. For engineering applications, single temperature or multi-temperature models (e.g. two temperature models) are usually considered for the design of TPS. The predictions provided by these physical models are inherently uncertain due to the limited state of our knowledge, the lack of experimental data at the specific flight conditions, and the complexity of the physics involved. Both types of models contain many model parameters, which need to be calibrated and whose uncertainties have to be quantified.

The main objectives here are (1) to quantify the prediction uncertainties resulting from the use of four different thermochemical models: one single-temperature model and three multi-temperature models, after a detailed calibration of the uncertain parameters and (2) to assess the validity of each of these models by using the proposed calibration, validation, and prediction processes and the data acquired at NASA Ames Research Center.

The classical process for model validation in science is related to data fitting: the closer the values computed by a model are to values measured in experiments, the better the model is considered to be. However, very often, the measured quantities from experiments are not necessarily connected to the QoI (e.g., the radiative flux in this study) and this results in a validation process that fails to take into account the QoI or the scenario at which one uses the model to make a particular prediction. In contrast, our point of view lies in the fact that propagation of uncertainties to the final prediction constitutes an important step in the validation of a given model. An alternative and systematic methodology for the validation of physical models under uncertainty has been proposed in [1]. It involves a statistical-based approach for the calibration of uncertain model parameters, the validation of the model itself, and the quantification of uncertainty associated with specific model predictions. It requires the use of experimental data for parameter calibration and model validation and ultimately appeals to expert opinion, through the definition of tolerances, for the interpretation of the results, i.e. a model is considered not invalid if, in view of the above-mentioned statistical process, one considers that it is capable of providing reliable predictions of QoIs under specific prediction scenarios. Otherwise, the model is deemed invalid. Estimation of the model parameters is carried out by solving an *inverse problem* based on Bayesian inference. Starting from a prior probability density function of the parameters, defined based on available information and belief about the parameters, and the likelihood function, that describes the probability that the model predicts observed (experimental) data for given values of the parameters, one can compute from Bayes' theorem the posterior probability density function (pdf) of the model parameters. Calculation of *posterior* pdf's for some uncertain model parameters of the single- and multi-temperature models is one focus of this investigation. Solution of the *forward problem* consists then in evaluating how uncertainties in the model parameters propagate onto the QoI(s) for a given prediction scenario.

The paper is organized as follows. The validation process is briefly illustrated on an abstract mathematical model in Section 2. The single- and two-temperature models are introduced in Section 3 while the treatment of uncertainties is briefly discussed in Section 4. A brief description of the data is also provided in that section. Finally, the numerical results obtained from the proposed validation procedure are presented in Section 5. The paper finishes with concluding remarks and a discussion about future work.

2. Brief description of the validation process

Predictive computational modeling for physical events presumes that observational data be acquired for the calibration and validation of models for simple scenarios of the theory. However, in addition, one needs to consider as well the predictive scenario, for which observational data may be unavailable and for which one hopes to be able to use the model to predict a given quantity of interest. We briefly describe below the calibration, validation, and prediction processes, in an abstract manner, as shown in Fig. 2, and based on the work presented in [5,6]. Other approaches for model validation in scientific computing have been proposed in [7,8] and in the references therein.

For the purpose of this presentation, we consider an abstract model problem that consists in finding the solution u such that:

$$\mathcal{A}(\boldsymbol{\theta}, S, u(\boldsymbol{\theta}, S)) = 0 \tag{1}$$

where $\mathcal{A}$ is an operator representing the model, usually in the form of partial differential equations and boundary conditions, $\boldsymbol{\theta}$ is a vector of model parameters that are unknown and need to be identified with respect to given data, and S denotes a scenario characterizing either an experimental setting or the prediction problem of interest. The scenario is described by input parameters such as the dimensions of the computational domain, the value of the forcing term, or boundary data. We also assume that the ultimate goal in using above model is to predict a quantity of interest $Q_p(u)$ on a scenario S_p, the so-called prediction scenario. The validation process consists of the following three stages: calibration, re-calibration, and model assessment.

Calibration. A first set of calibration scenarios S_c is considered in order to provide observables represented by data D_c (training set). One then needs:

1) to provide the prior probability density function $\pi_c(\boldsymbol{\theta})$ for the parameters based on available information and prior knowledge,