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Integrated data-model analysis facilitated by an Instrumental Model

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Abstract

A paradigm is described and demonstrated for rigorously evaluating model-versus-data agreement while extracting new insights for improving the model and experiment. "Bound-to-Bound Data Collaboration" (B2B-DC) is augmented with an Instrumental Model, integrating uncertainty quantification of the reactor model, chemical model, and data analysis. The subject of analysis is a fuel-lean $C_2H_2/O_2/Ar$ premixed laminar flat flame, mapped with VUV-photoionization molecular-beam mass spectrometry at the Advanced Light Source of Lawrence Berkeley National Laboratory. Experimental signals were modeled with a CHEMKIN flame code augmented with an Instrumental Model. Consistency of the model and raw experimental data are determined as a quantitative measure of their agreement. Features of the mole-fraction profiles are predicted for O, OH, C_2H_3, and background contributions to H_2O measurements. Also computed are posterior distributions of the initial targets and model parameters, as well as their correlations. This approach to model-versus-data assessment promises to advance the science and practical utility of modeling, establishing validity rigorously while identifying and ranking the impacts of specific model and data uncertainties for model and data improvements.
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Keywords: Uncertainty quantification; Model validation; Premixed flame; Data Collaboration; Instrumental Model

1. Introduction

Numerical modeling of combustion data has become a valuable tool for technology and science, yielding design and intellectual insights from "proven" physical and chemical models. The ideal proof is agreement of predictions with data from a range of reactors and conditions, but there are uncertainties in both the predictions and the data.

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The goal of developing uncertainty-quantified (UQ) predictive models [1,2] has become broadly accepted. In combustion chemistry, the UQ emphasis has been accuracy of the kinetic-model parameters (species thermochemistry, transport, kinetics). Uncertainty in combustor data is usually acknowledged, but mainly as a way of explaining apparent deviations of the predictions. We rely on data being accurate, if slightly imprecise.

Conventional testing of model agreement uses processed experimental data, such as species concentrations, which are obtained from raw data like pulse counts, currents, and voltages. As a result, in addition to raw-data aleatoric (statistical) uncertainty, analyzed data acquire epistemic (systematic, nonstatistical) uncertainties introduced via data-analysis assumptions and parameters. Some data analyses may be very precise, like spatial position from the turns of a precision-screw drive, while others may be much more uncertain, such as from factor-of-two calibration factors.

The present work provides a richer, more rigorous paradigm. Rather than simply observing model-data agreement or disagreement, it offers mathematical proofs that no points exist outside an interval where model and data are consistent, as well as insights into the extent of agreement, the sources of apparent disagreement, and specific further research needed to improve the models and the measurements. The key is to unify analysis of uncertainties from the physico-chemical combustion-experiment model and from the data processing, itself a model.

Benefits of such a more-direct analysis, extending model predictions to the actual experimental observables, have been noted in the past [3,4]. A formal way of analysis can be accomplished through an *Instrumental Function* [5], reversing the raw-data analysis and thus transforming modeled variables into directly measured quantities. Incorporating uncertainties of the data-analysis parameters broadens the concept to an Instrumental Model (IM), demonstrated in previous work [6] connecting shock-tube species concentration (a derived property) with the photodiode voltage (raw data) generated by laser light transmitted across the shock tube. To examine and demonstrate the benefits of the Instrumental-Model approach, here we turn to a more complex system, premixed laminar flat-flame data mapped with molecular-beam mass spectrometry.

2. Outline of the analysis protocol

One of the distinguishing features of the analysis presented here is that flame modeling is fully imbedded into the data analysis. In doing so, both measurements and modeling are intertwined into a single UQ analysis, and the extent of the agreement or disagreement is evaluated through rigorous UQ quantifiers rather than by comparison between the numerically simulated and data-based concentrations.

The general protocol of the approach is outlined first and applied and clarified in the subsequent sections and examples. A full model is developed, including both a proposed reaction mechanism (reactions, thermochemistry, kinetics, transport properties) and the Instrumental Model. From the flame measurements, particular features, referred to as *targets*, are chosen. For each experimental target, we identified model parameters that most influence the target value, referred to as *active variables*, and evaluated their respective ranges of uncertainties. Thus, another distinguishing feature of the analysis is that we do not necessarily rely on the parameter values but rather on realistically assessed parameter bounds.

Active variables in this protocol are from both the reaction and Instrumental Models. In addition, the Instrumental Model employs state variables of the reaction model. Thus, the flame model is integrated with processing of the experimental data.

For each target, a *surrogate model* is built, an algebraic representation of the relationship among active variables and the modeled target value. The purpose of surrogate models is to replace solving the flame differential equations with faster-evaluating functions. This approach speeds up function evaluation of the UQ analysis, and in the present case, it also allows use of more resourceful mathematical algorithms.

The composed data-model system is referred to as a *dataset*. The first question to pose is whether there exists at least one combination of active-variable values, all within their respective uncertainty bounds, such that the computed target values are reproduced within their respective uncertainty ranges. If such a point exists, the dataset is *consistent*, otherwise, the dataset is *inconsistent*. If the dataset is consistent, the entire collection of such allowable points, referred to as the *Feasible Set*, is examined to determine the range of variation of a given target when the model parameters are constrained to the Feasible Set. Such predictions can be made for active variables, dataset targets, as well as for a priori unmeasured targets, referred to as *blind predictions*. Further analysis is performed by sampling the Feasible Set, which produces *posterior distributions* for active variables and targets, along with the correlations among them.

3. Experimental data

3.1. Flame

This study employs data from a near-stoichiometric acetylene flat flame: equivalence ratio ϕ

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