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A paradigm shift in the interaction of experiments and computations in combustion research

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Abstract

A different approach to comparing experimental data and numerical simulation data is presented. Traditionally, when making comparisons with simulations, experimentalists have sought to measure the same fundamental quantities (e.g., mole fractions) that are output by numerical simulations. This approach often requires measurement of many variables to arrive at the desired quantity, and uncertainty may accumulate with each additional measurement. Because recent advances in computational resources have led to more detailed numerical models, more complete information is available within simulations. This allows for the possibility of using simulation results to derive predictions of measured signals (i.e., "computed signals") rather than measuring many quantities to derive a single fundamental quantity. Three examples of comparing measured and computed signals are presented: NO laser-induced fluorescence (LIF) images in both non-sooting and sooting diffusion flames, and luminosity images of sooting diffusion flames. For illustration, the non-sooting LIF data is treated both by the traditional method of comparing fundamental quantities and by comparing measured and computed signals. In each example, the comparison of measured and computed signals yields quantitative information similar to that obtainable through comparison of traditional quantities, along with reduced noise in the experimental data.

Keywords: Optical diagnostics; Computations; Comparison; Simulated signals

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1. Introduction

One important role for experiments in combustion research is to guide and verify computational models. The advances in lasers, detectors, and computers that occurred in the 1970's and 1980's led to the development of many new techniques for gathering data in the harsh environment of combustion. For a period of time, new diagnostic techniques were themselves of interest, and the relevance of the measured quantities to the theoretical and computational models under development at the same time was of secondary importance. In fact, quantities that were easy to measure were not usually the same quantities output by the models. However, as laser diagnostic techniques matured in the 1990's, the focus shifted to measuring fundamental quantities (e.g., mole fractions) that were of more significance to the modelers. Achieving this important goal has been much harder, often involving simultaneous measurement of many quantities (each with their own noise, uncertainties, and interferences) to get the fundamental quantity of interest to compare with simulations. Errors are often very difficult to estimate in these

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cases. In the meantime, computational models have become more sophisticated, more quantitative, and more complete. The availability of more complete information allows the possibility of using simulation results to derive predictions of measured signals rather than measuring many quantities to derive a single fundamental quantity. In some cases, comparison of computed and measured signals may be more informative and reliable than the comparison of computed and measured mole fractions, temperatures, mixture fractions, scalar dissipations, etc.

A few previous studies have compared measured and computed signals in an effort to validate computational fluid dynamics (CFD) models. Numerical simulation of experimental signals, known as computational flow imaging [1], is particularly useful under experimental conditions that do not allow for the direct measurement of a particular parameter. Boyce et al. [2] compared experimental interferometric data with theoretical maps computed from CFD results of a hypersonic flowfield. Danehy et al. [3] used CFD models to create theoretical planar laser-induced fluorescence (PLIF) images by determining the quenching dependence for the existing flow conditions. The study found that the theoretical images were useful for choosing the best excitation scheme for yielding signal intensities within the dynamic range of their detection system. This work was later expanded upon to look at PLIF images of mixing flowfields [4]. Amantini et al. [5–7] studied extinction and edge flame phenomena of counterflow diffusion flames both computationally and experimentally using OH and CO PLIF images, as well as velocities from particle image velocimetry (PIV) measurements. Simulated PIV velocity fields included predicted thermophoresis effects and the vaporization of oil droplets (used for seeding) to remove velocity vectors in regions with temperatures exceeding the boiling point of oil. Bell et al. [8] used numerical simulations to determine synthetic LIF images of NO by accounting for temperature and quenching effects for comparison with experimental results to look at NO formation pathways in both doped and undoped flames. Oftentimes, the comparison of measured and computed signals is seen as a last resort when direct measurements of fundamental quantities are impossible due to the complexity of the flow environment, the availability of diagnostics techniques, or simply limited resources.

The main premise of the “paradigm shift” is that, in designing experiments and choosing diagnostics, experimentalists should consider the accurate measurement of signals that can be calculated with little uncertainty as well as the more conventional approach of making direct comparison with computed results. It may be that deriving predictions of signals from numerical results is better than measuring the fundamental quantities that are normally output by simulations. Quantitative comparisons can easily be obtained by using appropriate calibration on both sides of the comparison. This approach clearly necessitates that modelers and experimentalists work together. Further, a detailed understanding of signal generation, as well as the effects of quenching, signal interferences, detector characteristics, and spatial resolution on signals is required. Below, three examples of comparing measured and computed signals are presented: NO laser-induced fluorescence (LIF) in both non-sooting and sooting diffusion flames, and luminosity images of sooting diffusion flames.

2. NO measurements in a non-sooting laminar flame

A non-sooting lifted methane/air coflowing non-premixed flame has been studied extensively both experimentally and computationally [9–13]. To test the ability of different kinetics schemes to predict NO formation in the flame, computations using two mechanisms (GRI 2.11 [14] and GRI 3.0 [15]) are compared to experimental measurements of NO using LIF. The computations were performed by using the numerical techniques and model described in [11], with the local rectangular refinement solution-adaptive gridding carried out to one additional level of refinement beyond that in [11]. The experimental procedures are outlined below. This comparison of computations and experiments is performed using two approaches: comparing computed and measured mole fractions, and comparing a computed fluorescence signal to the measured LIF signal.

The first approach of comparing computed and measured NO mole fractions requires measurement of the NO LIF signal as well as measurement of supporting data (temperature and major species concentrations) needed to apply Boltzmann and quenching corrections [16,17]. Two-dimensional images of NO fluorescence are created by tiling together a series of spectrally-resolved radial images of the (0,2) vibrational band [9]. Images of temperature and major species (N_2, O_2, CO_2, H_2O, and CO) mole fractions were measured using Rayleigh scattering and vibrational Stokes-shifted Raman scattering [13,18]. The quenching correction is calculated using the model of Settersten et al. [17]. The noise level of each component of the quenching and Boltzmann corrections (temperature, and N_2, O_2, CO_2 and H_2O mole fractions) is determined by calculating the rms fluctuation in a 4 mm × 3.5 mm area 5.5 cm above the burner (where the signals are reasonably constant) and dividing by the average signal in that region. The CO noise level is determined for a 4.2 mm × 3.3 mm area at a position 2.5 cm above the burner (around the CO maximum). The result is corrected for existing spatial gradients by sub-