A Benchmark Experimental Database for Multiphase Combustion Model Input and Validation – A Users Follow-up

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Abstract

Optimization of the performance of industrial combustion systems is relying increasingly on computational models and simulations to provide relevant process information in a cost-effective manner. Although computational fluid dynamics (CFD) offers a cost-effective alternative to experiments, the accuracy of the CFD models must first be assured. This is accomplished by two means: verification and validation. This paper describes a benchmark case suitable for validation of multiphase combustion models and submodels. The benchmark includes a reference spray combustor to provide well-defined input and boundary conditions, enabling measurements to characterize the fuel spray, combustion air, wall temperatures, exhaust gas temperatures and species concentrations. The characteristics (i.e., size, velocity, volume flux, etc.) of the methanol spray were determined using phase Doppler interferometry. Fourier-transform infrared spectroscopy was used to measure species concentrations in the reactor exhaust and the conversion of methanol. The inlet combustion air was characterized using particle image velocimetry and a five-hole pitot probe. The measurements constitute a database sufficiently complete for code validation; subsequently, several research groups have carried out simulations of the facility to varying degrees of success. This paper describes the development of the database and some of the modeling issues and needs.

Background

Two workshops were held at NIST, one in 1999 (Workshop on Validation of Multiphase Combustion Models) and the second in 2000 (Workshop on Metrology Needs for Multiphase Combustion Data) to assess the data needs for multiphase combustion modelers. Participants included representatives from code vendors/ developers, industrial/government users of codes, and university researchers. Priorities set by the participants of the first workshop provided direction for establishing the operating conditions and scale of the experimental configuration, and defining the data needs. Interest focused on the need to provide droplet size and velocity data at a station as close to the nozzle face as possible. Of critical need were the fluid flow characteristics (air stream velocity and turbulence intensity) at the inlet plane of the burner. Also, dimensions were required for the entire combustion facility, including the burner. It was clear from the workshop sessions that there was a wide range of specialized interests among the diverse groups, which indicated that a benchmark case would be chosen of interest to the general modeling community. Subsequent contacts with participants helped define a baseline case and data set finally chosen. We also employed a commercial CFD code to assist in the initial design of the combustor configuration before fabrication [1].

A second workshop was held after a preliminary data set was obtained to verify that the boundary, inlet, and flow measurements were sufficient to allow the modeling community to carry out simulation of the combustor configuration. The consensus among the workshop participants was that the defined benchmark case and measurements would be suitable for future simulation. The database was completed within the next two years and the results published subsequently in archival journals [2-4]. The operating conditions, facility schematics, boundary conditions, and NIST internal reports [5-7] were uploaded onto the Web (www.cstl.nist.gov/div836/836.02) for interested parties. Also note that, in addition to the workshops, several conference panel sessions were organized to discuss the different modeling issues and data needs with the modeling community. In particular, sessions were held at conferences of the American Society of Mechanical Engineers and American Institute of Aeronautics and Astronautics. Both of these organizations

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have active technical committees that deal with CFD issues and database needs, and publish standards for code verification and validation [8].

The full data set is available upon request simply via email. This path of communication also enables further contact with modelers by providing additional information upon request and follow-up of progress, which is a critical issue when using data published in the archival literature. The data set was also included in one of the NIST internal reports [5] on diskettes and mailed to numerous interested parties. Over 30 groups, including modelers from several different countries, have requested a copy of the data since its release. We are also aware of several groups that have obtained the database independently. In a recent follow-up with several of these groups, progress varied from deciding that the baseline case was not of sufficient interest to warrant the cost of carrying out a simulation (e.g., needed a different injector geometry, too low fluid flow to be handled by the flow solver, discontinued the effort), to still planning to use the database but have not done so at this time, to completed simulations and have reported results. Requests for additional information and data focused mainly on more detail of the combustion facility (including the burner) and some additional velocity and size/velocity correlation data, which was provided via email.

Elements of the Simulations

Most modelers use a variety of commercially available codes with the fundamental physics for multiphase combustion, which include the governing conservation equations of momentum, energy, and mass. In addition, models are coupled to these equations to include turbulence, chemistry, heat and mass transfer, and liquid atomization and transport (Lagrangian representation for droplet tracking, penetration and dispersion, and separate models for collision, secondary breakup, and vaporization), adding significant complexity to the problem. Two-way coupling is included to account for interactions between different processes (e.g., droplet/turbulence and turbulence/chemistry interactions). Although axisymmetry is used to simplify the simulation to two dimensions, reality dictates that three-dimensional complex configurations are important and thus adds another level of complexity. As a result of such complexities, the CFD community has derived over the years various novel numerical schemes and approaches to solve such sets of equations efficiently and robustly, using such approaches as unstructured/hybrid grids, and Reynolds-averaged, large-eddy, and direct numerical simulation approaches.

Elements of the Database

Experiments were conducted in an enclosed spray combustion facility, shown in Fig. 1 [4]. This benchmark was chosen because the level of complexity is simpler than a complete system, but allows simulation of key full-scale processes [8]. The operating conditions for the baseline case of the benchmark database are summarized in Table 1. The enclosed combustion chamber provided well-characterized boundary conditions. Measurements of the boundary conditions included the wall and exhaust gas-phase temperatures and exhaust gas species concentrations. Measurements within the reactor included gas-phase velocities, and the droplet size, velocity, and concentration. Inlet conditions included the air velocity, turbulence intensity, fuel flow rate, droplet size and velocity. Measurement uncertainties were determined to provide a level of confidence for the modelers. Spray measurements were obtained non-intrusively using phase Doppler interferometry. Data were obtained for the mean size, mean axial and radial velocity, number density, and volume flux of fuel droplets within the spray. Gas-phase temperature (using thermocouples) and species (using Fourier transform infrared spectroscopy) measurements were obtained at the reactor exit. To characterize the inlet combustion air, gas-phase velocity measurements were obtained using particle image velocimetry (PIV). Metrology issues associated with the various diagnostics are also discussed throughout Ref. [4].

The experimental facility includes a swirl burner with a movable 12-vane swirl cascade. The cascade is adjusted to impart the desired degree of swirl intensity to the combustion air stream that passes through a 0.10 m diameter passage and coflows around the fuel nozzle. The combustion air flows through an annulus located downstream of the swirl vanes before entering the reactor. The exit of the annulus, which surrounds the fuel line and nozzle, corresponds to the inlet of the reactor.

The liquid fuel was supplied through a pressure-jet atomizer and formed a hollow-cone spray with a nominal 60^o full cone angle. Methanol was used for these experiments, and the flow rate was maintained at 3.0 kg h^{-1} ± 0.02 kg h^{-1}. Methanol was chosen as the fuel because the thermodynamic and kinetics data necessary to model the gas-phase combustion are readily available [9], and the absence of soot in the non-luminous flame reduces the complexity of the modeling effort. The fuel and combustion air were introduced into the reactor at room temperature. The flame was fired in a vertical upwards configuration. The fuel flow rate, combustion air flow rate, wall temperatures, and exiting gas temperatures were monitored continuously and stored using a computer-controlled data acquisition system.

The burner is enclosed within a stainless steel chamber to isolate the flame from the ambient and define clearly the fuel/air ratio. The chamber height is 1.2 m and the inner diameter is 0.8 m. Several windows and ports provide access for optical non-intrusive measurements and other in-situ probes. A stepper-motor-driven traversing system translates the entire burner/chamber assembly, permitting measurements of spray properties at selected locations downstream of the atomizer. The reactor exit is off-axis to permit direct probing of the flame, which makes the problem non-axisymmetric.

Simulation Issues with the Database

Several research groups have initiated simulations of the facility for model validation, and have published results [10-12]. Users of the database include organizations representing 1) commercial software vendors, 2) universities in the US and abroad, 3) government agencies, 4) and industrial users of CFD codes. The following discusses some of their simulation issues, level of agreement between the simulated and measured parameters, additional experimental data needs, and new benchmark data needs.

As mentioned above, measurements carried out for the database were agreed upon from the results of two earlier workshops, which characterized the basic elements required to initiate a computational simulation. Due to limitations in obtaining experimental data for model input and validation (due to the need for measurements at conditions outside the instrument performance range, or computational parameters for which there are no measurement capabilities), modelers must represent boundary/inlet conditions in novel but in many times not physically accurate ways. This issue for the spray combustion modeler is of particular concern with regard to the initial (inlet) conditions, simply because of the computational sensitivity in simulating the exact case of interest. For example, one major issue for spray combustion simulations is the difficulty in describing the spray formation processes (i.e., liquid bulk breakup to a multitude of discrete droplets). Of course, parallel uncertainties also exist with regard to both the turbulence and chemistry submodels. The normal procedure is to describe the introduction of droplets in groups (referred to as "parcels") containing a number of discrete droplet size bins, and corresponding velocities (i.e., direction and magnitude), at specified spatial positions along the inlet. Thus, modelers require experimental data as close to the inlet as possible. It is generally difficult to provide experimental data for the spray characteristics at the atomizer since the fluid is still in the bulk or ligaments; both experimentally and numerically the liquid breakup process cannot be well characterized. What one does is provide experimental data as close to the inlet as possible (since generally the techniques available are based on measurement of spherical droplets). The modeler then assumes inlet conditions that will match through extrapolation the experimental results at the downstream position by varying the droplet (parcel) injection characteristics (size and velocity) - a procedure with great uncertainty. One modeling group commented that not accounting for the fluctuations in the liquid at the inlet might have contributed to disagreement of their results. Another group stated that the accuracy of the Lagrangian tracking and evaporation history were also dependent on the droplet initial conditions. In addition, they reported that the Sauter mean diameter and droplet velocities downstream are dependent on the initial spatial profile along the inlet. Representation of the initial conditions may also be compromised when the CFD model tracks a limited number of droplets.

Because accuracy of the inlet conditions is critical to a successful simulation, one response is to develop an atomizer that can inject discrete arrays of droplets. This may allow measurement of the droplet size closer to the atomizer or determination of initial droplet size by means of fundamental theoretical prediction via Rayleigh's theory for the breakup of capillary jets [13]. Such a reference atomizer would potentially be useful in providing initial spray conditions for modelers.

Level of Agreement of the Simulation with the Experimental Data

Generally, comparison of the fluid characteristics (including recirculation regions), spray volume flux, droplet axial and radial velocity components, and Sauter mean diameter were reported by different groups to be in relatively good agreement (i.e., within 15 %). For two groups, this was achieved through trial-and-error estimation of the initial droplet mean size and spray angle to optimize agreement with the experimental results, and was quite time consuming. Agreement was poor when constant droplet sizes and velocities were assumed at the inlet, especially with regard to droplet deceleration and dispersion of the spray in the radial direction. Another modeler reported that they were unable to match the extent of combustion. Experiments corresponded to 80 % conversion of fuel, but the combustion models examined were unable to capture this correctly. Some models failed due to "mixing-limited" assumptions. Combustion models that include chemical mechanisms should be able to reproduce the observed incomplete combustion, and related transport of larger droplets through the flame.

Modeling and Corresponding Measurements Needs

From the various interactions, discussions, support letters that were obtained from companies, government agencies, and modeling vendors, several specific data interests and needs are summarized below. Note the dichotomy of interests. For many modelers, in particular those from industry, simulation of soot formation and transport processes was of current interest, but leads to another level of complexity and uncertainty. On the other hand, model developers/vendors are interested in validation of more simplified cases, in particular turbulent nonreacting sprays, before addressing more complicated flows.

<u>Current database</u>

- flame gas temperatures and species concentrations (NO_x)
- axisymmetric configuration (at the exit plane)
- spray characteristics closer to the burner
- heat fluxes

<u>New or extended database</u>

- change –
  - operating conditions (chamber and inlet fuel pressure, temperature, fuel/air ratio, and swirl intensity)
  - atomization media (air, steam)
  - multicomponent fuels (Jet-A and diesel) and fuel properties (physical and chemical)
  - nozzles (air-assisted atomizer and multipoint injection)
- monodispersed spray flames
- nonreacting case
- sooting flame and characteristics
- transient injection

Summary

Various groups throughout the world are using the NIST benchmark multiphase combustion database successfully. Comparison of simulation results with the database has been favorable, and has helped modelers identify modeling issues that need further attention. Interaction with the users has also helped identify new measurement needs for the combustion modeling community. One benefit is the use of the database for a company's tutorial, which is exposing the data to the larger modeling community and enabling them to learn to model spray combustion. Currently, soot is being characterized in a heptane spray flame due to the interest in understanding and developing submodels of soot inception, growth, and transport.

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Table 1. Operating conditions for the baseline case of the NIST benchmark database.

Fuel	Methanol
Fuel Flow Rate	3.0 kg h^{-1}
Fuel Temperature	Ambient
Equivalence Ratio	0.3
Air Flow Rate	56.7 m^3 h^{-1}
Air Temperature	Ambient
Vane Angle	50^o
Swirl Number	0.58
Flame Standoff Distance	~ 5 mm
Chamber Pressure	Ambient

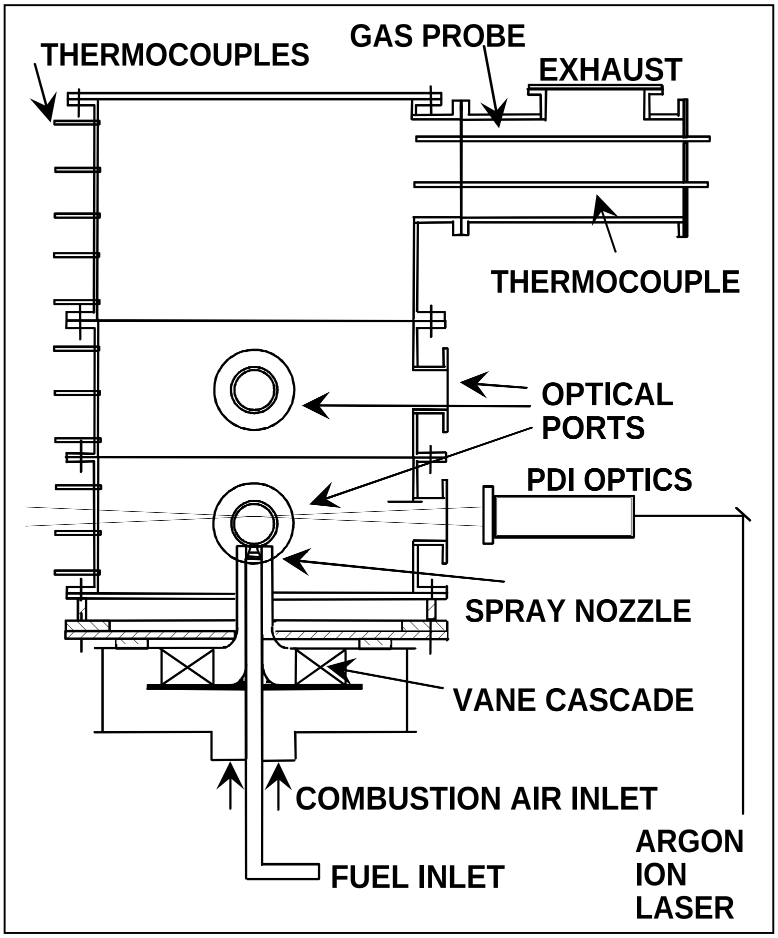

Figure 1. Schematic of the experimental facility.