JOURNAL OF PROPULSION AND POWER
Vol. 22, No. 5, September–October 2006

Technical Notes

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Application of a Benchmark Experimental Database for Multiphase Combustion Modeling

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DOI: 10.2514/1.21638

Introduction

OPTIMIZATION of the performance of industrial combustion systems is relying increasingly on computational models to simulate relevant physical processes and phenomena. Although computational fluid dynamics (CFD) techniques offer a cost-effective alternative to experiments, the accuracy of the CFD models must first be assured. This is accomplished through model verification and validation [1]. In the validation process, the collaboration of modelers and experimentalists is of utmost importance, as well as the use of databases that include data with specified uncertainties and follow a recommended format [2,3]. Without experimental uncertainties, one cannot assure the credibility of the simulation results [1]. In the modeling community, there is a wide range of specialized interests, ranging from the need for simple laboratory-scale experiments by software vendors to pilot-scale measurements by industrial modeling groups. Development of a benchmark database requires reliable measurements of the initial and boundary conditions, as well as within the flowfield, and at the same time simulates key features of the combustion process. Regarding spray combustion modeling, measurements need to focus upstream near the atomizer/burner face so that the inlet conditions can be specified accurately. Models require droplet size and velocity distribution data, as well as the fluid flow characteristics (airstream velocity and turbulence intensity) at the inlet plane of the burner. In response, a benchmark database was developed at the National Institute of Standards and Technology (NIST) and the results published in the literature [4–10]. The measurements constituted a database sufficiently complete for simulation of the experimental arrangement; subsequently, several research groups have carried out simulations of the facility to varying degrees of success. This article summarizes key aspects of the benchmark case and describes some of the modeling issues and needs that have arisen since its release.

Received 7 December 2005; revision received 27 March 2006; accepted for publication 4 April 2006.

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Elements of Multiphase Combustion Models

A variety of commercially available and in-house codes have been developed with the fundamental physics for multiphase combustion (namely, governing conservation equations for mass continuity, momentum, energy, and species [11,12]). In addition, models are coupled to the discretized conservation equations to include turbulence, chemistry, and liquid atomization and transport (droplet tracking, penetration and dispersion, and separate models for collision, secondary breakup, and vaporization), adding significant complexity to the problem. Two-way coupling may be included to account for interactions between the dispersed and continuous phases. Validation of the spray characteristics (i.e., volume flux, velocity, and size) is important because these characteristics play a major role in determining the gas-phase source terms [13]. 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 been developing over the years various novel numerical schemes and approaches to solve this set of equations efficiently and robustly, using such approaches as unstructured/hybrid grids, and Reynolds-averaged, large-eddy, and direct numerical simulation approaches [11]. However, one must recognize that many significant modeling uncertainties exist in describing the physics. These include providing a ligament breakup submodel for atomization, drag correlations for droplet transport, kinetics for the multiphase chemistry, and dissipation and length scales for turbulence. It is clear that an accurate representation of the initial and boundary conditions is essential to carrying out a successful simulation. Thus, the need for high-quality experimental data with carefully determined measurement uncertainties is highly sought for model validation.

Elements of the NIST Database

The enclosed spray combustion facility shown in Fig. 1 [4,5] served as our benchmark because the level of complexity was simpler than a pilot or full-scale system and allowed simulation of key physical processes [1]. The design of the facility followed these guidelines. 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 and turbulence intensity, fuel flow rate, and droplet size, velocity, and mass flux. Measurement uncertainties were estimated to provide a higher level of confidence [14], and the details of these estimates are given in [5]. Spray measurements were obtained nonintrusively 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, and uncertainty estimates, associated with the various diagnostics are also discussed throughout [5].

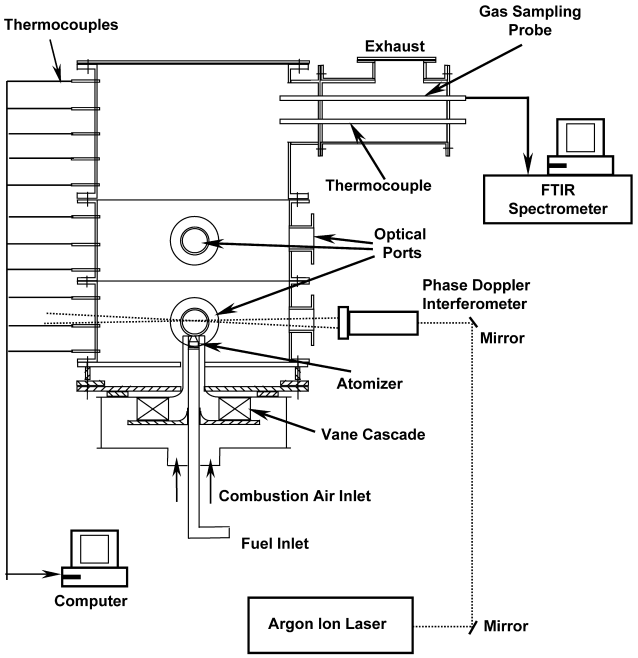

Fig. 1 Schematic of the experimental facility.

The experimental facility included a swirl burner with a movable 12-vane swirl cascade. The cascade was adjusted to impart the desired degree of swirl intensity to the combustion airstream that passes through a 0.10 m diameter passage and coflowed around the fuel atomizer. The combustion air passed through an annulus located downstream of the swirl vanes before entering the reactor. The exit of the annulus, which surrounded the fuel line and atomizer, corresponded 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 deg full cone angle. Methanol was used for these experiments, and the flow rate was maintained at 3.0 ± 0.02 kg h^{-1}. Methanol was chosen as the fuel because the thermodynamic and chemical kinetic data necessary to model the gas-phase combustion were readily available [15], and the absence of soot in the nonluminous flame reduced the complexity of the modeling effort. The fuel and combustion air were introduced into the reactor at room temperature. The steady state 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 was enclosed within a stainless steel chamber to isolate the flame from the ambient and define clearly the fuel/air ratio. The chamber height was approximately 1.2 m and the inner diameter was 0.8 m; the chamber dimensions were chosen to avoid impingement of the flame on the walls. Several windows and ports provided access for optical nonintrusive measurements and other in situ probes. A stepper-motor-driven traversing system translated the entire burner/chamber assembly, permitting measurements of spray flame properties at selected locations downstream of the atomizer. The reactor exhaust passage was off axis to permit direct probing of the flame, which made the problem nonaxisymmetric.

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
Airflow rate	56.7 m^3 h^{-1}
Air temperature	Ambient
Vane angle	50 deg
Swirl number	0.58
Flame standoff distance	~5 mm
Chamber pressure	Ambient

Some Simulation Issues Regarding Spray Combustion

Several research groups completed simulations of the facility for model validation and published comparative results [13,16,17]. Some of the simulation issues are described below, as well as the level of agreement between the simulated and measured parameters, additional data needs for the current database, and new benchmark data needs.

Acquiring experimental data for a quantity that will serve as input into a computational model may not always be available because the measurement capability may be nonexistent, or the measurement may be limited by instrument performance range. Thus, boundary/initial (inlet) conditions may have to be represented in novel ways. For example, one major issue for spray combustion modeling is validation of the spray formation process (i.e., liquid bulk breakup into a multitude of discrete droplets). Also, spray submodels have large uncertainty near the atomizer due to droplet/droplet interactions and grid dependence. Of course, analogous uncertainties exist with regard to both the turbulence and chemistry submodels. A procedure often used to represent the spray at the inlet is to introduce droplets in groups with uniform size and velocity (referred to as "parcels") [11], which makes simulation of the large number of droplets computationally palatable. A number of discrete droplet size bins are represented along with the corresponding velocities (i.e., direction and magnitude) and specified spatial positions along the inlet. Thus, models require experimental data as close as possible to, if not at, the inlet to specify properly the initial conditions.

Generally, one is unable to provide experimental data for the spray characteristics at the atomizer inlet since the fluid may still be in the bulk or forming ligaments; thus both experimentally and computationally the initial condition for liquid breakup is not well characterized. Experimental data are thus provided as close to the inlet as possible where the spray is established (because generally the techniques available are based on measurement of spherical droplets). Inlet conditions are assumed that will match through extrapolation of the experimental results at the downstream position by varying the droplet (parcel) injection characteristics (size and velocity), a procedure with considerable ambiguity. Additional issues that can contribute to the disagreement of results include the need to account for fluctuations in the liquid at the inlet, and the accuracy of the Lagrangian tracking and evaporation history is dependent on the droplet initial conditions. Also, the spray characteristics (i.e., Sauter mean diameter and droplet velocities) downstream are dependent on the initial spatial profiles 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, developing a reference atomizer that can inject discrete arrays of droplets to form a spray (for example, similar to that of acoustically driven atomizers [18]) may provide the necessary inlet condition for these models. Such an atomizer would 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 [19].

Level of Agreement between the Simulations and Experimental Results

Generally, comparison of the fluid characteristics (including recirculation regions), spray volume flux, droplet axial and radial velocity components, and Sauter mean diameter were reported to be in relatively good agreement (i.e., within 15%) [13,16,17]. This was achieved by some models through trial-and-error estimation of the initial droplet mean size and spray angle to optimize agreement with the experimental results and was time consuming. Comparison of computational and experimental results published by Itoh et al. [16]

was good for the mean airflow including simulation of the reverse flow regions. However, the root mean square values did not agree well, and likewise the turbulence diffusion. This was attributed to the fact that the velocity fluctuations were neglected at the inlet and because of the relatively course grid resolution. Simulations for which variation in the droplet position, velocity, and diameter was neglected, as shown in Fig. 2 (reproduced from [16]), indicated that agreement of the simulation with the experimental results upstream near the atomizer was good but the discrepancy grew with increasing axial position. Note that the experimental uncertainties are included in Figs. 2–6, as detailed in [5]. Details of the simulation uncertainties were not specified in the referenced articles.

Widmann and Bedford [17] improved the agreement between the experimental results and computational simulations by adjusting the spray angle at the inlet and sheet constant in the linearized instability sheet atomization (LISA) model [20], while the initial size distribution and the inclusion of a droplet collision model had little influence on the computation results. The LISA model is used to predict the most probable diameter for the injection of a Rosin–Rammler droplet size distribution. The model assumes that surface disturbances break the liquid sheet into ligaments and then droplets, and the aforementioned sheet constant is proportional to the ligament diameter. Figure 3 (reproduced from [17]) compares the Sauter mean diameter of the simulations with the experimental results for different initial size distributions. The results show reasonably good agreement after adjustment of the sheet constant and spray angle, and that the size distribution had little effect on the predicted mean size. 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. It was also difficult to match the extent of combustion. Experiments corresponded to 80% conversion of fuel [5], but the combustion models examined were unable to capture this correctly. It was thought that "mixing-limited" assumptions caused the discrepancy. Combustion models that include chemical mechanisms should be able to reproduce the observed incomplete combustion and related transport of larger droplets through the flame. It was speculated that failure to reproduce the experimental results was related to the larger droplets not being represented sufficiently in the model.

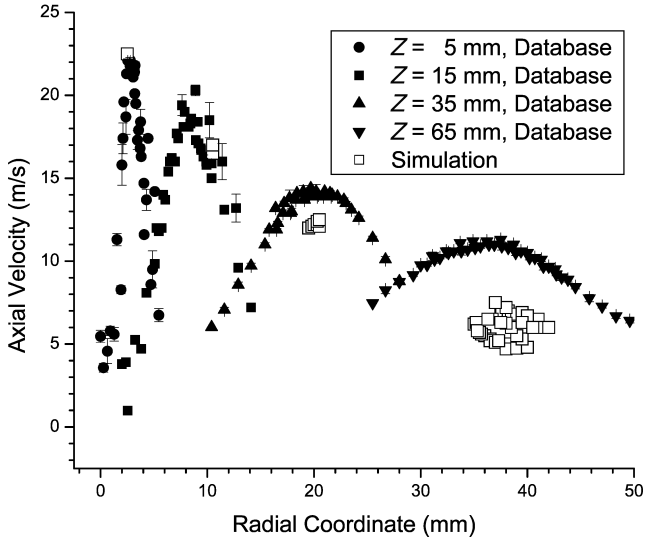

Fig. 2 Variation of the droplet axial velocity with radial position at different axial positions (Z). Comparison between the experimental results and computational simulation. Simulation by Itoh et al. [16].

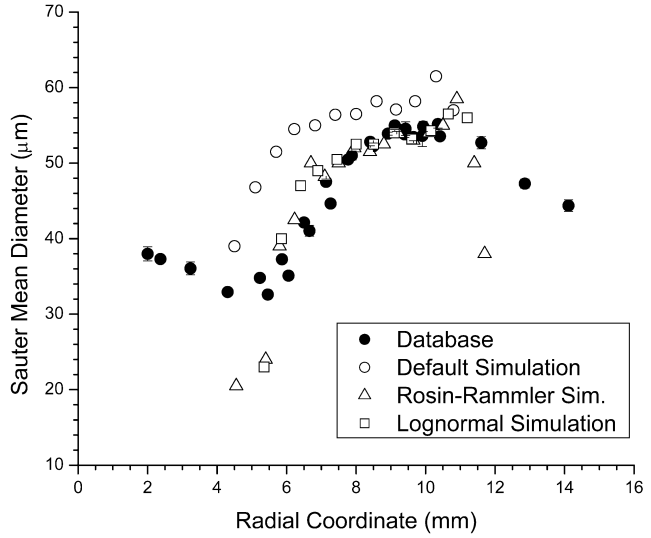

Fig. 3 Variation of the Sauter mean diameter with radial position at $Z = 15$ mm, assuming different initial size distributions for the simulations, which are compared with the experimental results. Simulation by Widmann and Bedford [17].

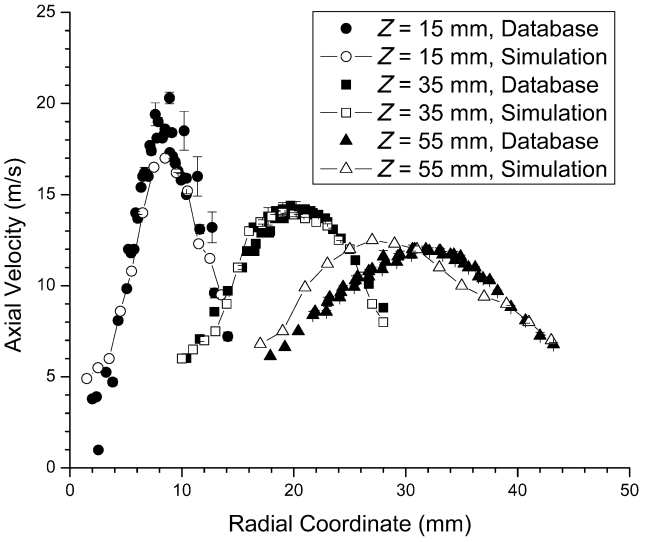

Fig. 4 Variation of the spray axial velocity with radial position at three axial positions, initial droplet Sauter mean diameter of 61 μm. Simulation by Crocker et al. [13].

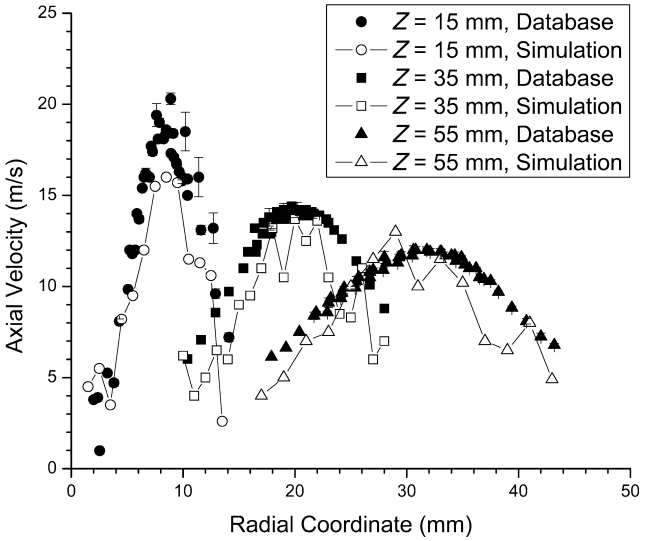

Fig. 5 Variation of the spray axial velocity with radial position at three axial positions, no spray angle distribution. Simulation by Crocker et al. [13].

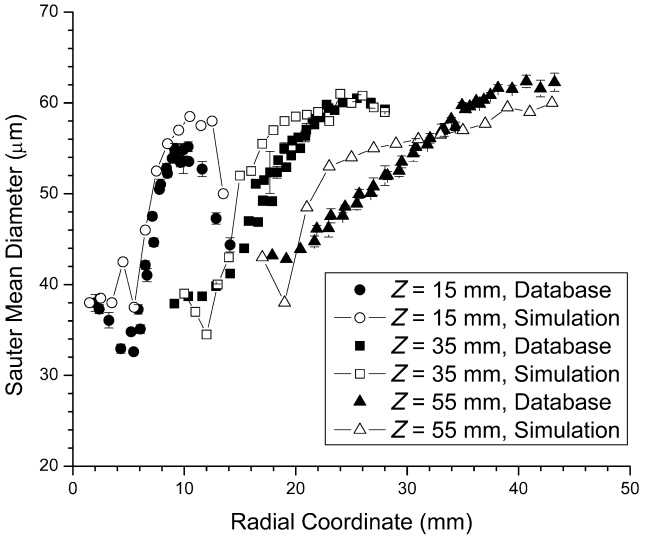

Fig. 6 Variation of the spray Sauter mean diameter with radial position at three axial positions, baseline case. Simulation by Crocker et al. [13].

A more extensive comparative study by Crocker and coworkers [13] achieved good agreement for the droplet sizes, velocities, and volume flux. The results indicated that small changes in the initial spray angle of a few degrees had a significant effect on the downstream dispersion of the spray, as shown in Figs. 4–6 (reproduced from [13]). The axial velocities were underpredicted at the peak values for the baseline case. When the initial droplet mean size was increased to 61 μm, better agreement was obtained at upstream axial positions, as shown in Fig. 4, and less agreement downstream. The baseline case used an assumed spray angle distribution as an initial condition, but when no distribution was used the peak locations were improved, as shown in Fig. 5 (note that the computed profiles are not smooth because 3000 parcels were used instead of 21,000 parcels for the baseline case). The Sauter mean diameters are shown in Fig. 6 for the baseline case with good agreement between the computational and experimental results. The simulation predicted somewhat higher values at the axial position of 15 mm, but this was expected because the experimental uncertainty at this location was much larger than further downstream. Thus, validation of computational results also requires knowledge of the experimental uncertainties, as well as those associated with the numerical computation.

Modeling Needs

Modeling needs are partitioned between supplemental data for the reported database and new or expanded databases. Regarding the reported database, droplet temperature, spatially and temporally resolved flame gas temperatures and species concentrations (including trace gases) for turbulence/chemistry interactions, heat fluxes, and parametric data at different operating conditions (including different liquid fuel temperatures) are of interest. Of primary importance is the characterization of the inlet conditions, in particular, the liquid sheet breakup (sheet thickness and breakup length), while of much less significance was the asymmetry in the exit plane of the experimental configuration. Regarding new data needs, simulation of soot inception, growth, oxidation, and transport is of current interest. Model developers/vendors are interested in validation of more simplified cases (in particular, turbulent nonreacting sprays, with and without vaporization, and monodispersed spray flames), before addressing more complicated flows. The dichotomy of interests also aspire for more extensive parametric studies with different operating conditions (chamber, ambient, and inlet fuel pressures, temperatures, fuel-air ratios, and swirl intensities), atomization media (air, and steam), fuel compositions (Jet-A, No. 6 fuel oil, and diesel), fuel properties (thermo, physical, and chemical), atomizer types (air-assisted atomization, multipoint, and transient injection), and changes in the reactor configuration.

The need is arising for a better understanding and estimation of the measurement uncertainties associated with instruments, different systemic biases, and suitability of measurement techniques for different applications. The need also exists for quantifying the numerical uncertainties associated with the various model approximations and boundary conditions.

Summary

Several groups have used the NIST benchmark multiphase combustion database for model validation. Comparison of simulation results with the database has been favorable and has helped identify modeling and measurement issues that require further attention. For example, unresolved issues regarding droplet breakup and soot formation processes command further attention by the community at large.

Acknowledgements

Thanks for the helpful suggestions by the participants of the 1999 Workshop on Validation of Multiphase Combustion Models and the 2000 Workshop on Metrology Needs for Multiphase Combustion Data that were held at the National Institute of Standards and Technology, and for the comments received by the database users. Thanks to J. F. Widmann and S. R. Charagundla who worked so diligently to acquire and publish the database.

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