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Benchmark Database for Input and Validation of Multiphase Combustion Models

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Introduction

Control of process efficiency and the formation of species byproducts from industrial thermal oxidation systems (e.g., power generation and treatment of liquid chemical wastes), is generally based on *a priori* knowledge of the input stream physical and chemical properties, desired stoichiometric conditions, and monitoring of a few major chemical species in the exhaust. Optimization of the performance of these systems is relying increasingly on computational models and simulations that help 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 model must first be assured. This should be accomplished in two ways: verification and validation. Verification involves ensuring that the algebraic and differential equations within the model have been accurately solved. In addition to verifying that the numerical code arrives at the correct solution, it is also necessary to determine if the chosen model accurately represents the physical process of interest. This is the validation step. The objective of this paper is to provide benchmark experimental data for CFD model and submodel validation.

This paper presents data obtained from a baseline spray flame within the reference spray combustion facility at NIST. The spray data presented were collected non-intrusively using phase Doppler interferometry (PDI). The size and velocity distributions of the fuel droplets, droplet number density, and volume flux of fuel droplets within the spray have been obtained. The enclosed combustion chamber provides well-characterized boundary conditions, and wall and ceiling temperature profiles have been measured. Gas temperature and species measurements obtained at the reactor exit can be used for boundary conditions or validation of computational results. The inlet combustion air has been characterized using a 3-D CFD simulation to determine the velocity and turbulence intensity profiles, and the simulation has been validated with experimental data. Gas-phase velocity, temperature, and heat flux measurements are planned for completing this baseline case.

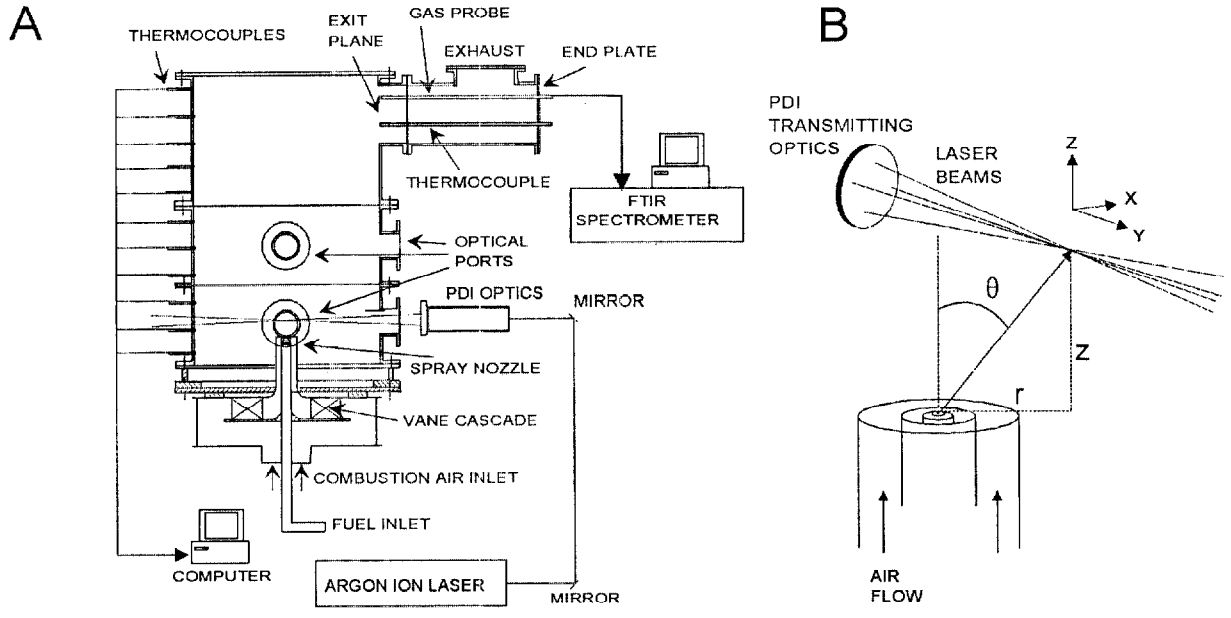

Figure 1. Schematic of (A) the reference spray combustion facility and (B) the nozzle used to generate the spray.

Baseline Case

Spray Combustion Reactor

Experiments were conducted in an enclosed spray combustion facility, shown in Fig. 1A. 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 swirl intensity is a measure of the angular momentum of the combustion air. It is characterized by the swirl number, S, defined as the ratio of the axial flux of angular momentum to the axial flux of linear momentum (Gupta *et al*., 1984). The vane angle and combustion air flow rate were $50^o \pm 2^o$ and 56.7 ± 1.7 m^3 h^{-1}, respectively. Recent CFD modeling of the burner results in a swirl number of S = 0.53.

Figure 1B presents a close-up view of the burner and nozzle. The liquid fuel flows through a pressure-jet nozzle and forms 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 ± 0.02 kg h^{-1}. Methanol was chosen as the fuel because the thermodynamic and kinetic data necessary to model the gas phase combustion are readily available (Afeefy *et al*., 1998; also available on the World Wide Web at *http://webbook.nist.gov/*). The fuel and combustion air were introduced into the reactor at room temperature. The fuel flow rate, combustion air flow rate, wall temperatures, and exiting gas temperatures were monitored and stored using a computer controlled data acquisition system.

The burner is enclosed within a stainless steel chamber to provide improved reproducibility and control of the spray flame. The chamber height is 1.2 m and the inner diameter is 0.8 m. Several windows provide optical access, and a stepper-motor-driven traversing system translates the entire burner/chamber assembly permitting measurements of spray properties at selected locations downstream of the nozzle. Additional details on the design of the burner are available in the literature (Presser *et al*., 1994). The relevant dimensions necessary for modeling the facility have been summarized in a NIST internal report (Widmann *et al*., 1999a). Note that the reactor exit is off-axis, which makes the problem non-axisymmetric.

The spray measurements were made using a two-component phase Doppler interferometer to measure the droplet size and velocity distributions and the spray intensity. The receiving optics were aligned at a 30^o scattering angle measured from the direction of propagation of the laser beams, and the transmitting and receiving optics were aligned at the same elevation. Additional details of the optical arrangement are available elsewhere (Presser *et al*., 1994; Widmann *et al*., 1999a).

Gas-phase species concentrations were measured using Fourier transform infrared (FTIR) spectroscopy. An FTIR spectrometer equipped with a deuterated triglycene sulfate (DTGS) detector was used for extractive sampling of chemical species in the combustor exhaust. A gas sampling system, consisting of an air-cooled sampling probe, a heated gas line, and a vacuum pump, facilitated the transport of the sample gas extracted from the combustion facility into the single-pass gas cell (10 cm path length) in a continuous manner. The sampling probe was designed to aerodynamically quench chemical reactions occurring within the gasses being sampled. The sampling gas line was also provided with a means for purging.

Operating and Boundary Conditions

The fuel flow rate into the reactor was measured with a turbine meter and maintained at 3.0 ± 0.02 kg h^{-1}. The rotation frequency of the turbine meter was calibrated as a function of methanol flow rate, and the analog voltage signal from the turbine meter was read into the data acquisition sytem and calibrated as a function of the turbine frequency. Combining the calibration uncertainties with the standard deviation obtained from repeated observations yields a combined standard uncertainty of 0.0157 kg h^{-1} for the fuel flow rate.

Thermocouples (K-type) were used to measure the wall temperatures and gas temperatures at the exit of the reactor (Widmann *et al*., 1999a). The gas temperature at the exit plane of the reactor was measured at the same locations as that of the species concentration data. The combined standard uncertainties for the measurements are 3 ^{o}C and 5.5 ^{o}C for the wall and gas temperatures, respectively.

The combustion air was delivered through the swirl burner at a rate of 56.7 ± 1.7 m^3 h^{-1}. The flow rate was measured using a 6.35 mm i.d. sonic nozzle for which the manufacturer reports a 3 % uncertainty. This uncertainty is significantly larger than those associated with the calibration of the pressure transducer, the uncertainty of the pressure gauge, or the random errors determined from repeated observations. The operating conditions for the baseline case are summarized in Table 1.

Fuel Type	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	0.49
Flame Standoff Distance	~ 5 mm
Chamber Pressure	Ambient

Table 1. Operating conditions for the baseline case.

Fuel Spray Measurements

Experimental data were collected at seven elevations downstream of the nozzle. Some of these data are presented in Figs. 2 - 4 and are available from the authors in electronic format. The mean axial velocity components of the droplets are presented in Fig. 2, and droplet Sauter mean diameters, D_{32}, are presented in Fig. 3.

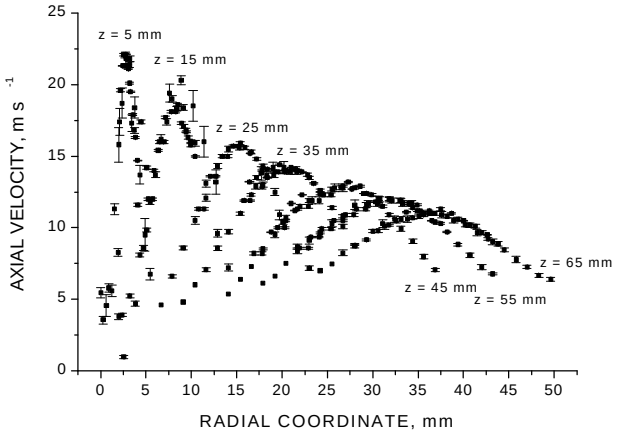

Figure 2. Droplet axial velocity, v_z, at seven axial locations downstream of the nozzle.

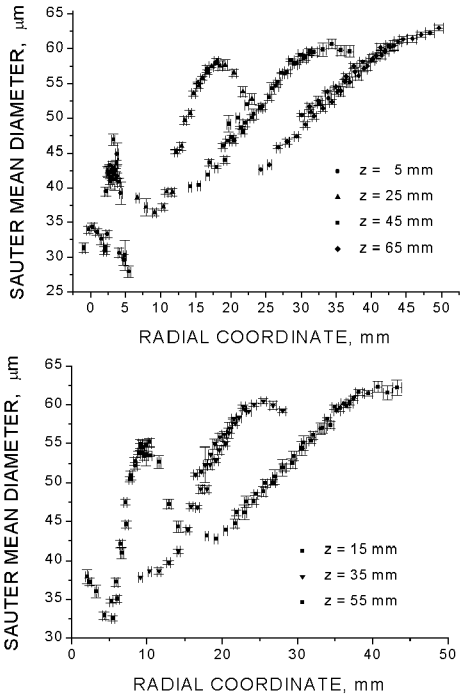

Figure 3. Droplet Sauter mean diameter, D_{32}, at seven axial locations downstream of the nozzle.

Figure 4 presents droplet number densities measured with the PDI at the downstream locations corresponding to data shown in Figs. 2 and 3. The number densities and volume fluxes are corrected for the instrument response time and rejected signals, which is discussed in detail elsewhere (Widmann *et al*., 1999b). The horizontal error bars express the uncertainty in the radial coordinate, and the vertical error bars correspond to twice the standard error of the mean ($2sn^{-1/2}$). Note that systematic errors associated with the instrument are not included in the figures at this time but should be considered when comparing the data to numerical results. Systematic errors associated with the PDI are discussed elsewhere (Widmann *et al*., 1999a)

Exhaust Chemical Species Measurements

The absorption spectra obtained with the FTIR spectrometer indicate that combustion was incomplete. Major species identified by the FTIR data include CO_2, CO and CH_3OH. No minor components or reaction intermediates were identified, which is attributed to the short instrument path length. Figure 5 shows the mole fraction of CO_2, CO, and CH_3OH at the exit plane of the reactor. The species concentrations are fairly uniform across the reactor exit plane, suggesting that there is good mixing in this region. Also, the concentration of CO_2 is approximately 50 times greater than that of CO, which indicates that the rate of methanol conversion to CO_2

and H_2O within the reactor is occurring at a rate approximately 50 times faster than the conversion to CO and H_2O.

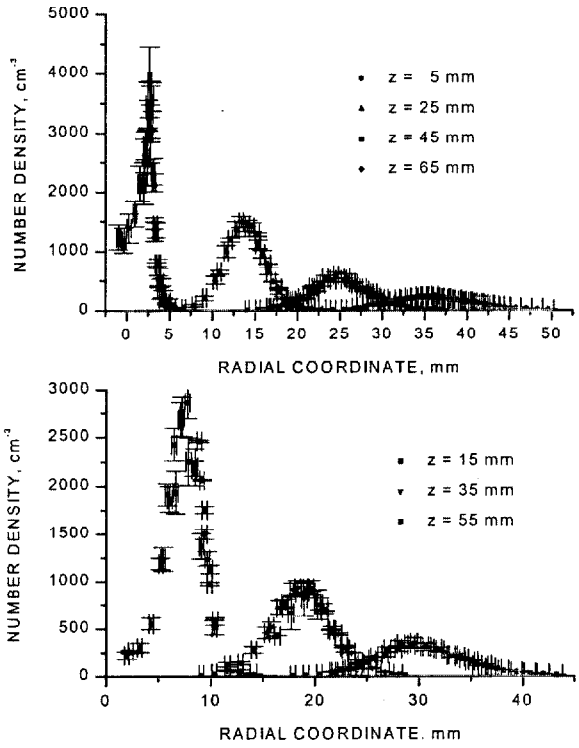

Figure 4. Droplet number density at seven axial locations downstream of the nozzle.

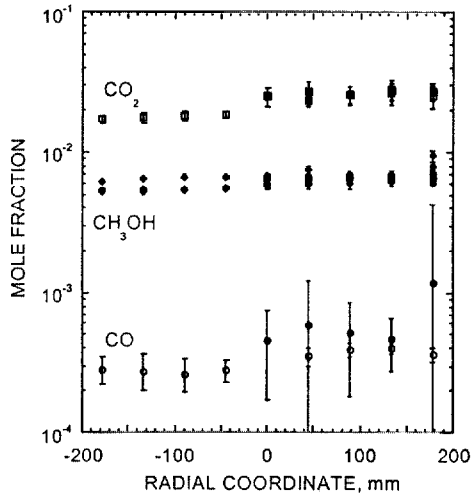

Figure 5. The exit concentrations of various species in the reactor.

Summary

Experimental data were obtained from a reacting methanol spray under well-characterized conditions for the purpose of validating multiphase combustion models and submodels. Droplet size and velocity distributions, number densities, and volume fluxes were measured, and uncertainties in the measurements were estimated. Gas-phase species measurements were made using FTIR spectroscopy, and provide exhaust concentrations of CO, CO_2, and CH_3OH. Wall temperature data are provided, as well as the temperature of the exhaust gas.

References

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