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Reference Spray Combustion Facility for Computational Fluid Dynamics Model Validation

John F. Widmann,* S. Rao Charagundla,† and Cary Presser‡
National Institute of Standards and Technology,
Gaithersburg, Maryland 20899

Introduction

THE operation of industrial thermal oxidation systems, for example, power generation and chemical waste incineration, is generally based on *a priori* knowledge of the input stream physical and chemical properties, desired stoichiometric conditions, and monitoring of a few major species in the exhaust. The optimization of these systems is relying increasingly on computational models and simulations to provide relevant process information in a cost-effective manner. However, for computational models to be used confidently, one needs reliable data for specifying model initial/boundary conditions and experimental/numerical comparative analysis of conditions within the reactor to validate the models. Discussion of these issues is the focus of the work carried out in the AIAA Computational Fluid Dynamics (CFD) Committee on Standards.[1]

The objective of this Technical Note is to introduce the reader to a new reference spray combustion facility being used to provide benchmark experimental data with associated quantitative uncertainties for the validation of multiphase combustion models and submodels. Reference 1 distinguishes between four levels of complexity when collecting data for CFD validation. These four levels are the unit problems, benchmark cases, subsystem cases, and the complete system. The four levels increase in complexity in the order stated. The current facility corresponds to a benchmark case and, therefore, is considerably less complicated than a complete thermal oxidation system. The benchmark case does, however, contain important elements of the system, such as multiphase flow, complex transport phenomena, and chemical reaction. Also, benchmark facilities have the flexibility to provide greater diagnostic analysis of flowfield phenomena than allowable in full-scale complex systems.

The current facility configuration and baseline operating conditions were defined in direct response to collaborations with modelers and their needs. A coupled experimental/computational approach is used to involve modelers directly in the program. Sample data are presented from the baseline case, and a more extensive compilation of the experimental data is available from the authors.[2]

Facility Design

The reference spray combustion facility, shown in Fig. 1, has evolved into a well-characterized and controlled system that can handle different 1) process liquid fuels and wastes, 2) atomizer designs, and 3) combustor configurations. A variety of state-of-the-art diagnostics are employed to characterize the input liquid stream, spray (droplet size, velocity, and number density), and exhaust emissions (particulates and chemical species). The facility permits examination of the effects of air swirl, atomizer design, fuel type, and air preheat on spray structure, combustion and emission characteristics. Experiments can be carried out under a variety of conditions, where the flow parameters (airflow rate, swirl number, and inlet air and fuel temperature) and fuel injector characteristics (fuel flow rate, spray angle, and atomizer configuration) are variable over a wide range. The unique aspect of this reference facility is the availability of advanced in-situ diagnostics that can be used to provide data for a wide range of operating conditions.

The experimental facility includes a stainless steel chamber with a variety of windows and ports for introducing both nonintrusive optical diagnostics and intrusive probes. The chamber allows for better-controlled evaluation of spray and emission data, as well as the study of different combustor configurations and heat transfer. The chamber height is 1.2 m, and the inner diameter is 0.8 m. All chamber inlet and boundary conditions are monitored to provide accurate data for modelers.

The facility includes a swirl burner with a movable 12-vane swirl cascade. The cascade is adjusted to impart the desired degree of swirl to the combustion airstream that passes through a 0.10-m-diam passage and flows around the fuel nozzle. The flow rate of the combustion air is monitored using a sonic nozzle, and a series of thermocouples are used to measure the temperatures of the reactor wall and exhaust gas. The fuel flow rate is measured with a turbine meter, and the pressurized liquid fuel is forced through an interchangeable spray nozzle. The fuel flow rate, combustion airflow rate, wall temperatures, and exiting gas temperatures are continuously monitored and stored on a personal computer.

The burner is fired upward along the vertical axis of the chamber. A stepper-motor-driven traversing system translates the entire burner/chamber assembly permitting measurements of the spray at selected locations downstream of the nozzle. Note that the reactor exit is off-axis, which permits insertion from the ceiling of thermocouples and gas-sampling probes facing directly into the flame, but also makes the problem nonaxisymmetric. Flexibility of the facility will allow for modification to the axisymmetric configuration. The relevant dimensions necessary for modeling the multiphase combustion within the facility are presented in Fig. 2. Additional details on the design of the burner are available in Ref. 2.

The reacting fuel spray is characterized with a two-component phase Doppler interferometer (PDI). Information provided by the system includes statistics on the droplet size, axial and radial components of velocity, number density, and mass flux. Air velocity measurements, that is, mean and rms values, are also carried out using the PDI by adding seed particles to the combustion air or by using hot-wire probes. Gas-phase species concentrations are measured using Fourier transform infrared (FTIR) spectroscopy. An FTIR spectrometer equipped with a deuterated triglycene sulfate detector is used for extractive sampling of chemical species in the combustor emissions. A gas-sampling system, consisting of an air-cooled sampling probe, a heated gas line, and a vacuum pump, facilitates the transport of the sample gas extracted from the spray combustor into the single-pass gas cell in a continuous manner. The sampling probe was designed to aerodynamically quench chemical reactions occurring within the gases being sampled. The sampling gas line was also provided with a means for purging. Typically, the gas-sampling probe is inserted into the exhaust gas stream in such a way to probe the conditions at the selected exit plane (see Fig. 1). The extracted gas samples are analyzed with the FTIR spectrometer, and

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*Chemical Engineer, Stop 8640, Fire Safety Engineering Division, 100 Bureau Drive. Member AIAA.

†Mechanical Engineer, Stop 8360, Process Measurements Division, 100 Bureau Drive.

‡Group Leader, Stop 8360, Process Measurements Division, 100 Bureau Drive; cpresser@nist.gov.

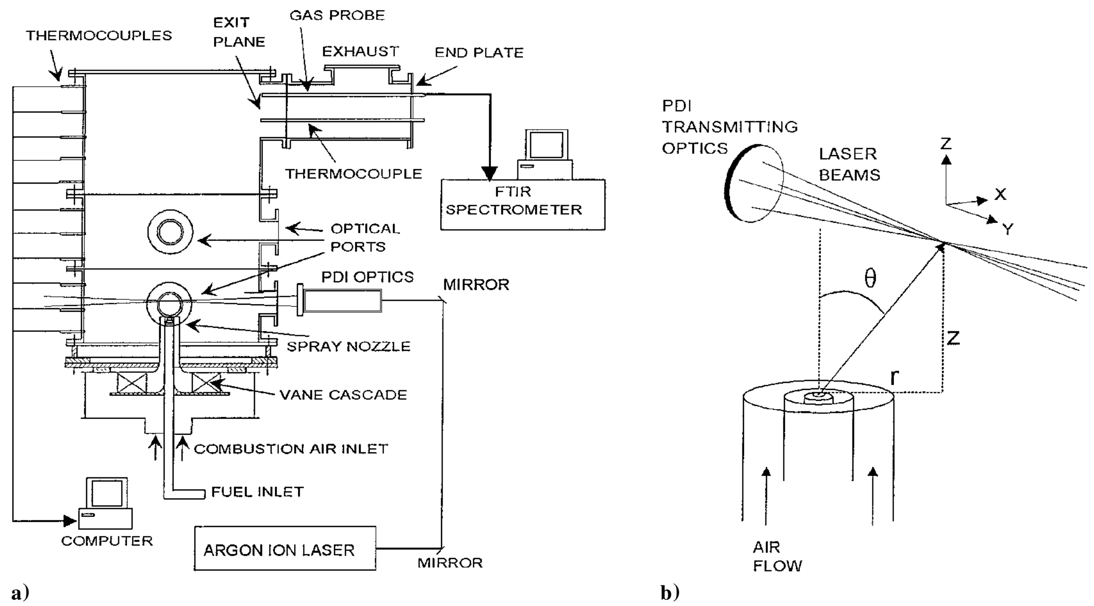

Fig. 1 Schematic of a) NIST reference spray combustion facility and b) downstream portion of the burner.

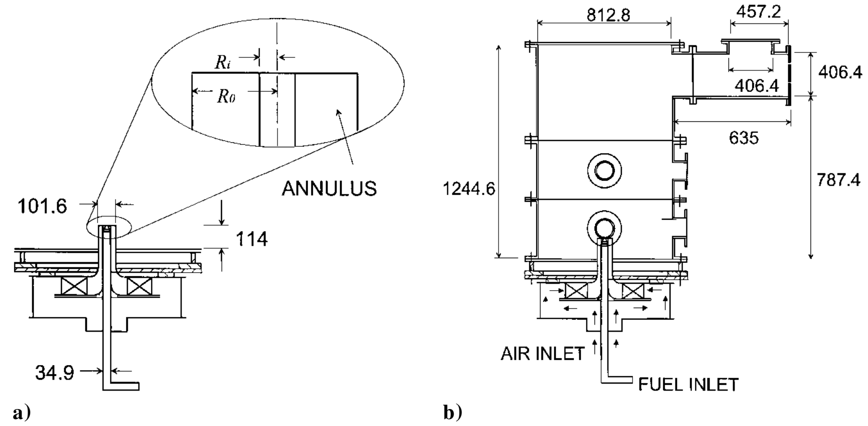

Fig. 2 Relevant dimensions (in millimeters) necessary to model the reference spray combustion facility.

the spectral data are recorded. These spectra are used to identify the major species present in the reactor emissions. Separately generated calibration spectra of each identified species are then used to quantify the species in the gas sample. A continuous emission monitor is used for monitoring NO_x in the exhaust gas.

Thermocouples (K type) are used to measure the wall temperature and the gas temperature at the exit of the reactor. The temperature of the exit gas is measured at the same locations where the species concentration data are obtained. The combined uncertainty is 3 and 5.5°C for the wall and gas temperatures, respectively. Fine-wire thermocouples (Pt–Pt/10% Rh) are used to estimate the gas temperatures within the reactor chamber. High-sensitivity heat flux microsensors are used to measure the radiation heat transfer to the chamber walls.

Baseline Case

The reference spray combustion facility at the National Institute of Standards and Technology (NIST) has been fabricated to develop a benchmark database that can be used for input and validation of multiphase combustion models. If such a database is to be used successfully for validation purposes, it is necessary that extensive measurements are made and that uncertainties in the measurements are quantified. Because of the vast amount of experimental effort required, it is prudent to initially limit the scope to a single operating condition (fuel flow rate, airflow rate, vane angle, etc.). After the system has been thoroughly characterized for the baseline case, new operating conditions will be chosen based on feedback from collaborators attempting to simulate the combustion process within the reactor.

All relevant information regarding boundary and operating conditions is presented in Ref. 2. Methanol was chosen as the fuel for the baseline case because the thermodynamic and kinetic data necessary to model the gas-phase combustion are readily available.[3] The fuel is forced through a pressure-jet nozzle and forms a hollow-cone spray with a nominal 60-deg full cone angle. A parallel program is underway to develop a reference atomizer with well-defined droplet size and velocity distributions. The atomizer will then provide known spray characteristics at the inlet, thus reducing the uncertainty in this very important inlet condition. The fuel and air are delivered to the reactor at ambient temperature and flow rates of 3.0 ± 0.02 $\mathrm{kg \cdot h^{-1}}$ and 56.7 ± 1.7 $\mathrm{m^3 \cdot h^{-1}}$, respectively. For the baseline case, the vane angle is maintained at 50 ± 1 deg. Recent CFD modeling of the vane cascade and combustion air passage yields a swirl number[4] of $S \approx 0.49$, and the predicted velocity profile at the inlet of the reactor is in good agreement with experimental measurements.[5,6] Turbulence intensity measurements at the combustion air inlet plane are in progress.

Sample PDI data characterizing the reacting fuel spray at seven elevations downstream of the nozzle are shown in Figs. 3 and 4. Figure 3 presents the mean axial velocity of the droplets as a function of radial position in the reactor. As expected, the mean velocity decreases with axial position due to the drag on the droplets, and

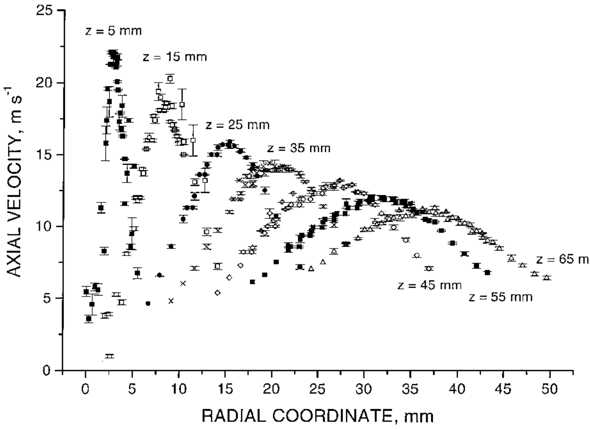

Fig. 3 Variation of the droplet mean axial velocity with radial position at seven axial positions downstream of the nozzle; measurements carried out with a PDI.

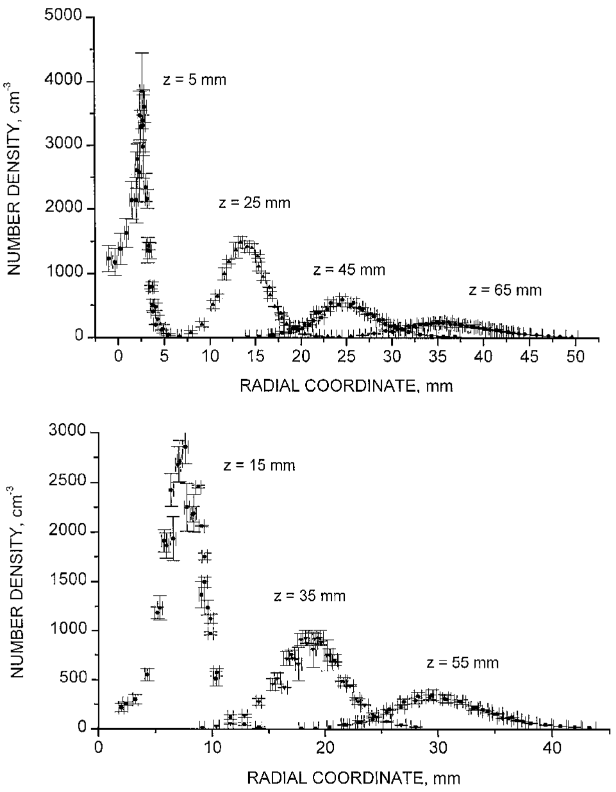

Fig. 4 Variation of the droplet number density with radial position at seven axial positions downstream of the nozzle; measurements carried out with a PDI.

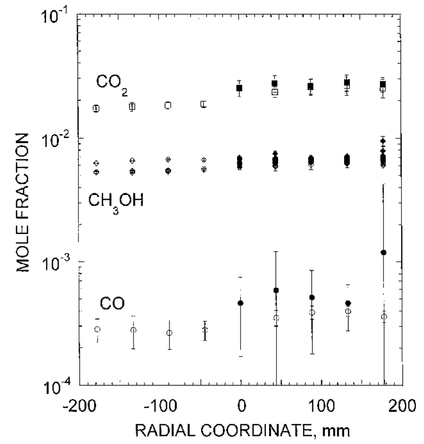

Fig. 5 Variation of major species concentrations with radial position at the reactor exit plane, measured using FTIR spectroscopy.

it peaks in the center of the spray where the droplets possess the highest momentum. Figure 4 presents the mean droplet number density measured in the spray at the same seven elevations presented in Fig. 3. The error bars in Figs. 3 and 4 correspond to type A uncertainties and do not include the type B uncertainties associated with the PDI. Type A uncertainties are those that can be quantified using a statistical analysis, whereas type B uncertainties are those related to the experimental technique that cannot be addressed using statistical methods.[7,8] The reader is referred to Ref. 2 for further details on the uncertainties in the measurements.

Measured species mole fractions in the exhaust gas are presented in Fig. 5. The measurements were obtained using the described extractive sampling method and analyzed using FTIR spectroscopy. Because an extractive sampling method is used, it is not possible to measure unstable reaction intermediates. The open and filled symbols in Fig. 5 correspond to the vertical and horizontal profiles, respectively. It is evident from Fig. 5 that the species concentrations for CO_2, CO, and CH_3OH are relatively uniform across the exit plane due to adequate mixing occurring within the reactor prior to the gases entering the exhaust duct (see Fig. 1). The error bars in Fig. 5 correspond to the expanded standard uncertainty with a coverage factor $k = 2$ and roughly indicate a 95% confidence interval.[7,8] The relatively large uncertainties in the CO concentrations (horizontal profile) are attributed to the relatively low concentrations, day-to-day fluctuations, and short path length of the absorption cell in the FTIR spectrometer. As is, the data are useful for model validation, and the uncertainty can be reduced with a longer absorption cell if numerical/experimental comparisons warrant it. Again, emphasis is placed on being receptive to the needs of the modeling community. The species concentration measurements presented in Fig. 5 were used to verify that mass was conserved during the experiments and to determine the extent of fuel conversion.

Conclusions

A reference spray combustion facility is currently operational and being used to develop a benchmark database for input and validation of multiphase combustion models and submodels. The baseline case consists of a methanol spray flame that has been characterized using a variety of diagnostics, including PDI and FTIR spectroscopy. In addition, considerable effort has been made to characterize completely the boundary conditions, including development of a reference atomizer and characterization of the combustion air that enters the reactor. Potential collaborators interested in modeling the facility or carrying out industry-specific experiments at NIST are encouraged to contact the authors for copies of Refs. 2, 5, and 6 that detail the results and include electronic files of the data. NIST also makes the reference spray combustion facility available to outside industrial and academic researchers wishing to participate in collaborative research.

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Role of Curing Agents on Decomposition and Explosion of Glycidyl Azide Polymers

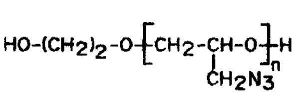
Surendra P. Panda,* Sanjay K. Sahu,† Dinkar S. Sadafule,‡
and Jyotsna V. Thakur§
Institute of Armament Technology,
Girinagar, Pune 411 025, India

Introduction

GLYCIDYL azide polymers (GAPs) (Fig. 1) cured with diisocyanates have been investigated rather extensively for use as propellants for ram rockets.[1–5] These propellants, in addition to being fuel rich and liberating large amounts of H_2, CO, and gaseous hydrocarbons on their burning in the primary chamber, are greatly insensitive to impact and provide high burning rates.[5] Their decomposition pattern is also not affected by increased pressure.[6] However, the decomposition products of cured GAPs contain HCN, which is highly toxic. Though attempts have been made to suppress HCN in the gaseous decomposition products by using copolymers of GAPs with high hydrocarbon content,[7] no attempt has been made to use diisocyanates to cure GAPs with increasing hydrocarbon content to achieve the same purpose. Further details of the explosive behavior of GAPs and their cured products are not available in the literature. In this Note, hydroxy-terminated GAPs with $\overline{Mn}$, 1100 and 2150 cured with toluene diisocyanate (TDI) (Fig. 2), isophorone diisocyanate (IPDI) (Fig. 3), and 4,4′-dicyclohexylmethane diisocyanate (H_{12}MDI) (Fig. 4) have been investigated to elucidate the decomposition mechanism, suppress HCN in the decomposition products, and generate data on their explosive behavior.

Materials and Methods

GAPs with two OH groups per molecule with average molecular weights 1100 and 2150 were synthesized by reacting the corresponding polyepichlorohydrin (PECH) with sodium azide in dimethyl sulfoxide (DMSO). Dihydroxy PECHs were in turn synthesized by activated monomer polymerization of epichlorohydrin using BF3-ethylene glycol complex as the catalyst.[8] These polymers were cured with TDI, IPDI, or H_{12}MDI with trimethylol propane (TMP) as a triol crosslinker and dibutyl tin dilaurate (DBTDL) as catalyst at 333 K to be used as ram rocket propellants. TDI, IPDI, and H12MDI (Fluka Chemika, laboratory grade) were obtained commercially and used as received for the cure of the GAPs.



$$HO\text{-}(CH_2)_2\text{-}O\text{-}\left[CH_2\text{-}\underset{CH_2N_3}{CH}\text{-}O\right]_n\text{-}H$$

Fig. 1 GAP.

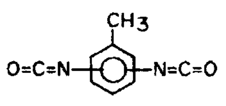


Fig. 2 TDI

(2, 4 isomer, 80% + 2, 6 isomer, 20%)

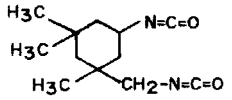


Fig. 3 IPDI.

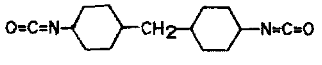


Fig. 4 H_{12}MDI.

Cured GAP samples were decomposed by taking about 270 mg of a sample in a 100-ml round-bottom flask fitted with a side tube and a vacuum tap and heating it after evacuation in a concentrated H_2SO_4 bath up to 543 K. The gases evolved were collected in an evacuated gas analysis cell of an IR spectrometer fitted with NaCl windows. Fourier transform infrared (FTIR) spectra were recorded using a Perkin–Elmer FTIR spectrophotometer, Model 1605, for the analysis of the gaseous mixture.

Ionodes (ion selective electrodes) are simple, potentiometric sensors that respond to the concentration of an ion in a solution. About 1.08 g of cured GAP ($\overline{Mn}$, 2150) was taken in a 100-ml flask fitted with a side tube and a vacuum tap. The flask was heated after evacuation in a concentrated H_2SO_4 bath up to 543 K. The water-soluble and acidic gases evolved were absorbed by 30 ml of 10% NaOH solution to convert HCN to CN^-. Three sets of test solutions with unknown CN^- content were prepared by using GAP cured with TDI, IPDI, and H_{12}MDI separately.

A standard AgCN solution (CN^- content 100 ppm) was taken in a beaker containing a reference electrode (polymer body Ag-AgCl type) and a CN^--sensitive electrode. A digital p_H meter was used to calibrate CN^- concentration in terms of mV. Three more readings were noted for the solutions containing CN^- diluted to 10, 1, and 0.1 ppm. Similarly, the test solutions were measured for their CN^- concentrations by converting mVs produced by the cyanide-specific ion electrode.

Measurements of temperature of explosion of uncured and cured samples of GAPs were carried out in a special apparatus. This apparatus consists of a 10-cm-diam cylindrical copper block with a 2.5-cm-diam and 7-cm-depth cavity. It contains Wood's metal with a melting point of 338 K as the bath material, which can be heated up to 623 K. Approximately 5 mg of sample material was taken in an aluminum cup with a 5-mm diam and 2-mm height. The cup was covered with an aluminum cap. The Wood's metal bath was then electrically heated. The heating rate was controlled by a dimmerstat, and the bath temperature was monitored by a thermometer. When the desired temperature was reached, the current was controlled. The aluminum cup containing the sample was introduced into the bath, and a stopwatch was started. After a certain time interval the sample exploded with flash, and the stopwatch was instantly stopped. This reading represented the explosion delay. Thus, readings were taken at successive temperature intervals of 1 K until a temperature was reached at which the explosion delay was less than 5 s. The temperature corresponding to the 5-s explosion delay is usually referred to as the explosion temperature.

Energy of activation for explosion was calculated by using the equation

$$t = Ce^{E/RT} \tag{1}$$

where t is explosion time lag, E is energy of activation, T is absolute temperature, C is a constant (depending on the composition of the explosive), and R is universal gas constant (1.986 cal/g). This expression can be rewritten as

$$\log t = B + E/(2.303 \times 1.986)T \tag{2}$$

where B is a constant.

On plotting $\log t$ against $1/T$, a straight line is obtained. The slope of the plot is equal to E/R, from which the energy of activation for explosion can be calculated.

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*Associate Director and Dean, and Chairman, Faculty of Explosives and Applied Chemistry; panda@iat.ernet.in.

†Senior Research Fellow, Faculty of Explosives and Applied Chemistry.

‡Technical Officer 'B,' Faculty of Explosives and Applied Chemistry.

§Technical Assistant 'B,' Faculty of Explosives and Applied Chemistry.