

EFFECT OF DODECANOL CONTENT ON THE COMBUSTION OF METHANOL SPRAY FLAMES

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The structure of a swirl-stabilized spray flame, fueled by a 75/25 mixture (by volume) of methanol and dodecanol has been examined. Spatially resolved information on droplet size and velocity distributions was obtained under burning conditions using a phase Doppler interferometry system. The effect of system gain (i.e., voltage setting of the photomultiplier tube detectors and laser power) on interpretation of the results was also assessed.

The relatively large volatility difference between methanol and dodecanol provided an opportunity to examine the occurrence of microexplosions within spray flames. Evidence of microexploded droplets was revealed by a sudden decrease in droplet size and velocity, and an increase in number density at different spatial positions within the flame. On this basis, results were obtained that indicated the occurrence of microexplosions in the 75/25 mixture flame, but at a reduced extent as compared to prior results reported for methanol flames containing a larger fraction of dodecanol.

1. INTRODUCTION

The combustion of liquids is important to many industrial processes involving energy conversion and disposal of liquid hazardous wastes via spray-fired incineration. In such practical applications, the fuel is invariably a blend of several constituents, which exhibit a range of physical properties and volatilities. Composition, in particular, can influence such aspects of spray combustion as atomization, vaporization, and particulate

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(e.g., soot) formation processes. Recent work has addressed the role of fuel composition on the combustion of sprays, using binary mixtures of miscible liquids that have well-characterized physical properties [1–3]. The present study builds upon these ongoing efforts to examine more fully the structure of spray flames generated from miscible mixtures of methanol and dodecanol. This composition represents a relatively nonsooting fuel that allows one to examine spray flame structure without the complicating effects of soot. Furthermore, the relatively large difference in volatility between methanol and dodecanol creates the potential for secondary atomization or “microexplosion” of droplets with the burning spray (the vapor pressure of methanol is approximately 203 kPa at 357 K, and dodecanol is about 0.1 kPa). This effect is considered to be beneficial to the combustion process, yet few prior studies have examined sprays (previous investigations have examined microexplosions from the perspective of single droplets [4, 5]).

Microexplosions are strongly dependent on the mixture composition, the volatility (boiling-point) difference between the mixture components, and the liquid-phase transport processes that contribute to internal concentration gradients within burning droplets. Composition plays a strong role, since the threshold temperature (the homogeneous nucleation limit) that triggers microexplosions is highly dependent on liquid composition. Internal concentration gradients, in particular, are a necessary condition for microexplosions to occur during gas-phase combustion of droplets that are miscible mixtures of liquids [4]. These concentration gradients are enhanced by internal circulation within the droplet [6], which is formed by the relative motion between the droplet and ambience.

Evidence from methanol/dodecanol single-droplet studies implies an important role for internal circulation; namely, microexplosions are found to occur for moving droplets [4], whereas none are detected for stationary droplets of the same mixture composition that burn under spherically symmetric conditions [5]. Certainly, the relative velocity between droplets and ambience is large at various positions within spray flames, which, in turn, promotes internal circulation. At such positions, microexplosions can conceivably occur as a result of the internal circulation pattern, which can distribute the mixture components in a manner favorable for achieving internal superheat conditions and microexplosions.

Evidence for microexplosions in studies of single droplets has traditionally been based on direct photographic imaging of single droplets [4, 5]. By contrast, the comparatively smaller size of droplets found in spray flames (generally under 100 μm) and relatively higher velocities (reaching values of 20 m/s) make it difficult to photograph individual droplets. Photographic methods applied to sprays provide images that are suggestive of the occurrence of microexplosions [1]. Therefore, alternative techniques to photographic imaging, such as the application of nonintrusive laser diagnostics, are of interest. Recent work [1, 2] used information obtained from phase Doppler interferometry [7] to infer the presence of microexplosions in spray flames. An equivolume mixture of methanol and dodecanol was studied because of the above-mentioned internal superheat arguments, which were thought to promote microexplosions. Spatially resolved measurements were carried out to obtain droplet size and velocity distributions within the spray flame. Evidence of microexplosions was indicated by a sudden decrease in droplet size and velocity, and an increase in number density when compared to a pure methanol flame. If microexplosions are not present, then droplet mean size and velocity would increase, and number density would decrease because of the presence of the more viscous dodecanol [2].

In the present investigation, the objective was to determine the extent to which microexplosions occurred during combustion of a particular mixture composition of methanol and dodecanol. The phase Doppler system was used under identical operating conditions to obtain spatially resolved information on droplet size and velocity for a 75/25 mixture (by volume) of methanol and dodecanol. The results were then compared with those of the aforementioned experiments.

2. EXPERIMENTAL ARRANGEMENT

Experiments were carried out in a spray combustion facility that was designed to simulate practical combustion systems. The facility includes a swirl burner with a movable 12-vane swirl cascade; the vanes are rotated simultaneously to impart the desired degree of swirl intensity to the co-flowing combustion air stream. The spray facility permits examination of the effects of combustion air swirl, atomizer design, fuel type, and air preheat on spray structure and combustion characteristics. The swirl strength introduced to the combustion air is given in terms of the swirl number, S , which is determined according to the theory outlined in [8]. Experiments were carried out for $S = 0.53$ under burning conditions.

A simplex pressure-jet nozzle was operated at total air and fuel flow rates of 64.3 kg/h and 3.2 kg/h, respectively. The pressure-jet nozzle provides a nominal 60° hollow-cone spray. The spray is injected vertically upward from the nozzle, located at the centerline and exit of the burner. A stepper-motor-driven, three-dimensional traversing arrangement is used to translate the burner assembly in the vertical (Z) and both horizontal (X and Y) directions. All optical diagnostics are fixed in position about the burner assembly, so that the burner can translate independently of the optical equipment. This arrangement permits precise alignment of the measurement volume within the spray (see Fig. 1). Measurement of radial profiles of the spray flame properties, e.g., droplet size and velocity distributions, can then be carried out at different axial positions. The radial profiles are obtained for the same nozzle orientation. Further details on the experimental arrangement are given elsewhere [9].

Droplet size and velocity distributions were measured using a single-channel phase Doppler interferometer [7]. The instrument provides in-situ nonintrusive measurements at different positions within the spray. For these experiments, an off-axis light collection system was used, with the optics positioned at a scattering angle of 30° (see Fig. 1). The focal lengths of the transmitting and receiving optics were 495 and 500 mm, respectively. The focal length of the collimating lens was 300 mm. A 10-mW He-Ne laser, operating at a wavelength of 632.8 nm, provided the light source for the methanol and 50/50 methanol/dodecanol mixture flames. An upgraded system, incorporating a 4-W cw Ar-ion laser and operating at a wavelength of 514.5 nm was used for the 75/25 mixture flame. The laser was operated at 400 mW for the measurements presented in this article. The signal data rate was kept at a relatively low value (approximately 200 Hz) by adjusting the supply voltage to the photomultiplier tube (PMT) detectors. The approach kept the sample duration time relatively constant across the entire radial profile. Data were also acquired by optimizing the system gain to detect the maximum number of droplets without saturating the PMT detectors and thus affecting the signal-to-noise level. This was accomplished by setting the PMT voltage (for a specified laser beam intensity) at a level

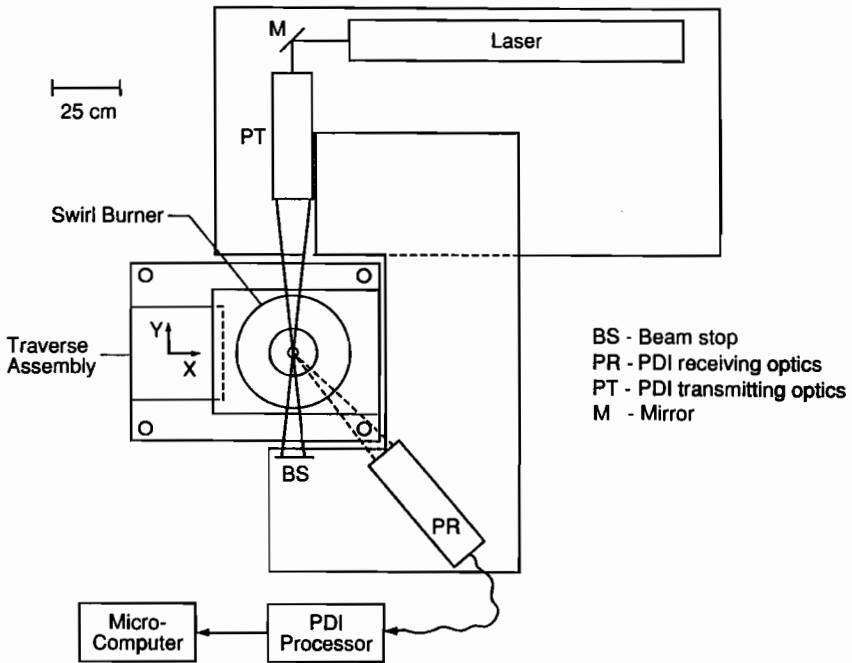


Fig. 1 Schematic of experimental spray combustion facility: BS, beam stop; M, mirror; PR, PDI receiving optics; PT, PDI transmitting optics.

commensurate with the maximum value of volume flux [10, 11]. This value generally corresponded to the instrument operating procedures recommended by the manufacturer. Although these two approaches may have certain constraints, they represent extremities in the operation of the instrument. Generally, the instrument is calibrated with well-characterized monodispersed sprays, and therefore it is expected that the results will be accurate and have minimal data rejection. For these polydisperse sprays, the data rejection rate was within 15% of the total number of recorded points and was similar for both systems. Measurements were repeated several times on both sides of the flame. The measurement repeatability was generally better than 5% near the nominal spray boundary.

3. RESULTS AND DISCUSSION

3.1 Effect of System Gain

Fundamental to the use of a phase Doppler system is selection of the appropriate system gain. Detection of microexplosions was considered to rest on the ability to resolve comparatively small differences in the measured values of droplet mean size, velocity, and number density at various positions within the examined spray flames. Spray flames generally contain a wide range of droplet sizes, ranging from submicrometer droplets to droplet diameters of several hundred micrometers. Detection of all droplets encountered in the measurement volume of the phase Doppler interferometer can be a formidable task

in dense regions of the spray. To optimize detection of droplets in these regions, the system gain is set such that the PMT detectors are not saturated by the larger droplets and yet remain sensitive enough to detect the smaller sizes. Alternatively, multiple measurements must be recorded and combined during postprocessing of the data to determine the appropriate statistics. The system gain of the phase Doppler instrument can be affected by the PMT voltage setting, laser power, and other parameters. It is therefore important to determine how the system gain influences the measurements, especially with regard to the occurrence of microexplosions.

Data from the phase Doppler instrument were recorded at two different operating conditions. In the first case, the data rate was kept low, at approximately 200 Hz (i.e., "low-data-rate" case), in order to keep the sample duration time relatively constant across the entire radial profile. The results presented in this article were recorded for this condition. In the second case, the PMT voltage was changed to optimize detection of the droplets (i.e., "optimum-gain" case), such that the voltage at each point was adjusted to achieve a maximum in volume flux [10]. This criterion appeared to parallel, in most regions of the spray flames, the procedures recommended by the manufacturer (i.e., when the PMT detectors begin to saturate).

Figures 2–4 present the results obtained for droplet Sauter mean diameter (D_{32}), number density (\bar{N}), and axial velocity (\bar{U}), respectively, at axial positions (z) of 10, 25.4, and 76.2 mm. The solid boxes along the abscissa indicate the position of the burner passage walls, with the fuel nozzle located at the centerline. Data were recorded for the 75/25 mixture flame at the two above-mentioned instrument operating conditions. The results indicate that, at $z \leq 25.4$ mm, there are significant differences in the values of D_{32} , \bar{N} , and \bar{U} measured across the profiles. This is to be expected, since the optimum-gain case detects more smaller droplets (resulting in a strong signal with a high data rate); the threshold level for the low-data-rate case is too high to detect smaller droplets. For example, Fig. 5 presents the size and velocity distributions at a radial position (r) of 15.2 mm and an axial position of 25.4 mm for the two cases. The optimum-gain case (see Fig. 5B) shows the detection of many smaller droplets and development of a second lower-velocity peak in the distribution as compared to the low-data-rate case (see Fig. 5A). As a result, the mean value for D_{32} decreases from 58.5 to 46.3 μm , \bar{U} decreases from 19.3 to 14.2 m/s, and \bar{N} increases from 4.2×10^2 to 2.2×10^3 particles/cm³ for the optimum-gain setting. At $z \geq 50.8$ mm, the results indicate negligible difference between the two readings. This is to be expected because of droplet vaporization and dispersion with increasing axial position. The measurement therefore requires a high PMT voltage to maintain a low data rate; i.e., the two instrument settings are essentially the same at downstream positions. The relevance of these results is that, at $z = 50.8$ and 76.2 mm, the instrument system gain has negligible influence on the measured trends.

Variation of the mean droplet properties (i.e., D_{32} , \bar{N} , and \bar{U}) with axial position is also dependent on the instrument operating conditions (see Figs. 2–4). For the low-data-rate case, the maximum value of D_{32} near the spray boundary (defined by the peaks in the D_{32} profiles) decreases with increasing axial position from approximately 80 μm at $z = 10$ mm to 60 μm at $z = 76.2$ mm (see Fig. 2). This is attributed to detection of primarily larger droplets as they undergo vaporization. This trend is opposite to that indicated by the optimum-gain case (the maximum value of D_{32} changes from approximately 40 to 60 μm with increasing axial position, since the rapid vaporization of the smaller droplets tends to increase the mean diameter), and to observations generally reported in the literature for

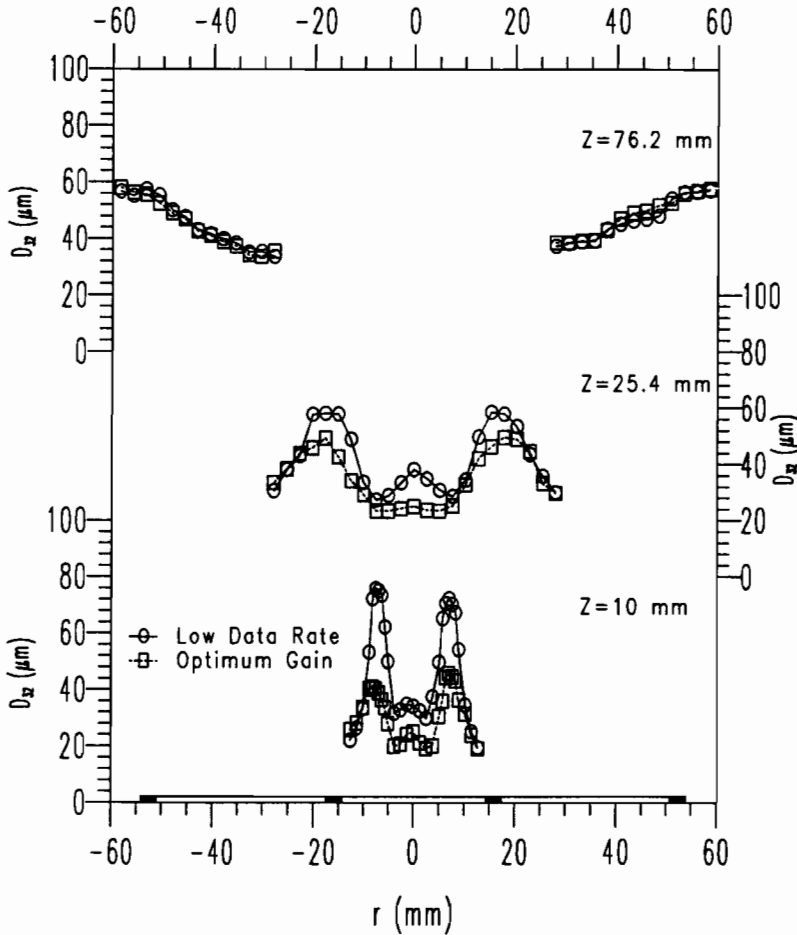


Fig. 2 Variation of droplet Sauter mean diameter (D_{32}) with radial position (r) at different axial positions (z) at two different instrument operating conditions for the 75/25 methanol/dodecanol mixture flame.

nonburning sprays [9]. The maximum value of number density near the spray boundary (see Fig. 3) decreases with increasing axial position for the optimum-gain case (from $\bar{N} \approx 2 \times 10^4$ particles/cm³ at $z = 10$ mm to 5×10^2 particles/cm³ at $z = 76.2$ mm) and remains relatively unchanged for the low-data-rate case (at $\bar{N} \approx 5 \times 10^2$ particles/cm³). The maximum value of mean axial velocity decreases with increasing axial position for both cases (from $\bar{U} \approx 25$ m/s to 6 m/s for the low-data-rate case, and from $\bar{U} \approx 18$ m/s to 6 m/s for the optimum-gain case). The relevance of these trends is that at downstream positions there are primarily larger droplets. If there is a sudden abundance of smaller droplets, this may be indicative of the occurrence of microexplosions.

In addition to PMT voltage, it is also important to ascertain that the laser power does not influence the results, since two different phase Doppler systems (with lasers of

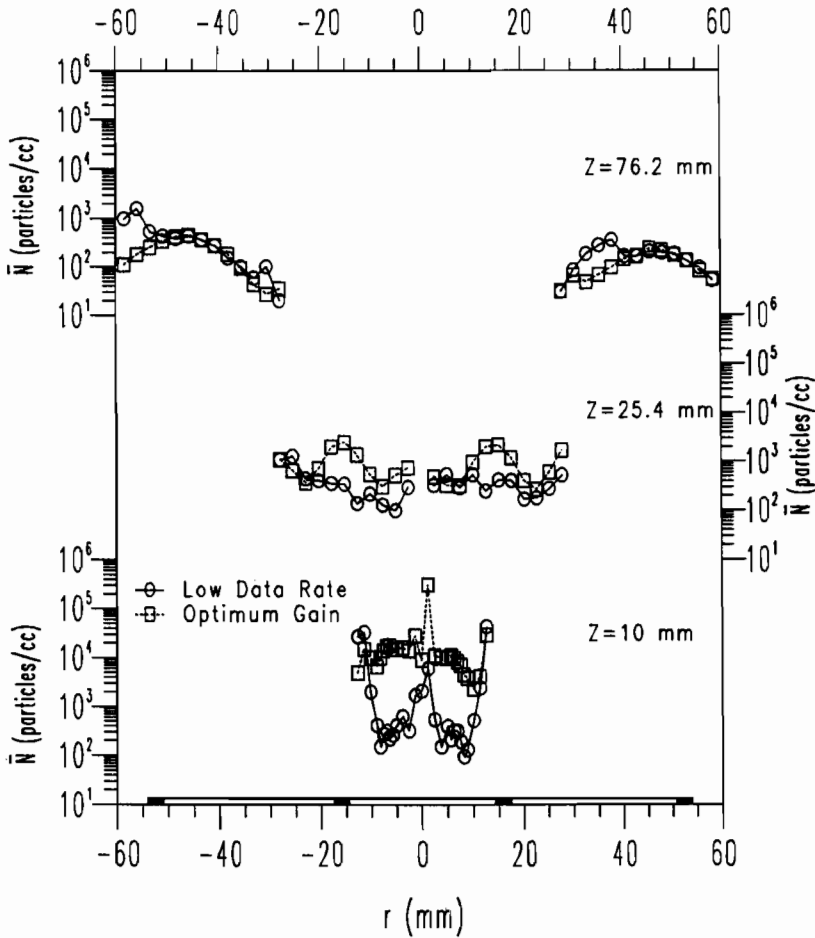


Fig. 3 Variation of droplet number density (\bar{N}) with radial position (r) at different axial positions (z) at two different instrument operating conditions for the 75/25 methanol/dodecanol mixture flame.

different power) were used. Figure 6 presents the effect of PMT voltage on the droplet mean size (see Fig. 6A) and axial velocity (see Fig. 6B) at four different laser beam intensities of 10, 125, 200, and 400 mW, and for $r = 0$ and $z = 10$ mm. The results indicate that the PMT voltage has a significant effect on the values of D_{32} and \bar{U} for a preset laser power. This effect is the same for the droplet number density (data not presented). It is also observed that the number density (and volume flux) does not reach a maximum value at each measured position. A maximum value is generally achieved in regions near the spray boundary, where the data rate is high. For the case when no maximum value is found, the PMT voltage is set according to the recommended procedures of the manufacturer. Figure 6 indicates that as the laser power increases, lower PMT voltages are required to maintain a particular value of droplet mean velocity (or size).

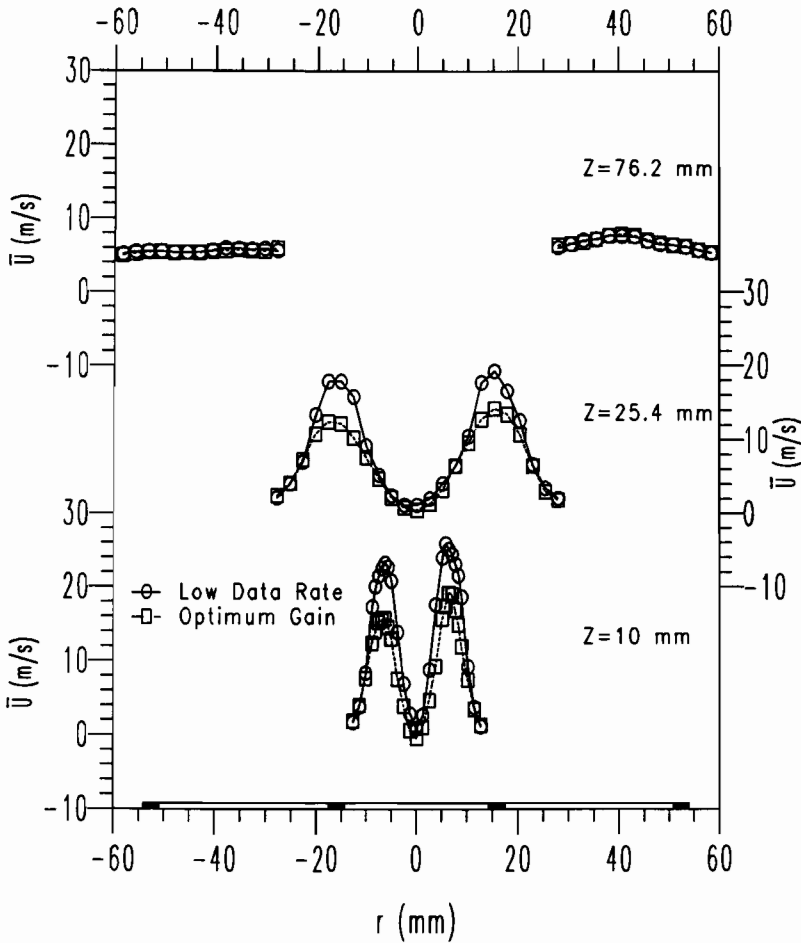


Fig. 4 Variation of droplet mean axial velocity (\bar{U}) with radial position (r) at different axial positions (z) at two different instrument operating conditions for the 75/25 methanol/dodecanol mixture flame.

Therefore, the use of two different lasers with the phase Doppler system should have negligible influence on the results, provided the detector voltage is adjusted appropriately.

3.2 Droplet Mean Diameter, Number Density, and Velocity

The Sauter mean diameter (D_{32}) and number density (\bar{N}) are presented in Figs. 7 and 8 for the pure methanol, 50/50, and 75/25 methanol/dodecanol mixture flames at axial positions of $z = 10, 25.4, 50.8,$ and 76.2 mm. The measurements were carried out with the phase Doppler system operating under the low-data-rate condition. A limited data set is presented for $z = 50.8$ and 76.2 mm because of the very low data rate in the central region of the spray flame. The variation of D_{32} with spatial position is typical of hollow-cone, pressure-atomized spray flames. The droplets near the spray boundary are larger

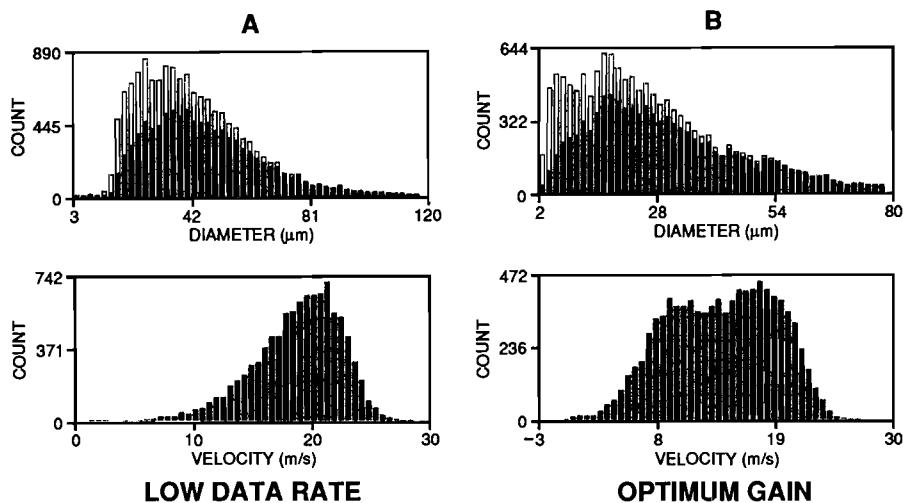


Fig. 5 Distribution of droplet size and velocity for the (A) low-data-rate and (B) optimum-gain operating conditions of the phase Doppler system with the 75/25 methanol/dodecanol mixture flame at $r = 15.2$ mm and $z = 25.4$ mm.

than those near the spray centerline in the upstream portion of the spray. The profiles become more uniform with increasing axial position. At $z = 10$ mm the values of D_{32} are similar for all three flames near the spray boundary and toward the center of the spray.

Variations in the spray characteristics as a result of droplet vaporization and dispersion results in an increase in droplet mean size and decrease in number density with increasing axial position. If microexplosions occur at a particular spatial position in the methanol/dodecanol mixture flames, one expects a different trend, namely, a decrease in the value of D_{32} and an increase in \bar{N} . In addition, dramatic changes in these properties would provide further evidence for the presence of microexplosions. As a basis of comparison, methanol is used because of its similar chemical properties to the mixtures and its inability to microexplode during combustion (since it is a single-component liquid).

Microexplosions are not present at upstream positions, because the droplets do not experience the necessary period of liquid-phase heating; the threshold temperature that triggers microexplosion is not reached within the droplet. Farther downstream (at $z \geq 50.8$ mm), the droplet mean diameter (see Fig. 7) for the 50/50 mixture flame becomes significantly smaller and number density becomes noticeably higher (see Fig. 8) near the spray boundary than for the methanol flame. The value of D_{32} was determined to lie within the range of ± 1 μm for these data with a 95% confidence level, indicating that the variation in the measurements is not responsible for the reported trends. The reduced mean size and increased number density for the 50/50 mixture flame is indicative of the occurrence of microexplosions, as discussed earlier [1]. It is expected that droplet mean size would be larger than the sizes obtained for the methanol flame if microexplosions are not present (the increase in the values of D_{32} would be at least 8 μm , see Fig. 7). The droplet mean size and number density for the 75/25 mixture flame remain similar to that of methanol. These results suggest that microexplosions occur near the spray boundary at

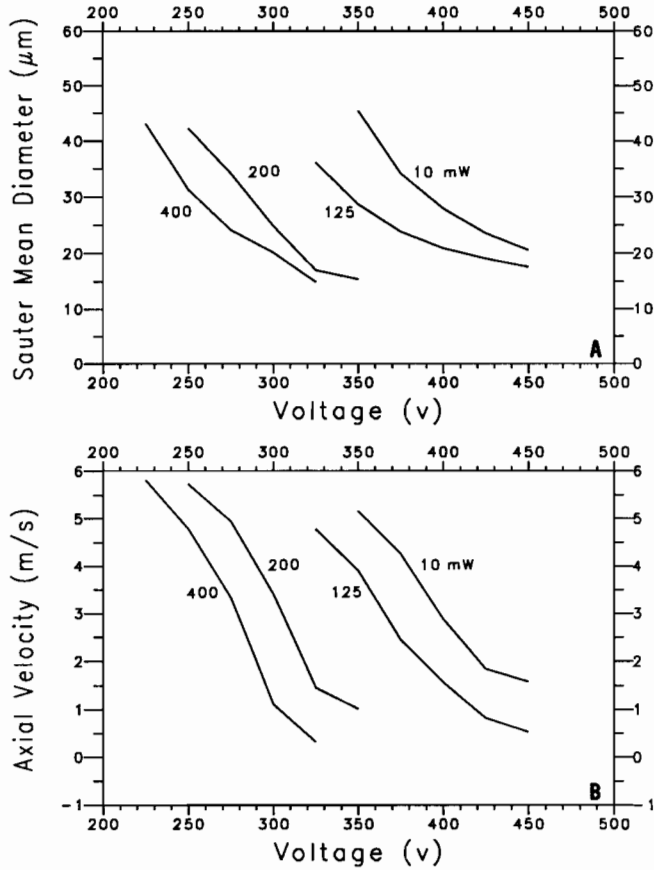


Fig. 6 Variation of droplet mean (A) size and (B) axial velocity with PMT voltage at different laser powers for the 75/25 methanol/dodecanol mixture flame at $r = 0$ and $z = 10$ mm.

$z \geq 50.8$ mm for the 50/50 mixture flame, whereas the mean properties provide little or no evidence of microexplosions in the 75/25 mixture flame. It is noted that the decrease in the value of D_{32} presented in Fig. 7 for the 50/50 mixture flame relative to methanol or the 75/25 mixture flame at $z = 50.8$ and 76.2 mm is not believed to result from a shear-induced breakup of the droplets. The droplet velocities and diameters, and corresponding Weber numbers, were significantly smaller than the value considered necessary for such a breakup mechanism to be operative (the maximum value of Weber number was approximately 2 near the spray boundary at $z = 10$ mm) [12].

Radial profiles of droplet mean axial velocity (\bar{U}) for methanol and the two mixture flames are presented in Fig. 9 at $z = 10, 25.4, 50.8,$ and 76.2 mm. The mean velocity profiles are characteristic of the overall structure of hollow-cone spray flames, viz., the highest droplet velocities are found near the spray boundary. The results indicate that the value of \bar{U} decreases with higher dodecanol content near the spray boundary. This trend may be reasonable, since denser fuels will create larger droplets with lower velocities

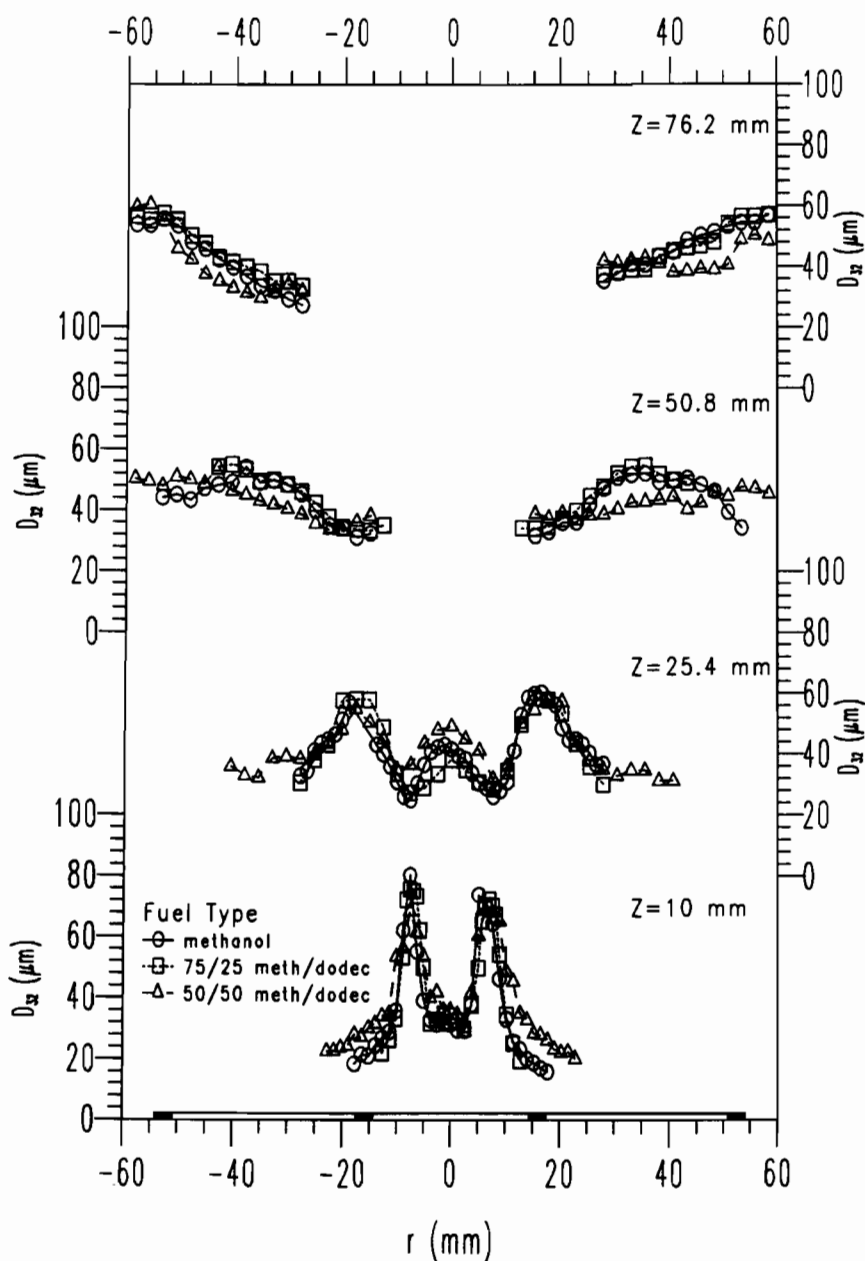


Fig. 7 Variation of droplet Sauter mean diameter (D_{32}) with radial position (r) at different axial positions (z) for the methanol and two methanol/dodecanol mixture flames.

(during the atomization process) for a given initial droplet momentum. However, since droplet mean size is expected to decrease in regions where microexplosions occur, the corresponding decrease in droplet velocity may be attributed to rapid droplet entrainment

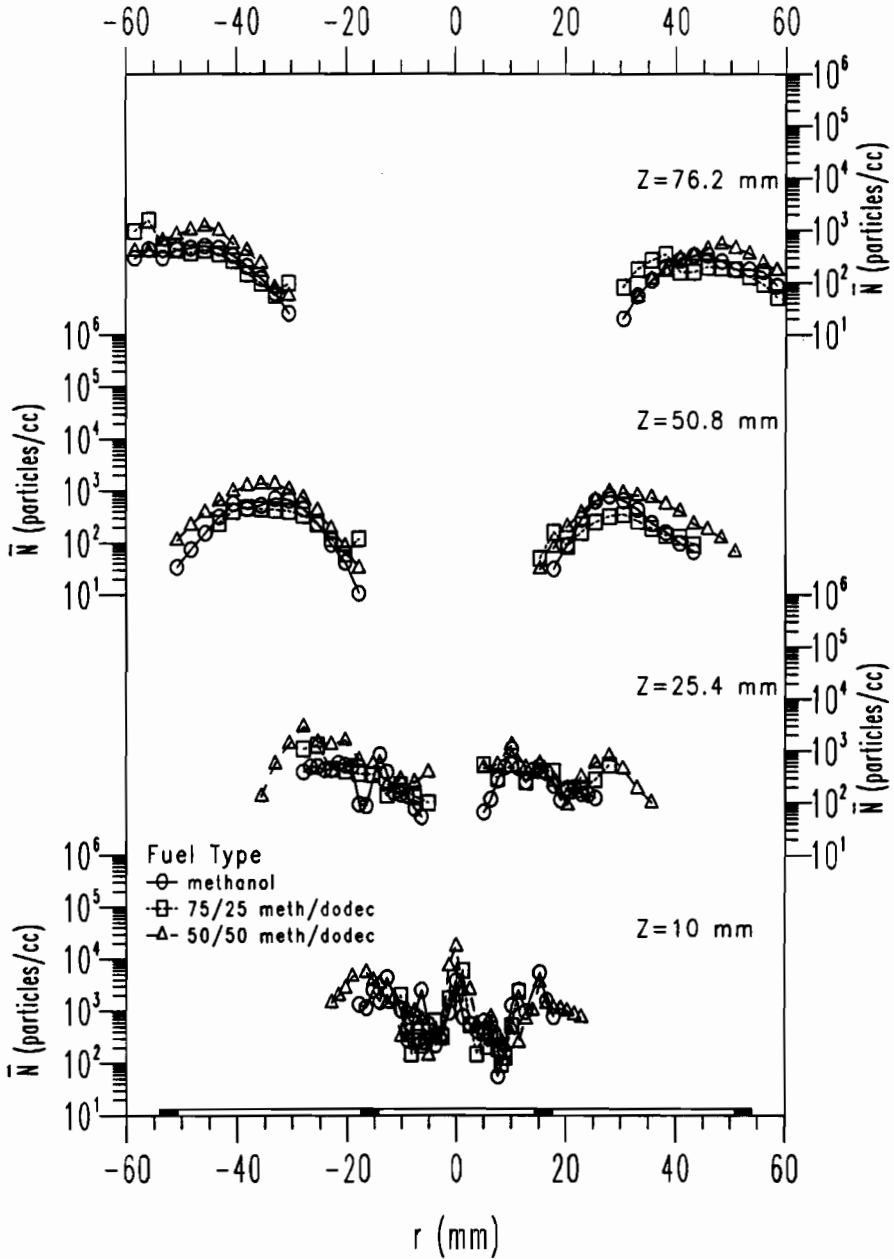


Fig. 8 Variation of droplet number density (\bar{N}) with radial position (r) at different axial positions (z) for the methanol and two methanol/dodecanol mixture flames.

into the air flow field and subsequent deceleration. These trends may be further substantiated by examining changes in the size and velocity distributions, and size/velocity correlations with spatial position, as discussed in the next section.

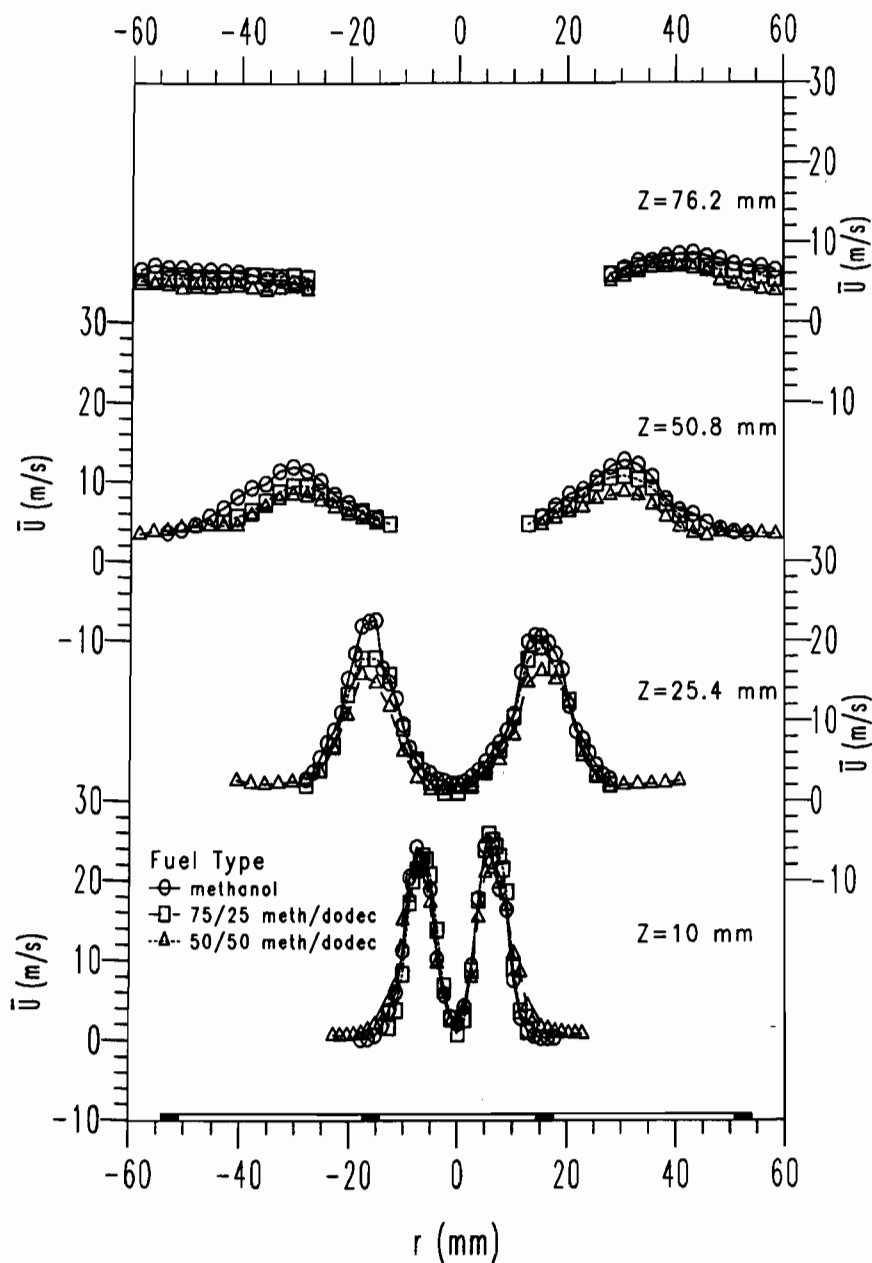


Fig. 9 Variation of droplet mean axial velocity (\bar{U}) with radial position (r) at different axial positions (z) for the methanol and two methanol/dodecanol mixture flames.

3.3 Size and Velocity Distributions

The droplet size and velocity distributions were found to vary significantly with spatial position in the investigated spray flames. A typical set of size and velocity dis-

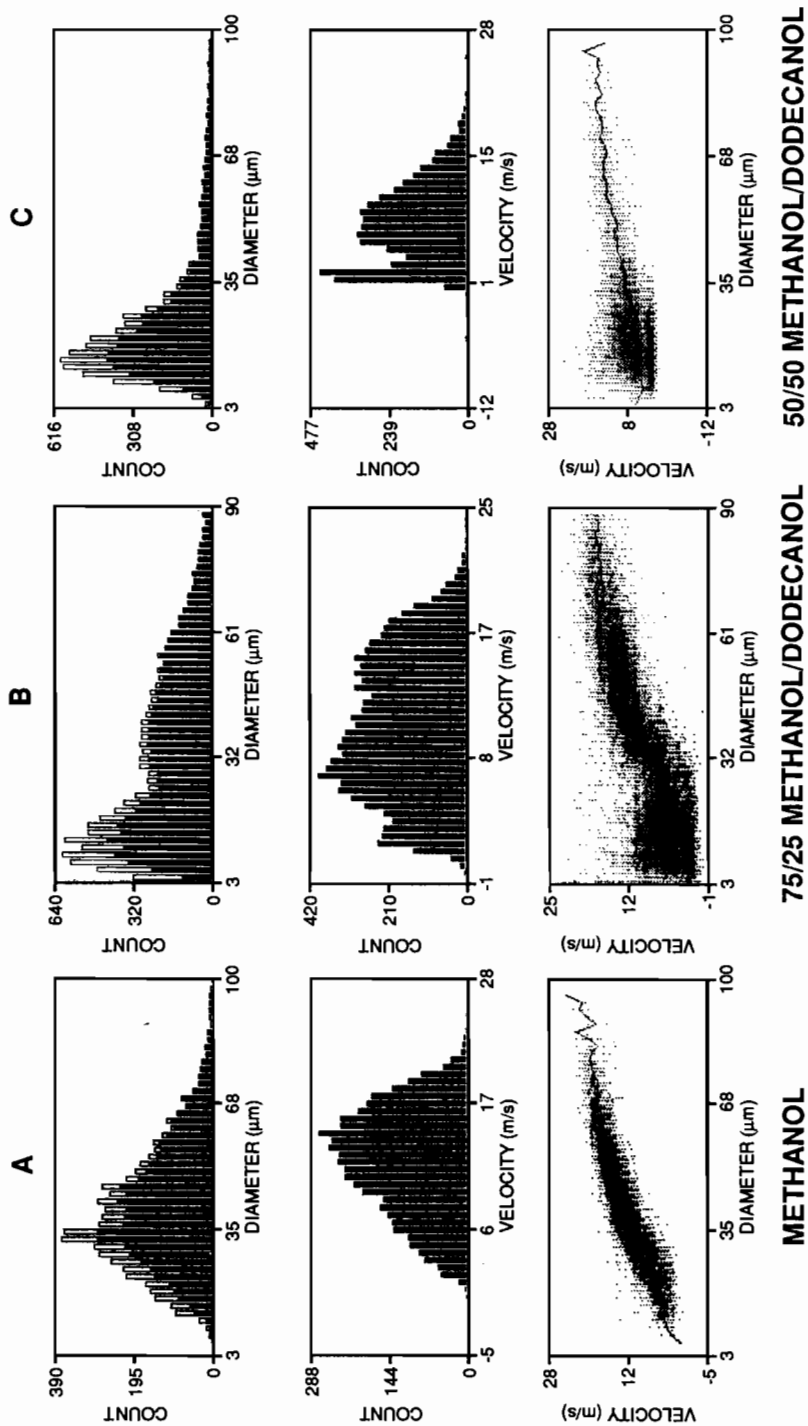


Fig. 10 Distribution of droplet size, velocity, and velocity/diameter correlations for the (A) methanol, (B) 75/25 methanol/dodecanol, and (C) 50/50 methanol/dodecanol flames at $r = 33.0$ mm and $z = 50.8$ mm.

tributions, and velocity/size correlations obtained for the three spray flames, is presented in Fig. 10 at $r = 33.0$ mm and $z = 50.8$ mm. This radial position was chosen because it represented a position where microexplosions were expected to occur for the 50/50 mixture flame (see Figs. 7–9). The solid bars of the distributions represent the measured data on a flux (or temporal) basis, while the open bars represent the data corrected for variations in the effective measurement volume [7]. Also note the change in axes scales between distributions. The results indicate that the size distributions for the methanol and 50/50 methanol/dodecanol mixture flames generally remain monomodal (see Figs. 10A and 10C); however, a significant increase is observed in the number of detected smaller droplets and a decrease in the larger sizes for the mixture. The 75/25 mixture flame appears to be an intermediate case, i.e., a bimodal distribution that corresponds to a combination of the other two flames (see Fig. 10B).

The velocity distributions for the methanol and 50/50 mixture flames indicate a dramatic increase in the number of lower-velocity droplets for the mixture. The bimodal velocity distribution for the 50/50 mixture flame (see Fig. 10C) appears to result from a combination of faster-moving larger droplets that originate from the nozzle and slower-moving smaller droplets that form during microexplosions. The velocity/size correlation indicates the presence of two separate regions, with the formation of the lower-velocity region as a result of microexplosions. Further details are presented in [1] and [2]. Again, the trend for the 75/25 mixture flame appears to be a combination of the methanol and 50/50 mixture flames; a trimodal velocity distribution results for this composition (see Fig. 10B). The velocity/size correlation shows the initial formation of this second lower-velocity region. These trends are also present at $z = 76.2$ mm. The results indicate that the 75/25 methanol/dodecanol mixture flame does not appear to be a composition that enhances microexplosions, but perhaps an intermediate case that corresponds to incipient occurrence of microexplosions. Evidence for the presence of microexplosions appears to be strengthened with higher dodecanol content; the optimum methanol/dodecanol mixture composition remains to be determined. Other properties to consider in future studies include examination of mixture composition (volatility of the mixture components), residence time, temperature (air and fuel preheating), and approaches to augment the occurrence of microexplosions in spray flames.

4. SUMMARY

Measurements of droplet mean size, velocity, and number density were obtained using a phase Doppler interferometry system. The measurements were carried out in pure methanol, 50/50, and 75/25 methanol/dodecanol mixture flames. The study examined the effect of dodecanol content on the occurrence of microexplosions in methanol flames. Comparison of the results obtained in these three flames indicates that the tendency for microexplosions is strengthened with higher dodecanol content. The effect of system gain (i.e., PMT voltage and laser power) on the measurements has been found to influence dense regions of spray flames, but has a negligible effect at downstream positions where microexplosions are expected to occur.

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