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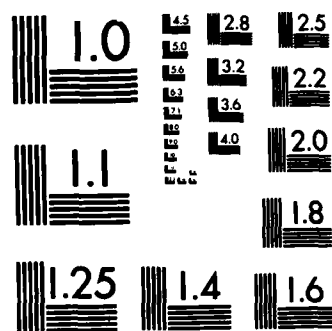
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MECHANISMS OF SKINNEE PRODUCTION AT HIGH PRESSURE COMPRESSION OF ANISOTROPIC POLYMER FILMS

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report documents progress made during the second year of a three-year study of the atomization and evaporation characteristics of emulsified and alternative fuels at conditions typical of those found in gas turbine engines. The development of experimental techniques suitable for drop size measurements in realistic polydisperse fuel sprays in high pressure/temperature air has been the first goal of this year's program. The second														

Area of interest has been the development of detailed drop models which predict the heat-up, evaporation, and trajectory of fuel sprays and the resulting size distribution parameters. In addition to these two areas, a facility was constructed during the first year of this program to allow for the containment of sprays in high pressure/temperature moving air with optical access for spray size measurements. These experimental and analytical tools have and will continue to be used to study the differences in atomization/evaporation of emulsified and neat fuels, and various other fuels of interest to the U.S. Navy.

Significant results of the second year of this study include the following. A commercial forward-angle laser light-scattering instrument has been modified to measure drop sizes in evaporating and burning sprays. Using this apparatus it has been shown that emulsified and neat fuels initially atomize to about the same drop sizes, but at elevated temperatures and pressures, both Jet-A and hexadecane emulsions evaporate in such a way so as to produce drops of significantly smaller Sauter mean diameter (SMD) than their neat fuel counterparts at the same distance from the nozzle. The difference between the emulsified and neat fuel drop sizes only appear at elevated pressures (greater than about 3-1/2 atm) for the fuels and temperatures examined. These results are consistent with those that might be expected if microexplosions were occurring in the emulsified fuels.

A computer model has been developed based on single drop heat-up and evaporation theory. Sixteen to twenty-one size classes are used to characterize the spray and the complete heat-up, evaporation, and aerodynamic interactions are included in the model. The model is incomplete in that the inhomogeneities of the spray along the line-of-sight have not yet been included. However, the steady state drop temperature has been computed and compared with the spontaneous nucleation temperature of water for a number of conditions. These calculations suggest that the steady state drop surface temperatures at conditions where differences are seen in the evaporation characteristics of the emulsified and neat fuels are somewhat below (approximately 30K) the kinetic superheat limit for water. Spontaneous nucleation is expected to occur somewhat below the superheat limit.

TABLE OF CONTENTS

	<u>Page</u>
INTRODUCTION AND BACKGROUND.....	1
EXPERIMENTAL APPARATUS.....	3
SPRAY TRAJECTORY AND EVAPORATION MODEL.....	8
EXPERIMENTAL RESULTS AND DISCUSSION.....	22
Atomization/Evaporation Results for Emulsified and Neat Jet A.....	23
Atomization/Evaporation Results for Emulsified and Neat Hexadecane.....	31
Drop Size Measurements in Flames.....	40
CONCLUSIONS.....	43
RECOMMENDATIONS FOR NEXT YEAR.....	44
ACKNOWLEDGMENTS.....	46
REFERENCES.....	47

APPENDIX A
APPENDIX B

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LIST OF ILLUSTRATIONS

<u>Figure</u>		<u>Page</u>
1	COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-HEXADECANE.....	14
2	COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-DODECANE.....	15
3	COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-OCTANE.....	16
4	COMPUTED EVAPORATION CONSTANT AT QUIESCENT CONDITION FOR N-HEXADECANE.....	18
5	COMPUTED EVAPORATION CONSTANT AT QUIESCENT CONDITION FOR N-DODECANE.....	19
6	COMPUTED EVAPORATION CONSTANT AT QUIESCENT CONDITION FOR N-OCTANE.....	20
7	EFFECT OF AIR TEMPERATURE ON ATOMIZATION AND EVAPORATION- SMD VERSUS DISTANCE FROM NOZZLE.....	24
8	EFFECT OF AIR TEMPERATURE ON ATOMIZATION AND EVAPORATION- RELATIVE SMD VERSUS DISTANCE FROM NOZZLE.....	25
9	EFFECT OF AIR PRESSURE ON ATOMIZATION AND EVAPORATION- SMD VERSUS DISTANCE FROM NOZZLE ($T_{AIR} = 589 \text{ K}$, $V_{REF} = 14.6 \text{ m/SEC}$).....	28
10	EFFECT OF AIR PRESSURE ON ATOMIZATION AND VAPORIZATION-SMD VERSUS DISTANCE FROM NOZZLE ($V_{REF} = 8.5 \text{ m/S}$, 547K).....	30
11	COMPARISON OF RELATIVE SMD FOR EMULSIFIED AND NEAT HEXADECANE AT CONSTANT PRESSURE (4.42 atm , 448 kPa) AND VARIOUS TEMPERATURES.....	32
12	RELATIVE SMD FOR NEAT HEXADECANE AT FIXED TEMPERATURE (644 K) AT VARIOUS PRESSURES.....	34
13	RELATIVE SMD FOR EMULSIFIED HEXADECANE AT FIXED TEMPERATURE (644 K) AT VARIOUS PRESSURES.....	35
14	RESULTS OF FIGURES 12 AND 13 COMPARED.....	36
15	COMPARISON OF PREDICTED AND MEASURED SMD's AT DIFFERENT AIR TEMPERATURES ($P = 4.42 \text{ atm}$) (448 kPa).....	41

LIST OF TABLES

<u>Table</u>		<u>Page</u>
1	Some Properties of Fuels Used.	7
2	Example Output from Computer Model	11
3	Computer Predicted Steady State Drop Surface Temperatures for Hexadecane at Conditions Corresponding to Figure 11. . .	33
4	Computer Predicted Steady State Drop Surface Temperatures for Hexadecane at Conditions Corresponding to Figures 12- 14	33
5	Computer Predicted Spray Characteristics for a Condition of $T_{Air} = 700$ K, $P_{Air} = 448$ kPa.	39

**MECHANISMS OF SMOKE REDUCTION IN THE HIGH PRESSURE
COMBUSTION OF EMULSIFIED FUELS;
VOL. II: EXPERIMENTAL AND THEORETICAL STUDY OF EVAPORATING
EMULSIFIED AND NEAT FUEL SPRAYS**

INTRODUCTION AND BACKGROUND

High quality petroleum derived fuels are not as widely available as they were in the past. Future fuels derived from petroleum and non-petroleum sources such as coal and shale-oil will tend to be lower in hydrogen content and more viscous with more residual components. These fuels will be more difficult to atomize effectively and will tend to produce more soot during combustion. The purpose of this contract is to conduct fundamental research which addresses two separate aspects of the problems associated with atomization and burning of lower quality fuels. The first aspect is the experimental study of atomization and evaporation of water/oil emulsified fuel sprays in a real combustion environment, with a specific effort to verify the proposed "microexplosion" phenomena. The second goal is to examine the atomization and evaporation of "out-of-spec" fuels which are too viscous or non-volatile to meet the standard fuel specifications for gas turbine combustion. Both of these goals required the development of experimental techniques not previously available to study drop-size distributions of fuel sprays in high pressure evaporating and combusting systems. This report covers progress made during the second year of a three year effort to study atomization in combustors.

The first aspect of the atomization problem deals with the study of emulsified fuels. It has been shown (Refs. 1 and 2) that the increased soot formation resulting from combustion of low-hydrogen-content fuels

can be somewhat offset by mixing water or alcohol with the fuel. Several theories have been offered to explain this soot-reduction phenomena. These include: (a) better atomization of the emulsified fuel due to "microexplosions" caused by superheating and violent boiling of interior water micro-droplets; (b) a change in the chemical kinetics leading to soot production due to the increased OH or the increase in H/C ratio; (c) the reduction of liquid-phase pyrolysis processes due to lower drop temperatures resulting from the lower boiling point of water; or (d) the reduction of gas-phase pyrolysis processes due to the lower flame temperature from either strictly dilution effects or other chemical processes. One of the goals of this contract was to develop techniques to verify the existence of microexplosions in real combustion systems. Microexplosions have been observed for large emulsified drops burning in quiescent atmospheres, but no direct measurements have been successfully performed on realistic sprays in turbulent air. Some of the observed microexplosion phenomena have been criticized as unrealistic for several reasons: nucleation introduced by the supporting wire; the large size of the drops (when compared with real spray size distributions); and the lack of high aerodynamic shear forces which promote internal mixing and reduce the possibilities for microexplosions and also extend the heat-up period relative to the total lifetime of the drop. The purpose of the first part of this program was to develop methods to examine the behavior of sprays of emulsified fuels in a more realistic combustion environment.

The second part of this program involves a study of the atomization and evaporation of alternative fuels, which generally will be more difficult to atomize and evaporate when compared to present-day petroleum-based fuels. Some correlations exist for predicting the change in spray quality for small variations in fuel properties, and some models have been developed for fuel spray evaporation in combustors, but experimental data are lacking to verify these models and extend them to alternative fuels. The same experimental techniques developed for the first part of the program will be used for the second part.

EXPERIMENTAL APPARATUS

The combustor facility and test section were described in some detail in the previous yearly progress report (Ref. 3). That system was used for these tests except that the disc, which provides recirculation for flame stabilization, was replaced with a fuel nozzle alone for the evaporation tests, and a window purge was added. These modifications, as well as a brief description of the overall system are discussed below.

Unvitiated compressed air is supplied to the test cell by three compressors and a gas-fired preheater which provide up to 1.1 kg/sec at pressures ranging from 138 kPa (1.36 atm) to 1620 kPa (16.0 atm) and temperatures up to 1090 K.

The test section consists of a type 316 stainless steel pipe, 16.83 cm OD, 12.50 cm ID, 2.17 cm wall thickness, with quartz windows on each side having a clear aperture of 9.2 cm by 6.7 cm. A smooth transition section 5.5 cm long is provided on each end of the windows to reduce recirculation zones. Each window is purged by air on both top and bottom. Air is supplied to each window by a total of 10 tubes of nominal 0.635 cm OD and then diffused and exhausted by a convergent section parallel to the window surface.

For the evaporation tests, the flame stabilizing disc has been replaced by a fuel nozzle alone mounted about even with the upstream edge of the windows. The nozzle is supported with a 12.7 mm OD stainless steel tube which follows the test section centerline for a distance of about 250 cm upstream from the nozzle and then makes a right angle bend and exits from the test section. The 12.7 mm OD tube carries cooling water and a separate parallel 6.35 mm OD stainless steel tube is the water return line. Another 6.35 mm OD stainless steel tube is mounted inside the 12.7 mm water cooling tube and carries fuel to the nozzle.

Fuel temperature is regulated by controlling the water cooling temperature.

The nozzles used were simplex pressure atomizers producing a hollow cone spray. The model type was Delavan Corp. WDA 450 hollow cone with nominal flow rates of 3.79 liters/hour (1 gallons/hour) and 11.3 liters/hour (3 gallons/hour) at 862 kPa (125 psi) differential pressure using water.

The operation of the test cell is monitored with a Hewlett-Packard 9820 programmable calculator which is coupled to a 50 channel scanner. A test report including the average and statistical variation of all the important parameters is available immediately after a test. The sensing systems consist of strain-gage pressure transducers, thermocouples, and turbine flowmeters.

Drop size data were obtained with a Malvern Model 2200 Particle Sizer based on the diffraction angle produced by drops when illuminated by a beam of monochromatic, coherent, collimated light from a HeNe laser. The smaller drops diffract light at larger angles to the optical axis than the larger drops. Detection is accomplished with a 30 annular ring set of solid state detectors. Detector outputs are multiplexed and the data signal-averaged with a Commodore PET computer. A fairly complex (and proprietary to Malvern) computer routine is used to interpret the light scattering pattern of the polydisperse drop systems. The drop-size data are available as either a set of two parameters defining a Rosin-Rammler, log-normal, or normal distribution, or as a histogram of 15 size classes of drops without any assumption about the shape of the distribution. Although all of the distributions have been tried, the Rosin-Rammler has generally provided the best fit and was used throughout this program. A 300 mm focal length $f/7.3$ lens was used to collect the scattered light. The laser beam diameter was 9 mm with a Gaussian intensity distribution truncated at its edge by the 9 mm aperture.

Several modifications were made to the Malvern drop sizer for these measurements to avoid problems associated with flame radiation during the burning spray measurements, and laser beam steering problems during both non-burning evaporation tests and burning sprays.

Three modifications were made to discriminate against flame radiation. First the laser beam was chopped at 667 Hz and the differential signal at each detector ring was sampled for 20 cycles. This necessitated slowing the multiplexing rate in the electronics from about 1.3 ms/channel to 30 ms/channel. It was also necessary to sample only the "clean" part of the signal when the beam was completely blocked or completely transmitting as the chopper blade edge produces a large spurious signal when passing through the laser beam due to its own diffraction pattern. The second modification was the use of a 3 nm band pass interference filter centered at the HeNe laser wavelength of 632.8 nm in front of the lens on the drop sizer. All measurements were made with the 300 mm focal length lens which has a maximum effective acceptance angle of about 2.7° from the normal axis for light reaching the detector. The transmission of the filter changes less than one percent for rays at this angle or less relative to the normal axis through the filter. However, if the 100 mm or 63 mm focal length lenses (the other standard sizes) were used, the acceptance angle increases to about 8.1° or 12.8° , respectively, and wider band pass filters would be necessary. The third modification involves the use of an aperture of diameter 32 mm located about 130 mm from the lens to block radiation from the flame which is not within the scattering volume of the laser beam.

In addition to problems with flame radiation, there are substantial problems even in non-combusting sprays in high temperature air due to steering of the laser beam caused by refractive index changes in the scattering volume resulting from thermal and compositional gradients near the drops. This results in excess spurious signals on the inner detector rings, getting worse at higher evaporation rates and finally limiting, at

some distance from the nozzle, the application of this technique for drop sizing. A technique has been developed for blocking light on the inner detector rings and extrapolating values from the outer rings. Radiation data on up to eight of the thirty rings is blocked, but even this becomes insufficient at some point in the evaporation process.

The significant fuel property data are given in Table 1. The emulsions were first blended using a homogenizer, and were also continuously recirculated through an ultrasonic cavity during use to maintain a consistent blend.

Table 1. Some Properties of Fuels Used

JET A (AL-10112F)

Viscosity at 40°C 1.72 cS
 Specific gravity at 60°F 0.8049
 Heat of Combustion 46.904 MJ/kg
 Hydrogen Content 14.15%
 Flash Point: 355K
 Boiling Point Distribution (GC)

<u>Wt% Off</u>	<u>Deg K</u>
0.1	436
10	468
20	484
30	490
40	494
50	502
60	506
70	510
80	518
90	527
99	548
100	796

20% H₂O/2% Surfactant/78% Jet A (AL-10112F)

Viscosity at 40°C 4.47 cS
 Specific gravity at 60°F 0.8618

Hexadecane (95% purity)

Viscosity at 40°C 2.98 cS
 Specific gravity at 60°F 0.7774
 Boiling point (nominal) 560K

20% H₂O/2% Surfactant/78% Hexadecane

Viscosity at 40°C 5.55 cS
 Specific gravity at 60°F 0.8249

SPRAY TRAJECTORY AND EVAPORATION MODEL

A computer model based on an array of different-sized, noninteracting drops has been developed to study the heat-up, final "wet-bulb" drop temperature, evaporation rates, trajectories and resulting size distribution parameters at locations downstream from the nozzle. The trajectory part of the model should be considered as a straightforward and simple one based on an average drop path (neglecting turbulent statistical fluctuations) in a one-dimensional flow field. This corresponds to the experimental situation being studied. The thermodynamic part of the model, however, is very detailed and computes the transient heat-up and final drop temperature in greater detail than most spray models. The environment surrounding the drop is calculated based on the properties of both the fuel vapor and air rather than air alone as in some spray models. The convective effects on evaporation are included and constantly updated as the different size drops are decelerated to the air-stream velocity. The effects of temperature and pressure on air and fuel properties is included, and the steady-state "wet-bulb" temperature is iteratively calculated using the equations for the vapor pressure and temperature-dependent fuel and air properties. This model assumes uniform drop temperatures (infinite heat transfer rates within the drop) and single-component fuels.

Some spray models have predicted the change in drop-size distribution for a quiescent spray as a function of time, but results from this model show the considerable distinction between drop-size distributions as measured at a given location along the nozzle axis, at which drops arrive after different transit times (depending on diameter), as contrasted with the variation with time. For example, in this experiment, the spray initially has a higher axial velocity than the air and the small drops decelerate more rapidly than the large ones, resulting in a higher concentration in the measurement volume for the small drops and a longer time-of-arrival. These effects must be included

in any model which is intended to be used for comparison with experimentally measured changes in size distribution.

In developing a model which can be used to compare with experimental results, it is necessary to consider the interaction of the measuring device with the spray. The added weighting of the small drops due to their more rapid deceleration has been discussed. In addition, the small drops are caught up in the air stream and tend to populate the center of the spray while the large drops maintain their initial velocity longer and tend to fill the outer edges of the spray. This disparity is magnified by the fact that at the exit of a hollow-cone swirl nozzle (the type used in these tests) the majority of the fluid consists of larger drops in the outer cone of the spray, while smaller drops fill in the less dense spray in the center of the cone. Thus, it is necessary to model these inhomogeneities in size distribution through the spray and also the location, diameter, and intensity distribution of the laser beam relative to the spray. At this time, the model does account for the different trajectories of the large and small drops, but assumes that all the spray is initially at a fixed cone angle. The drop size distribution is calculated for a complete cross section of the spray at a given axial location, without regard for the laser beam sampling volume. The model also assumes that spray breakup is complete and no secondary atomization or drop agglomeration occurs beyond some point from the nozzle exit. An initial size distribution at that point is an input to the model. Thus, the model is not applicable very close to the nozzle ($\lesssim 10\text{mm}$).

Results from the model are presented in the following sections, while the detailed mathematics of the model are presented in Appendix A. A general flow chart of the model is presented in Figure A-1. while a listing of the Fortran source code is given in Appendix B. Most of the model has been constructed from pieces of existing models. The thermodynamic part of the model follows closely the work of Chin and Lefebvre at Purdue University, while the aerodynamic equations for drag,

velocity, etc. are based on a model developed at the University of Sheffield by Swithenbank, Boyson, Ayers and others. (See Appendix A for detailed references.)

The capabilities of the model can probably be best understood by examining some typical output data and also comparing the model results with experimental results. Some information available from the model is shown in Table 2 which represents a spray of n-hexadecane into air at 644 K and 4.42 atm. The air velocity was assumed to be a uniform one-dimensional axial flow of 8.54 m/s, while the initial fuel velocity was 20.76 m/s at an angle of 22.5° to the axis (45° cone angle) and a fuel temperature of 311 K. The computed drop size data assuming a Rosin-Rammler distribution are shown on the top line and include the two Rosin-Rammler parameters, $\bar{x}$ and N which specify a size and a width for the distribution, and the Sauter mean diameter (SMD) which is an "average" drop size. By definition, if all drops in the spray were equal in size to the SMD, then the volume-to-surface-area ratio of the imaginary monodisperse spray would be equal to the actual spray. This ratio is chosen because surface area regulates evaporation rates while the volume indicates the quantity of fuel. The initial drop sizes are shown in column 1 and the initial relative population of drops in each size class were computed to correspond exactly to a Rosin-Rammler distribution specified as an input to the program. (Those values were $\bar{x} = 57$ and $N = 1.5$ for the example shown.) Because of evaporation and the more rapid deceleration of the small drops (resulting in an increased weighting for the small drops), the size distribution changes at positions downstream from the nozzle. The drop-size distribution no longer corresponds exactly to the Rosin-Rammler distribution, and the degree to which it does fit that distribution is given by the correlation coefficient. For the cases examined, the correlation coefficient has been in excess of 0.97, but under some conditions it could be worse. These distribution parameters are calculated from information shown for individual drop size classes in the lower part of Table 2.

Table 2. Example Output from Computer Model

Initial DIAM	R-R XBAR (UM)	68.9	R-R N	2.52	CORR.COEF.	.991	SMD	46.51	RE			
DIAM	TIME	X	DROP	Y	DROP	Z	DROP	U-VEL	V-VEL	W-VEL	FTEMP	RE
5.6	.9	.00026	.0074	.0021	0.0000			8.540	.000	0.000	520.4	.0
7.0	.9	.00040	.0088	.0023	0.0000			8.540	.000	0.000	520.4	.0
8.8	.9	.00062	.0110	.0025	0.0000			8.540	-.000	0.000	520.4	.0
11.1	.9	.00095	.0142	.0028	0.0000			8.540	.000	0.000	520.4	.0
14.0	.9	.00145	.0191	.0033	0.0000			8.540	-.000	0.000	520.4	.0
17.6	1.3	.00220	.0264	.0041	0.0000			8.540	.000	0.000	520.4	.0
22.2	18.6	.00202	.0264	.0053	0.0000			8.658	.088	0.000	505.6	.3
28.0	27.4	.00179	.0264	.0068	0.0000			9.310	.575	0.000	460.2	3.1
35.2	35.2	.00157	.0264	.0082	0.0000			10.811	1.696	0.000	411.3	12.4
44.4	44.4	.00142	.0264	.0091	0.0000			12.708	3.112	0.000	377.2	30.7
55.9	55.9	.00135	.0265	.0096	0.0000			14.156	4.193	0.000	355.5	54.9
70.5	70.5	.00131	.0264	.0098	0.0000			14.913	4.759	0.000	341.1	81.2
88.8	88.8	.00129	.0265	.0100	0.0000			15.372	5.101	0.000	331.6	112.3
111.9	111.9	.00126	.0264	.0101	0.0000			15.830	5.443	0.000	325.0	153.6
141.0	141.0	.00125	.0265	.0103	0.0000			16.230	5.742	0.000	320.7	206.3
177.6	177.6	.00123	.0265	.0104	0.0000			16.617	6.031	0.000	317.7	275.2
223.8	223.8	.00121	.0264	.0104	0.0000			16.971	6.295	0.000	315.6	363.8
282.0	282.0	.00120	.0264	.0105	0.0000			17.276	6.523	0.000	314.2	476.6
355.2	355.2	.00119	.0264	.0106	0.0000			17.549	6.727	0.000	313.2	620.7
447.6	447.6	.00118	.0264	.0106	0.0000			17.790	6.907	0.000	312.5	804.3
563.9	563.9	.00118	.0265	.0107	0.0000			17.992	7.057	0.000	312.1	1036.5

The initial drop sizes (in μm) are shown in column 1 while the instantaneous drop sizes are shown in column 2 at a distance from the nozzle of 26.4 mm as shown in column 4 and a time (in seconds) as specified in column 3. When the drops reach a diameter of $0.9\ \mu\text{m}$ they are assumed to be completely evaporated and the diameter is fixed at $0.9\ \mu\text{m}$ to keep some of the computations from becoming undefined. For those cases, the time and location are frozen at the point where the drop disappeared and those drops are not used in calculating the Rosin-Rammler parameters. Note that this model calculates spray data at a given axial distance from the nozzle (X DROP) and not at a given time from injection. The smaller drops take longer to reach the specified location due to their lower velocity as specified in column 7 by U-VEL in m/s. The smaller drops decelerate to the air stream velocity of 8.54 m/s more rapidly than the large drops. The coordinate system is cylindrical with the axial coordinate being x with velocity u, the corresponding radial components y and v, and the corresponding angular components (assumed zero presently) z and w. Distances are in meters and velocities in meters/second.

Note the difference in trajectories and velocities for the different size classes. All non-evaporated drops are at the same axial (X DROP) location but the radial location (Y DROP) of the small drops is less than the large ones due to their being caught up in the air stream sooner as shown by the axial (U-VEL) and radial (V-VEL) velocities. The wide variation in Reynolds numbers (RE) is shown in the last column. The importance of convective effects in heat and mass transfer is obvious from these values, and hence, the shortcomings inherent in quiescent spray models.

The instantaneous drop temperature (FTEMP) is shown in the next to the last column. The initial fuel temperature was 311 K and the "wet-bulb" final steady-state drop temperature is 520 K at these conditions. The normal boiling point of n-hexadecane is 560 K. Note that the small

heat up and evaporate almost instantaneously while the "uniformly mixed" temperature of the largest drops is predicted to be close to the initial fuel temperature. Due to finite rate heat transfer the surface temperature of the large drops would be higher, but experimental evidence is lacking to predict temperature profiles within the drop. Complex models have been developed to predict these profiles, but they are too cumbersome for this effort and generally lack verification.

Note the importance of modeling the transient nature of the drop before it reaches the steady-state temperature. Of the 21 drop size classes shown in Table 2, only one nonevaporated size class has reached the steady-state temperature. As the pressure and convective effects are increased, the length of the transient period relative to the steady-state period increases (Ref. 4). Thus, models that assume no mass transfer until the drop reaches its steady-state temperature are not representative of many realistic conditions in gas turbines and are insufficient to compare with experimental results generated in this program.

In addition to the drop array data just discussed, the model has been used to examine the steady-state "wet-bulb" temperature and the quiescent, evaporation rate of the fuel, which are both independent of drop size, as a function of air pressure and temperature. At atmospheric pressure, the steady-state drop temperature is lower than the normal boiling point due to the cooling effect of energy used in vaporizing the fuel. As the pressure increases, the boiling point increases and the steady-state temperature increases. Obviously the fuel and air properties are important in determining this temperature. Steady-state temperatures for three normal paraffins - octane (C_8H_{18}), dodecane ($C_{12}H_{26}$), and hexadecane ($C_{16}H_{34}$) - were calculated over a range of conditions with the results as shown in Figures 1 to 3. At low air temperatures, the drop temperatures converge to the air temperature. As the air temperature increases, the increased vaporization cools the drop below the air temperature, but increased pressure markedly increases the

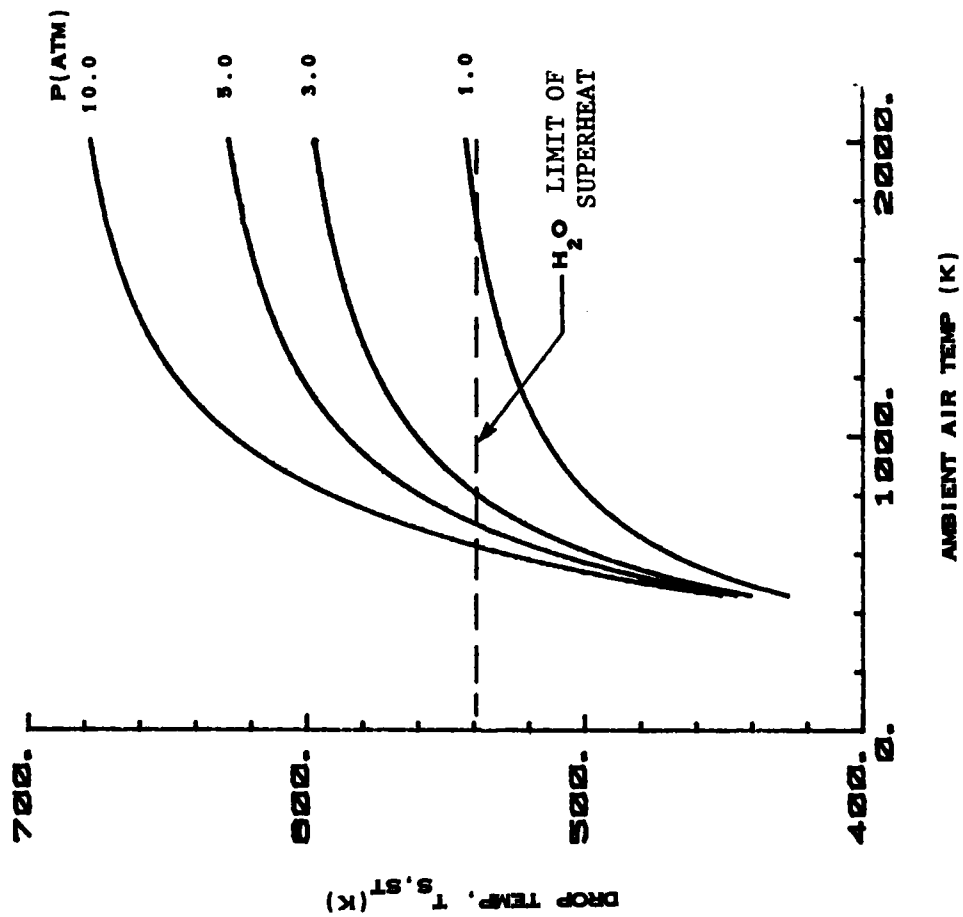


FIGURE 1. COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-HEXADECANE

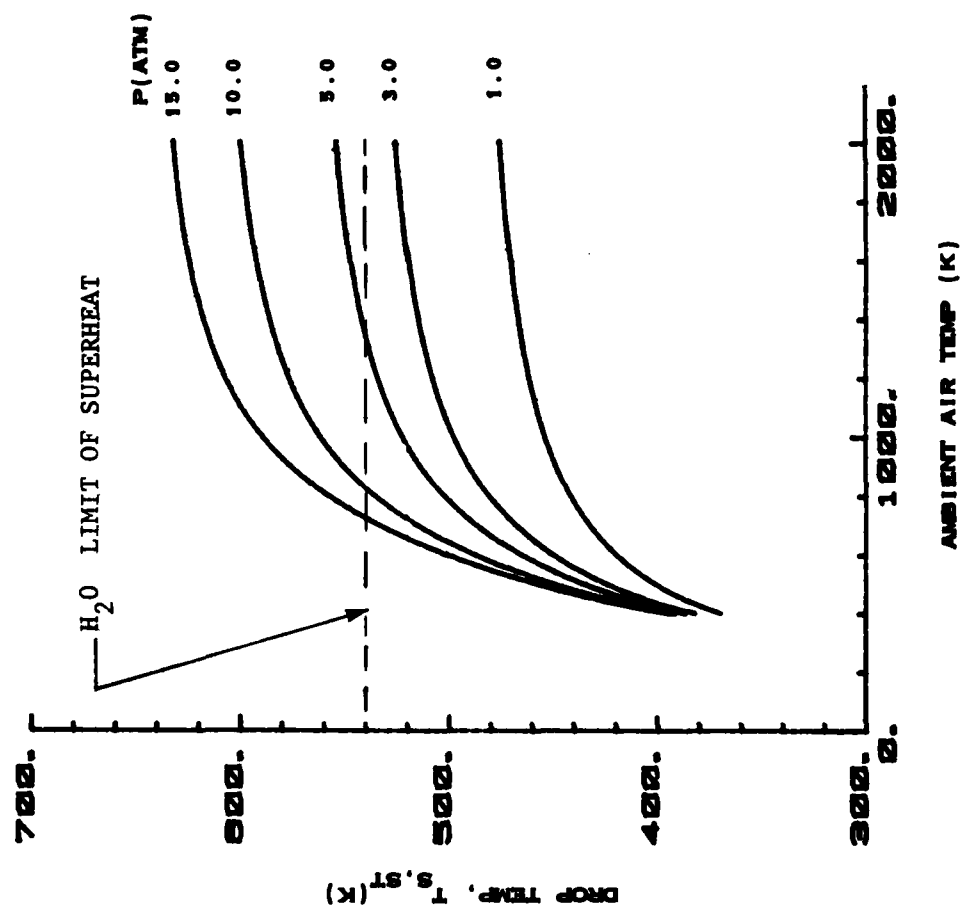


FIGURE 2. COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-DODECANE

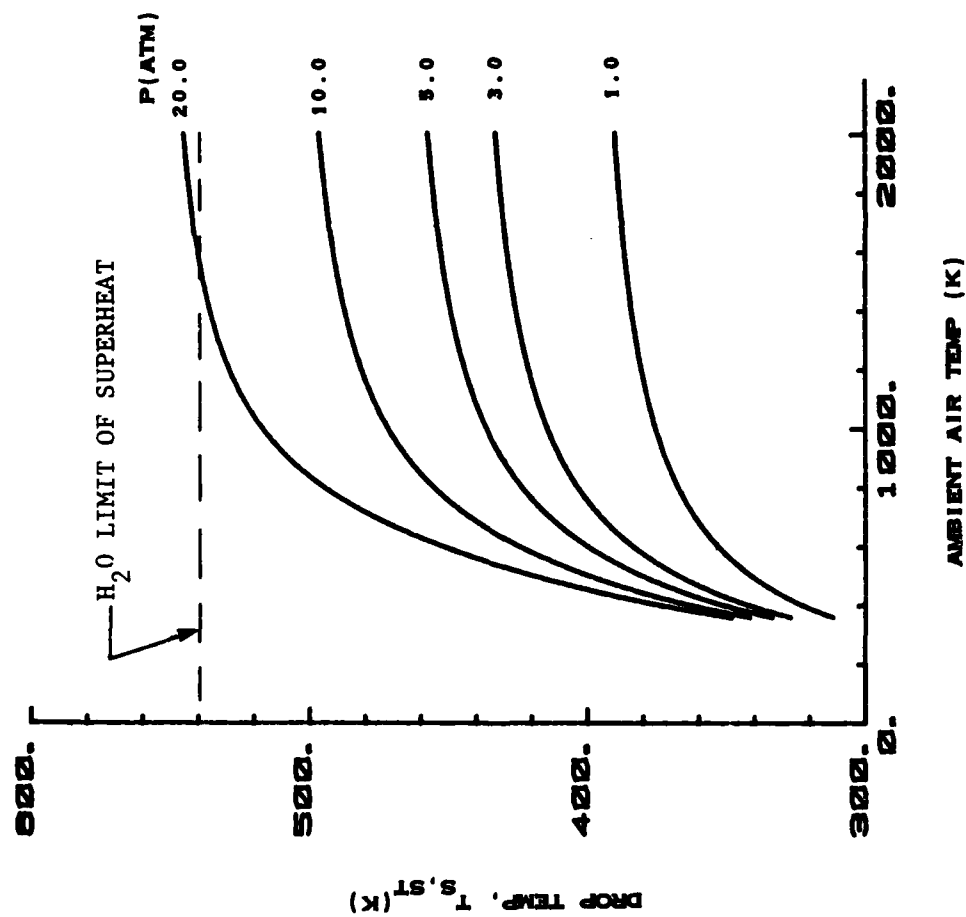


FIGURE 3. COMPUTED STEADY STATE DROP SURFACE TEMPERATURE FOR N-OCTANE

allowable drop temperature. The kinetic limit of superheat for water indicated in the figures is discussed in a later section. The critical pressure for hexadecane is 1421 kPa (14.02 atm) and for dodecane 1820 kPa (17.96 atm), and data are not shown for pressures higher than the critical pressure.

Droplet evaporation follows a D-squared law which relates the drop diameter D to the initial size D_0 and the time t by (Ref. 5)

$$D^2 = D_0^2 - \lambda t \quad (1)$$

where the proportionality constant λ is the evaporation constant. The mass transfer rate of fuel from the drop, $\dot{m}_F$, at quiescent conditions is related to the evaporation constant by

$$\dot{m}_F = (\pi/4) \lambda \rho_F D \quad (2)$$

where ρ_F is the fuel density. The evaporation constant is increased by convection, with a correction factor given by Frossling (Ref. 6) for cases where heat transfer rates are controlling of,

$$\lambda_{\text{Conv.}} = \lambda_{\text{Quies.}} (1 + 0.276 \text{Re}_D^{0.5} \text{Pr}_g^{0.33})$$

where Re_D is the Reynolds number of the gas relative to the drop and Pr_g is the Prandtl number of the gas. The correction factor depends on drop size and must be calculated using the drop array part of the program, but it is instructive to examine the temperature and pressure dependence of the quiescent evaporation constant which is independent of drop size and velocity. The quiescent evaporation constants for n-octane, n-dodecane, and n-hexadecane are shown in Figures 4 to 6. It can be seen that there is a strong temperature dependence, as there must be, and a pressure dependence which is weak over the conditions used in these experiments but which increases at elevated temperatures.

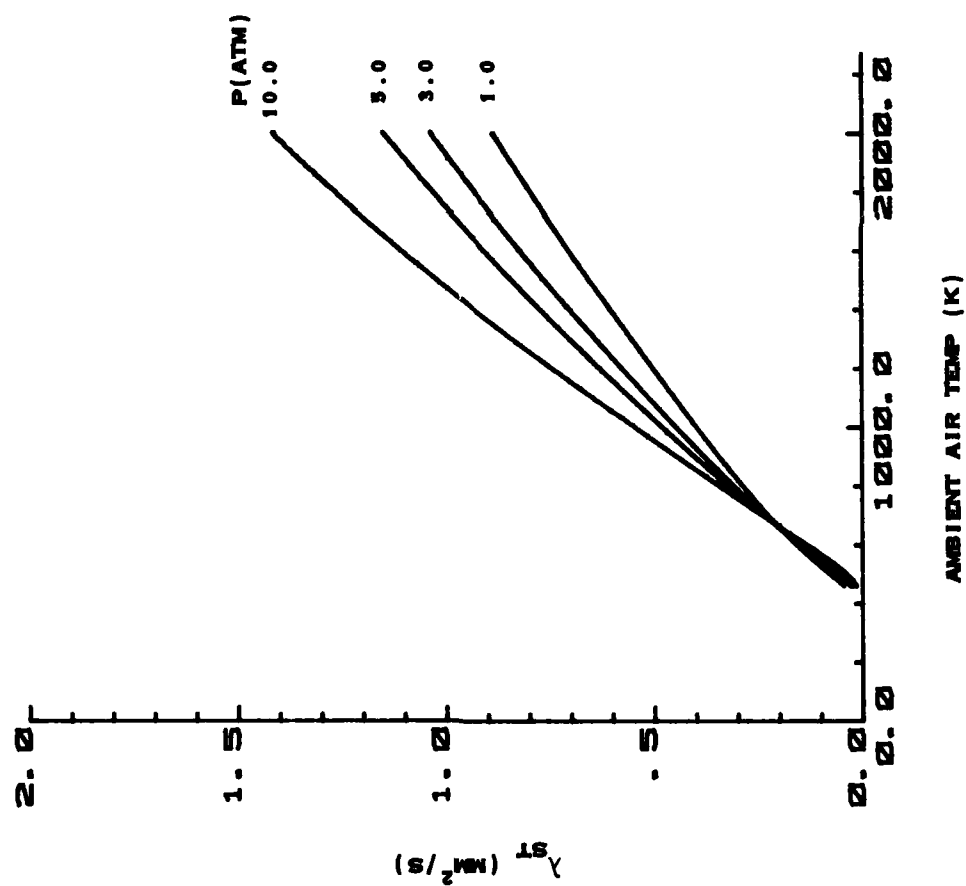


FIGURE 4. COMPUTED EVAPORATION CONSTANT AT QUIESCENT
CONDITION FOR N-HEXADECANE

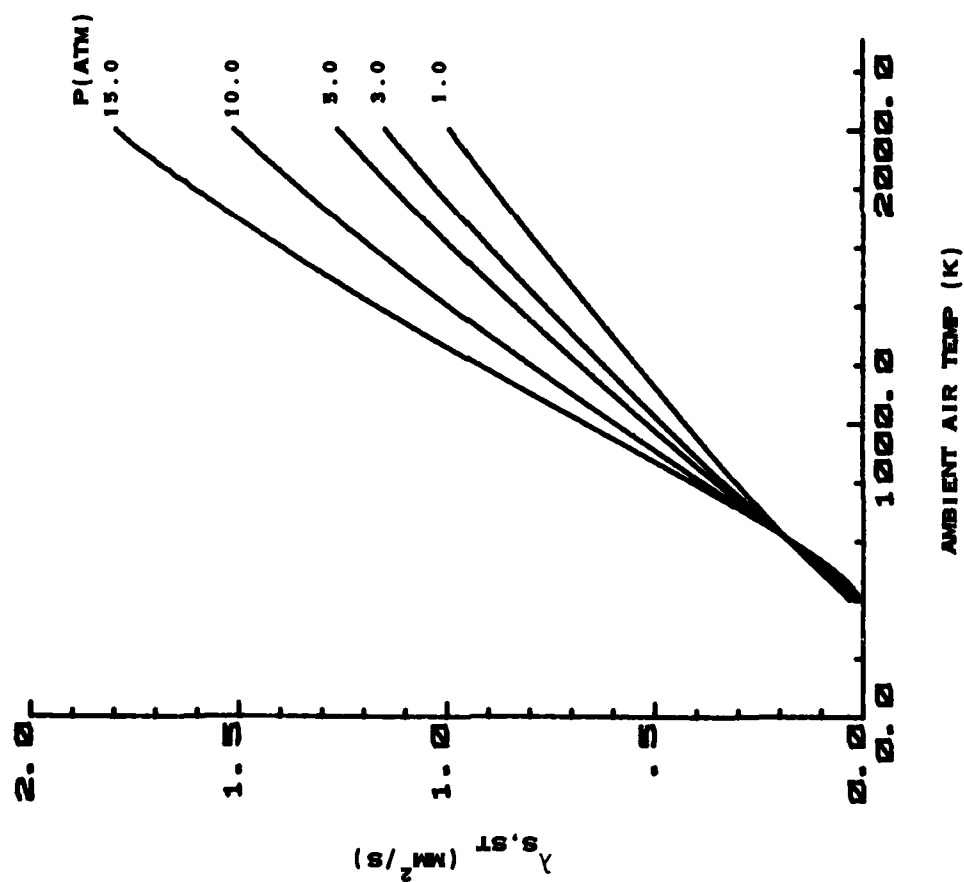


FIGURE 5. COMPUTED EVAPORATION CONSTANT AT QUIESCENT
CONDITION FOR N-DODECANE

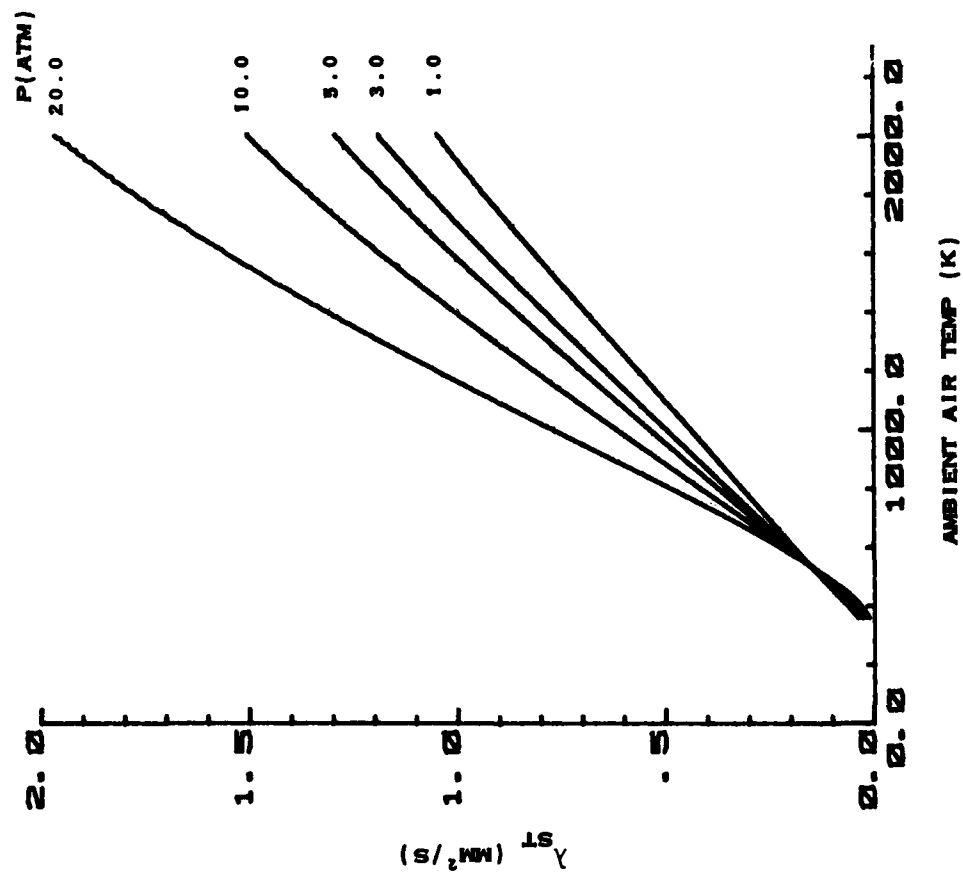


FIGURE 6. COMPUTED EVAPORATION CONSTANT AT QUIESCENT
CONDITION FOR N-OCTANE

In summary, the computer model, while not completely comparable with experimental results in its present form, does provide insight into much of the thermodynamics affecting drop evaporation. It also shows quantitatively how the smaller drops are caught up in the air stream much more quickly than the larger ones. It also indicates the importance of modelling evaporation during the transient heat-up phase, particularly for realistic sprays at high pressures and Reynolds numbers. It shows the effect of air pressure on the steady-state drop temperature, and how increasing air pressure leads to increased drop temperatures which enhances the probability of initiating microexplosions.

EXPERIMENTAL RESULTS & DISCUSSION

Experiments determining the change of drop size distribution with distance from the nozzle for emulsified and neat Jet A and n-hexadecane in high pressure/temperature flowing air have been performed. Initial experiments were performed with Jet A and showed that the emulsified fuels initially atomize to about the same size as the neat fuels and evaporate in a similar manner at low temperature and pressure conditions. However, at elevated temperatures and pressures, the emulsified fuels evaporated in such a way so as to develop smaller drop sizes than the neat fuel. Because Jet A is a multi-component fuel, as are all commercial fuels, the evaporation of even neat Jet A requires several important assumptions about the distillation process to model. For that reason, further tests were conducted with a single component fuel, n-hexadecane, and the evaporation process for a spray of that fuel has been modelled and is compared with experimental results.

The experimental results presented in this section all have the same general form consisting of graphs showing the average drop size, represented by the Sauter mean diameter (SMD), upon initial atomization close to the nozzle, and after varying amounts of evaporation moving downstream from the nozzle. In most of the plots, the SMD's were normalized near the nozzle so that the relative effects of evaporation on the emulsified and neat (without water) fuels could be seen more clearly. Each graph shows the change in average drop size as a function of distance from the nozzle for a series of air temperatures, all at a fixed air pressure, or visa versa. Data for neat fuels are shown as open symbols with solid lines drawn through the data, while data for emulsified fuels are closed symbols with dashed or dotted lines. Lines through comparable data for the emulsified and neat fuels at the same condition are called out in the figures. Drop size data are shown as close as 6.35 mm (1/4 inch) from the nozzle, in cases where the spray density was not too great, to a distance of 31.35 mm (1-1/4 inches) or

56.35 mm (2-1/4 inches) from the nozzle. Data are not shown beyond a point where excessive noise due to beam steering of the laser beam prevented reasonable results.

Atomization/Evaporation Results for Emulsified and Neat Jet A

The effects of air temperature and pressure on the atomization and evaporation of Jet A emulsions and neat fuels were examined using nominal 3.79 liter/hr (1.00 gph) and 11.4 liter/hr (3.00 gph) nozzles. Drop size data for the 11.4 liter/hr nozzle spraying into air at 310 kPa (3.06 atm) with a velocity of 14.6 m/s over a temperature range from 308 K to 644 K are shown in Figure 7. Similar data for the 3.79 liter/hr nozzle spraying into higher pressure air (448 kPa or 4.42 atm) moving at 8.5 m/s are shown in Figure 8. In Figure 8, the SMD's have been normalized so that the first point (high temperature cases) or average of first two points (lower temperatures cases) is equal to unity to show the relative evaporation more clearly. The initial average drop sizes in Figure 8 were smaller than in Figure 7 and equal to about $31\text{ }\mu\text{m}$. (The smaller drop sizes are typical for a smaller capacity nozzle.)

These results point to a substantial difference in the evaporation characteristics of emulsified jet fuel when compared with neat jet fuel. When the air temperature is low (308 K), evaporation is relatively unimportant and microexplosions are not possible; the two fuels show a similar trend in drop-size distribution, indicated by the Sauter Mean Diameter (SMD). These data and the more extensive results presented in Ref. 3 show that the room temperature atomization characteristics of the two fuels are quite similar with the emulsified fuel usually producing slightly larger fuel drops due to the higher viscosity. This fact along with the observation that the SMD's near the nozzle tend to be approximately the same for the two fuels and diverge in moving away from the nozzle for the higher temperature cases indicate that the differences in SMD are due to differences in evaporation rather than initial

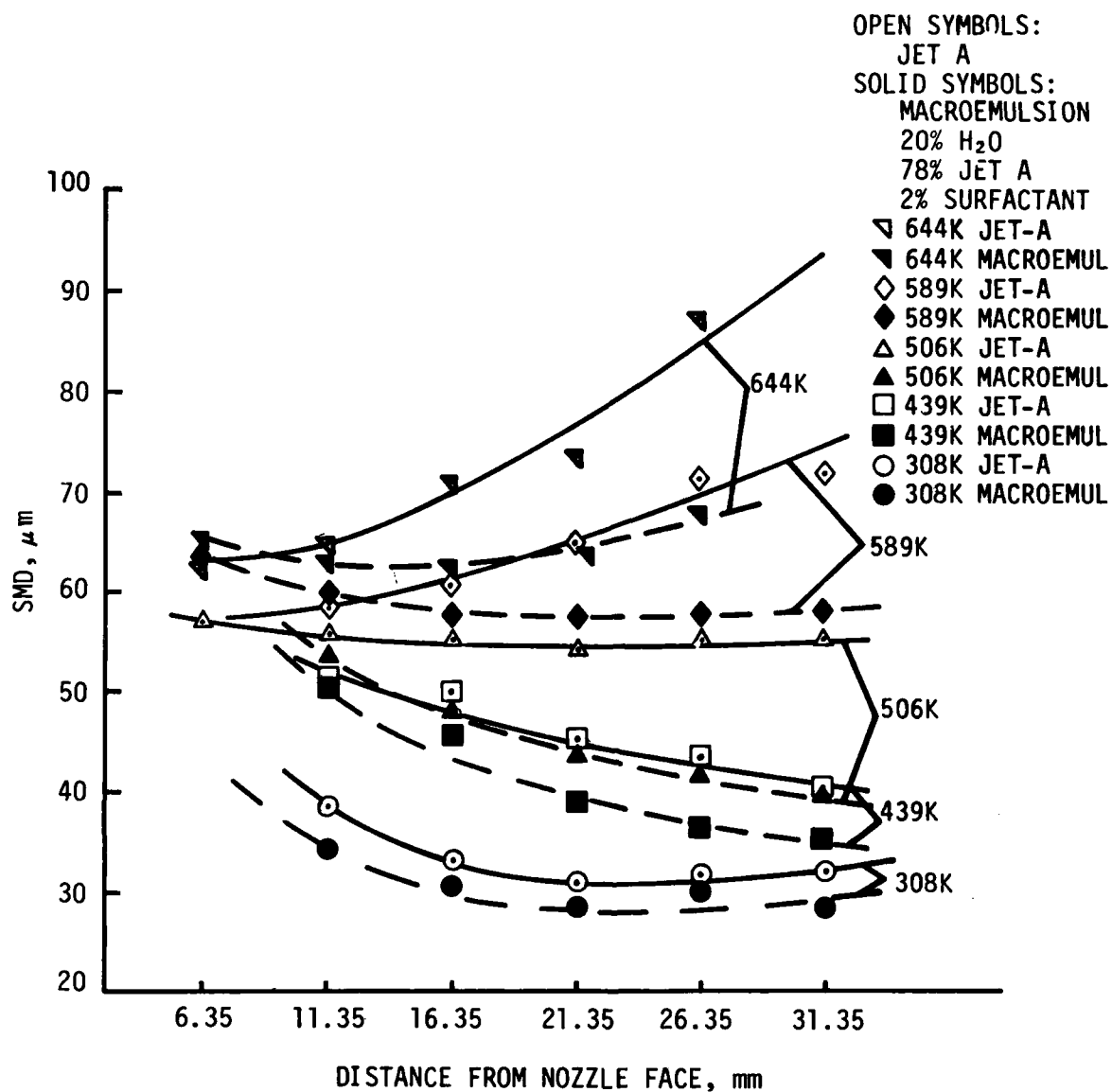
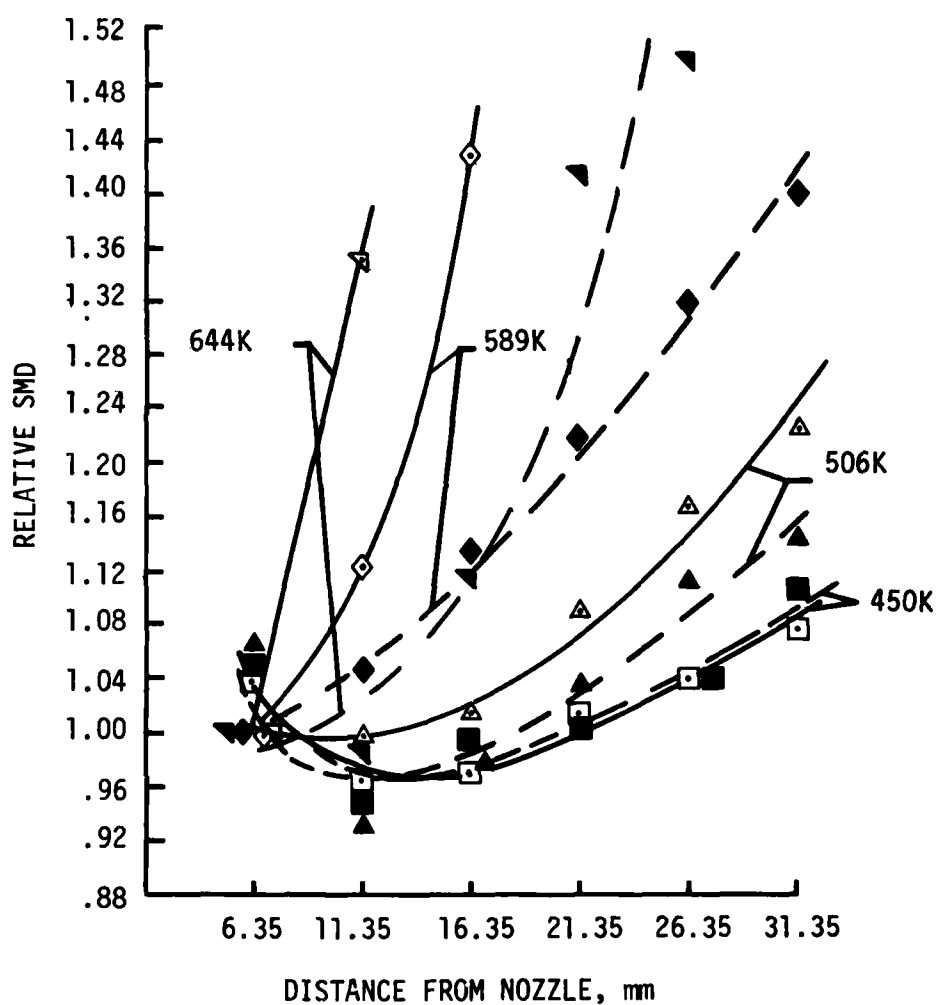


FIGURE 7. EFFECT OF AIR TEMPERATURE ON ATOMIZATION AND EVAPORATION -
SMD VERSUS DISTANCE FROM NOZZLE

P = 310 kPa (~3 atm), V_{REF} = 14.6 m/S
DELAVAL 11.4 liters/hr 45° HOLLOW CONE WDA NOZZLE @ 862 kPa

OPEN SYMBOLS: JET A
 SOLID SYMBOLS: 78% JET A
 20% H₂O
 2% SURFACTANT

NEAT EMULSION
 □ 450K
 △ 506K
 ◇ 589K
 ▽ 644K



EFFECT OF AIR TEMPERATURE ON ATOMIZATION AND EVAPORATION-
 RELATIVE SMD VERSUS DISTANCE FROM NOZZLE
 3.8 liters/hr, 45°HC DELAVAN NOZZLE, 8.5 m/s, 448 kPa

FIGURE 8.

atomization. At elevated temperatures there is a systematic difference between two, with the emulsified fuel always showing a much lower average drop size. This is consistent with the microexplosion hypothesis, but it is necessary to diverge a bit and try to explain the general behavior of all the data in Figures 7 and 8 to better understand what other phenomena could cause the same results.

First, consider that these drop-size data were obtained with a laser-diffraction technique which measures drop characteristics along its 9 mm diameter line-of-sight, and that the measurement method can affect the results. The drop-size data in Ref. 3 for an almost nonevaporating spray in room temperature air show that the average drop size sampled by the instrument drops rapidly after leaving the nozzle, then levels out, then increases slightly. The initial reduction in SMD near the nozzle is due to at least three phenomena. First, in a hollow cone nozzle the majority of the spray volume is in the outer part of the cone composed of relatively larger drops, while a smaller amount of spray made up of smaller drops fills in the inner core. Near the nozzle the laser beam intercepts more of the outer cone increasing the average drop size. Secondly, secondary atomization may occur after the initial breakup which further reduces the large drops as distance from the nozzle increases. Third, for cases where the air velocity is lower than the initial fuel velocity as in Figures 7 and 8 and Ref. 3, the small drops rapidly decelerate to the air velocity increasing their relative concentration in the sample volume and decreasing the SMD. The differences in the drag effects on large and small drops were shown dramatically in the results of the computer model presented earlier. These three factors contribute to the decrease in SMD when moving away from the nozzle for the room temperature case where evaporation is negligible.

Now consider the elevated temperature data in Figures 7 and 8 which indicate an increase in SMD as the temperature is raised and the evaporation rate increased. This result is due to the fact that although

all drops decrease in size with evaporation, the smaller drops evaporate much more quickly and the resulting average drop size actually increases. Thus at higher air temperatures the SMD increases in moving away from the nozzle relative to the room temperature case. This is demonstrated qualitatively by results from the computer model. Data in Figures 7 and 8 show only initial trends in the change in SMD relative to the total spray lifetime. The computer model predicts and some of the data indicate that the SMD initially increases and then levels out further into the evaporation process. Also the largest SMD's shown are, in some cases, biased on the high side due to uncorrectable beam steering problems. This study is directed at the relative evaporation characteristics of emulsified versus neat fuels and the largest SMD's reported may be erroneously high.

Having qualitatively examined the phenomena responsible for the trends shown for neat Jet-A in Figures 7 and 8, it is possible to consider the reasons for the differences between the emulsified and neat jet fuel. Since the two fuels show a similar SMD near the nozzle and then the emulsified fuel shows a smaller SMD away from the nozzle, it is entertaining to speculate that microexplosions are occurring after the emulsified drops heat up and cause the larger drops to subdivide into smaller drops. However, the heat of vaporization of water is about eight times that of Jet A and the heat capacity of water is also higher so that the water may be absorbing much of the thermal energy available and reducing the evaporation rate of the emulsified fuel so that the rate of increase in drop size is reduced. This effect must be balanced against the lower boiling point of water which would tend to increase its evaporation rate. An analysis of this effect will be performed using the computer model modified to handle two fuel components.

Further tests were performed with emulsified and neat Jet A at constant air temperature with varying air pressure. Law (Ref. 7) has suggested that an increase in air pressure at constant temperature should

favor the occurrence of microexplosions because the steady state drop temperature increases with air pressure as was shown in Figures 1 to 3. The limit of superheat of water, also shown in Figures 1 to 3, is one of the criteria used to predict the condition for the onset of microexplosions. Spontaneous nucleation occurs below or at the limit of superheat (about 88 to 90 percent of the critical temperature) above which fluids will always film boil. Many liquids may be heated well above their "boiling points" and close to their predicted limit of superheat where they boil explosively. The details of the interface between the fluid and its surroundings usually determine where the fluid begins to boil in the range between the boiling point and the limit of superheat. Several investigators have chosen different temperatures to represent the condition for vaporization of the water and drop disruption; Birchley and Riley (Ref. 8) have chosen the normal boiling point, Jacques (Ref. 9) and Gollahall (Ref. 10) use that temperature where surface tension forces are exceeded by the forces due to the internal pressure of the drop, and Law (Ref. 7) assumes drop disruption occurs at the limit of superheat. Measured values for spontaneous nucleation of water have been reported by Avedisian (Ref. 11).

Thus, although there is disagreement about the drop temperature where microexplosions occur, a higher drop temperature, as allowed by an increase in air pressure, should favor a divergence in drop sizes for emulsified and neat fuels if drop disruptions are occurring. In order to examine this possibility, tests were performed at 589 K at pressures of 207 kPa (2.04 atm) and 310 kPa (3.06 atm) with the 11.4 liter/hr nozzle, and at 547 K with pressures from 165 kPa (1.63 atm) to 448 kPa (4.42 atm) for the 3.79 liter/hr nozzle, as shown in Figures 9 and 10, respectively. These results suggest that the emulsified and neat fuels evaporate in a similar manner at the lower pressures but tend to diverge as the air pressure is increased with the emulsified fuels producing smaller drops than the neat fuels, consistent with the microexplosion hypothesis.

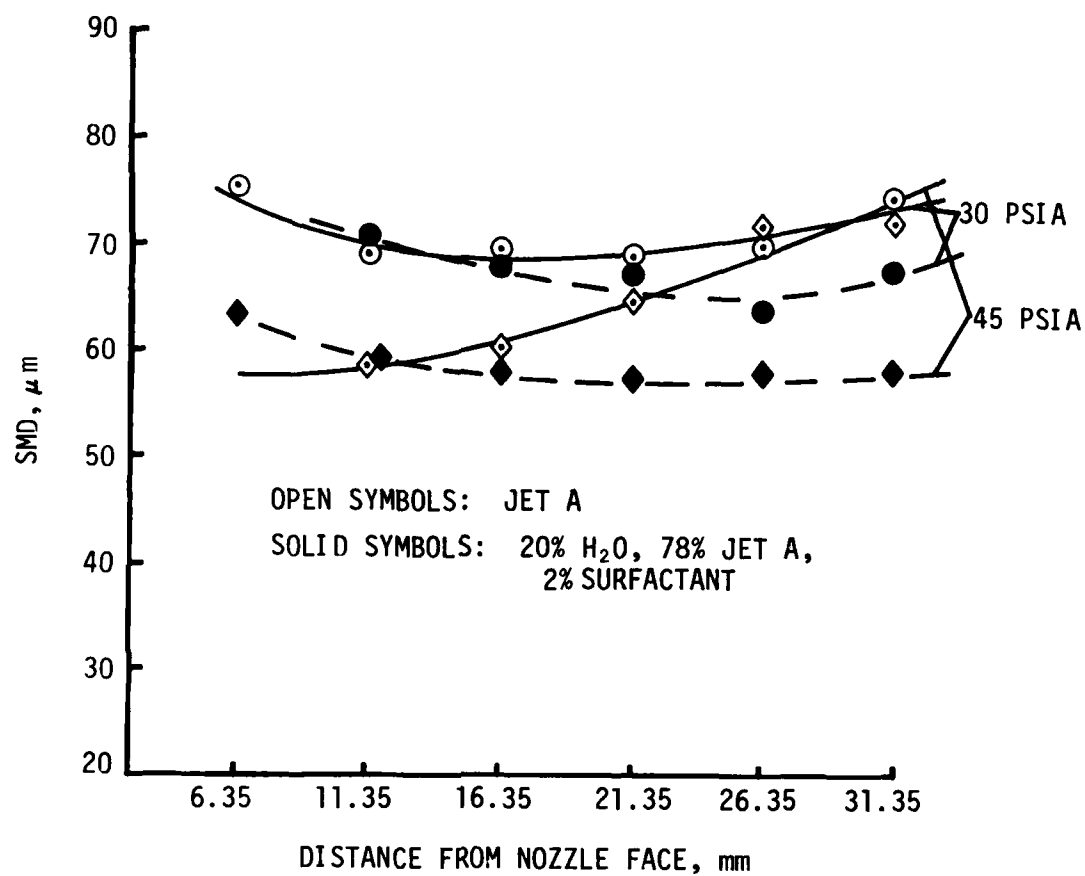
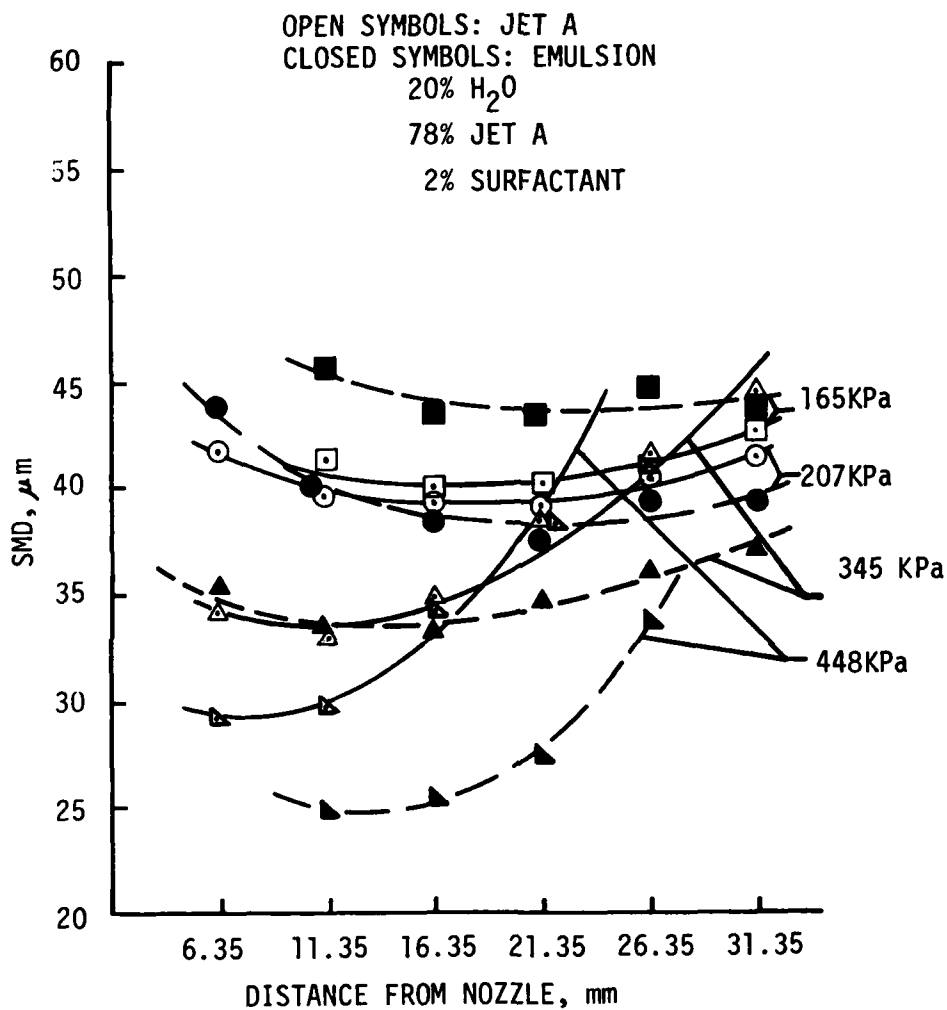


FIGURE 9. EFFECT OF AIR PRESSURE ON ATOMIZATION AND EVAPORATION -
 SMD VERSUS DISTANCE FROM NOZZLE
 ($T_{AIR} = 589$ K, $V_{REF} = 14.6$ m/SEC)



EFFECT OF AIR PRESSURE ON ATOMIZATION AND VAPORIZATION-
SMD VERSUS DISTANCE FROM NOZZLE

3.8 liters/hr 45°HC DELAVAN NOZZLE, 8.5 m/s, 547K

FIGURE 10

As an aside to the comparison of neat and emulsified fuel evaporation, consider the effect of pressure on the evaporation of neat fuel. Figures 4 through 6 indicate that the evaporation constant at quiescent conditions is approximately independent of air pressure at temperatures used in these experiments, while Figures 9 and 10 show that neat fuels evaporate faster as the pressure is increased (assuming that evaporation rates can be inferred from the rate of initial increase in SMD). This contradiction can be partly explained by three factors. First, as the air pressure increases the initial SMD decreases by a factor proportional to about $P^{-0.4}$, and the smaller drops evaporate much faster according to the d^2 -law. Secondly, the computations in Figures 4 through 6 are for the quiescent evaporation constant while Eq. 3 shows that the convective evaporation constant depends on pressure through the Reynolds number. Third, the transit times for the drops to a fixed measurement location increase slightly with pressure due to increased drag at higher pressures, allowing more time for evaporation.

Atomization/Evaporation Results for Emulsified and Neat Hexadecane

In order to make these arguments more quantitative, it was necessary to repeat the previous experiments with a single component fuel whose evaporation process could be modelled with greater certainty. Three single component fuels were obtained: n-hexadecane, n-dodecane, and n-octane, but experiments have been performed only with the n-hexadecane at this time. The evaporation of hexadecane drops was investigated at fixed air pressure and varying air temperature and visa versa. At a fixed pressure of 4.42 atm (448 kPa) the Sauter mean diameter (SMD) of the spray varied with distance from the nozzle as shown in Figure 11. A comparison of the size distribution of emulsified and neat fuels at 506 K and 547 K indicates no difference within the precision of the measurement. (Data for the emulsion at 506 K were essentially identical with those for the emulsion at 547 K and were omitted in Figure 11.) At 589 K the emulsified fuel produces smaller drops and the difference

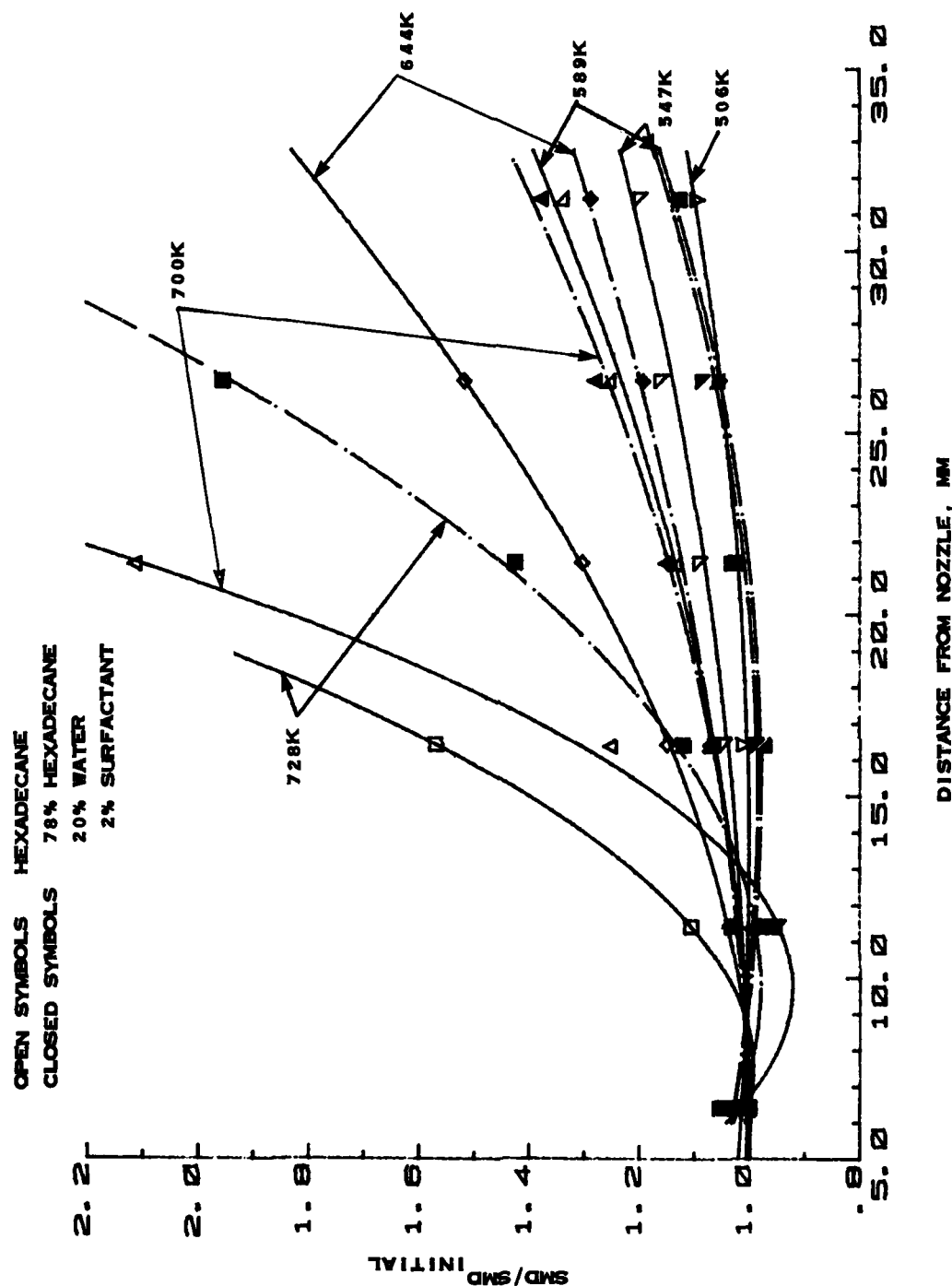


FIGURE 11. COMPARISON OF RELATIVE SMD FOR EMULSIFIED AND NEAT HEXADECANE AT CONSTANT PRESSURE (4.42 atm, 448 kPa) AND VARIOUS TEMPERATURES (DELAVAN WDA 3.8 LITERS/HR 45° HOLLOW CONE, $\Delta P=483$ kPa). $SMD_{initial} \approx 2 \mu m$

increases at the higher temperatures. The corresponding predicted maximum steady-state surface temperatures of the drops as computed by the model are shown in Table 3. At a fixed temperature of 644 K the drop sizes of neat and emulsified fuels were studied as a function of air pressure with the results as shown in Figures 12-14. Examination of Figure 14 indicates that at the lower pressures of 165 kPa (1.63 atm), 241 kPa (2.38 atm), and 345 kPa (3.40 atm), the drop sizes in sprays of neat and emulsified fuels are about the same, but that at higher pressures the sprays of emulsified fuels have smaller SMD's during the heat up and evaporation process. Table 4 presents the computed droplet temperatures for these experiments.

Table 3. Computer Predicted Steady State Drop Surface Temperatures for Hexadecane at Conditions Corresponding to Figure 11
($P_{air} = 448 \text{ kPa (4.42 atm)}$)

Air Temperature (K)	Drop Temperature (K)
506	488
547	503
589	520
644	535
700	541

Table 4. Computer Predicted Steady State Drop Surface Temperature for Hexadecane at Conditions Corresponding to Figures 12-14
($T_{air} = 644 \text{ K}$)

Air Pressure		Drop Temperature
(kPa)	(atm)	(K)
165	1.63	491
241	2.38	502
345	3.40	512
448	4.42	520
586	5.78	529

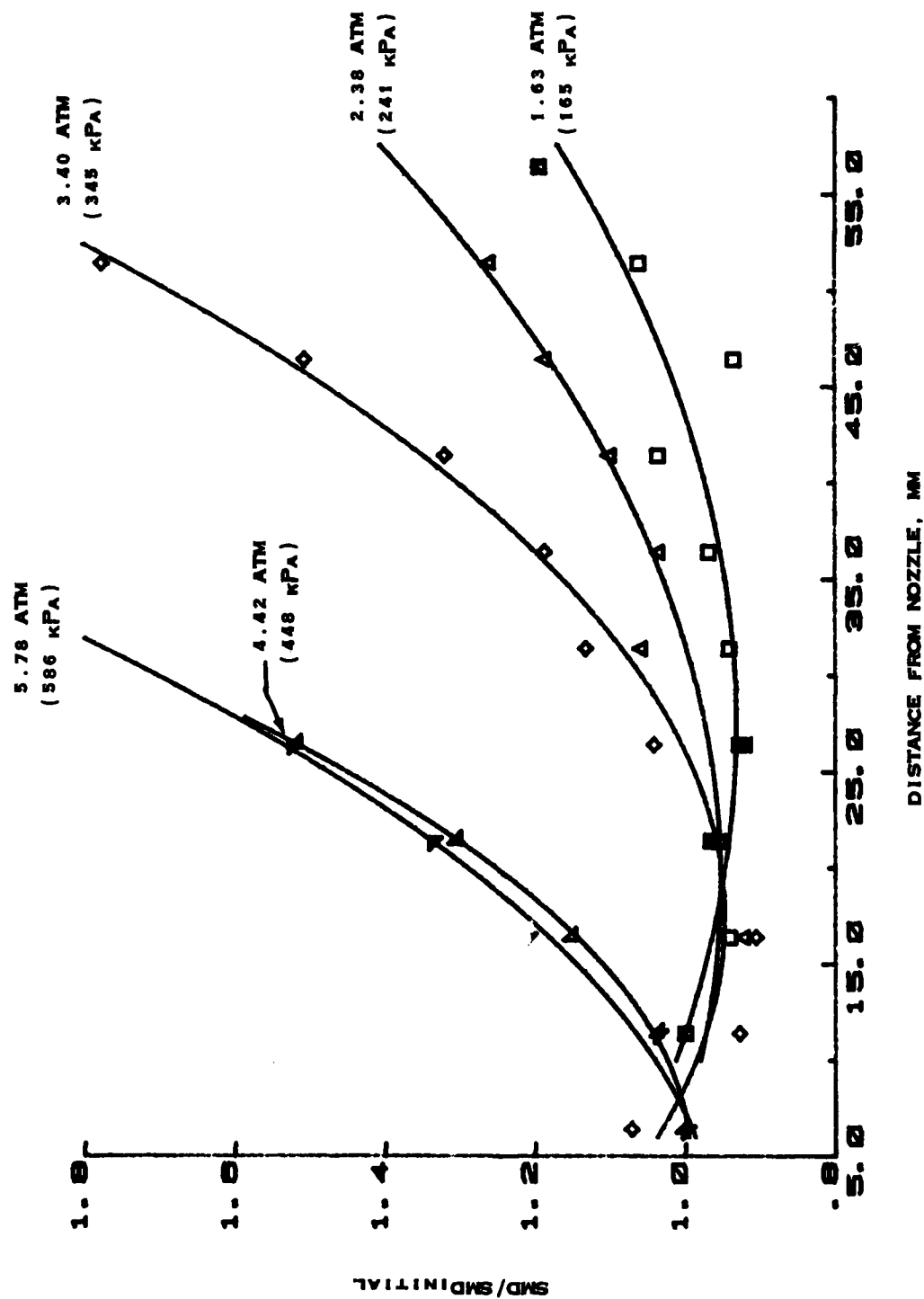


FIGURE 12. RELATIVE SMD FOR NEAT HEXADECANE AT FIXED TEMPERATURE (644K)
AT VARIOUS PRESSURES (DELAVAN WDA 3.8 LITERS/HR 45° HOLLOW CONE,
 $\Delta P = 483 \text{ kPa}$). $SMD_{\text{initial}} \approx 152 \text{ Pa}$ (kPa)^{-0.250}

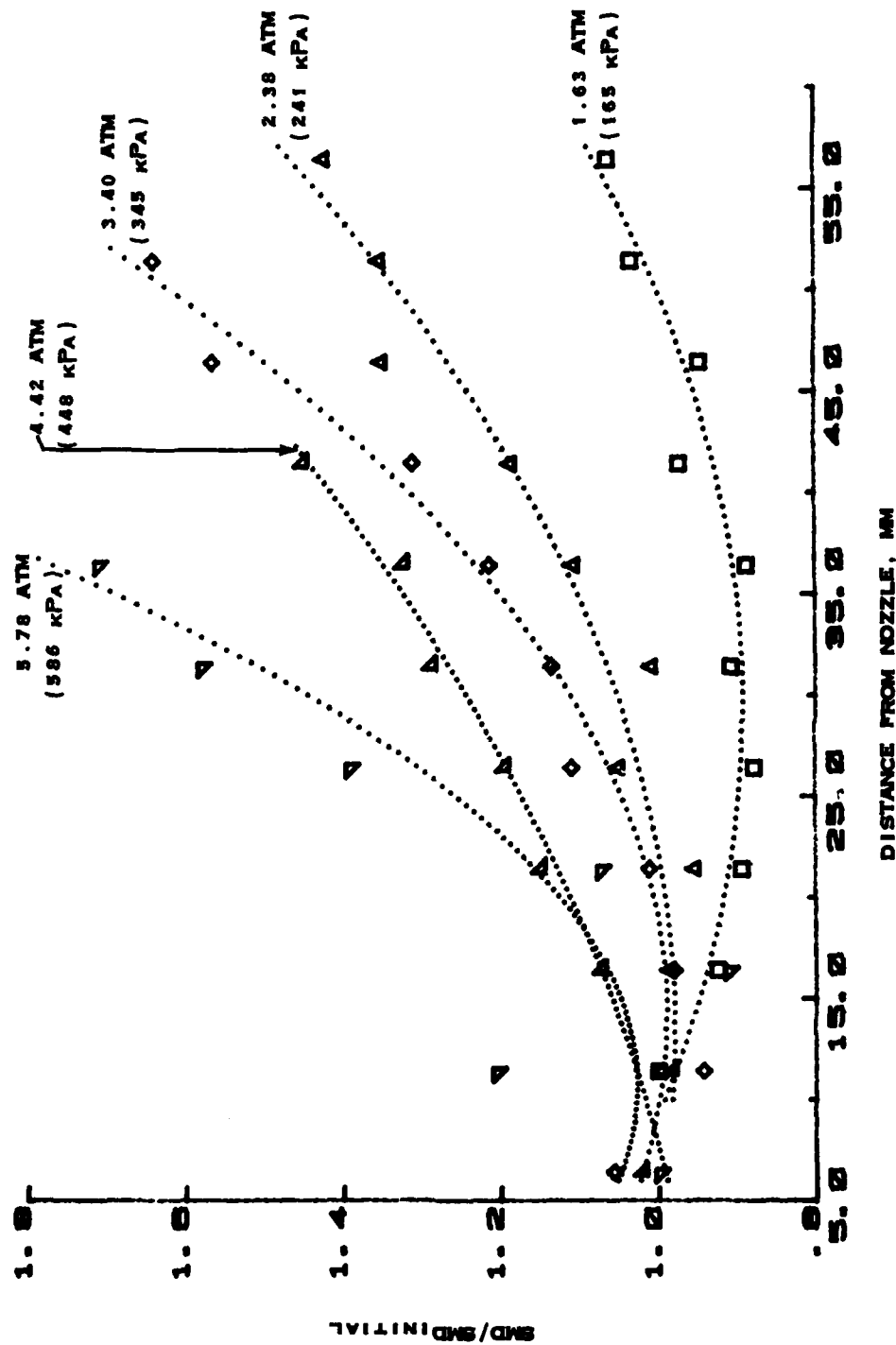


FIGURE 13. RELATIVE SMD FOR EMULSIFIED HEXADECANE AT FIXED TEMPERATURE (644K)
AT VARIOUS PRESSURES (DELAVAN WDA 3.8 LITERS/HR, 45° HOLLOW CONE)

$\Delta P = 483 \text{ kPa}$. $SMD_{\text{initial}} \approx 152 P_{\text{air}}^{-0.250}$

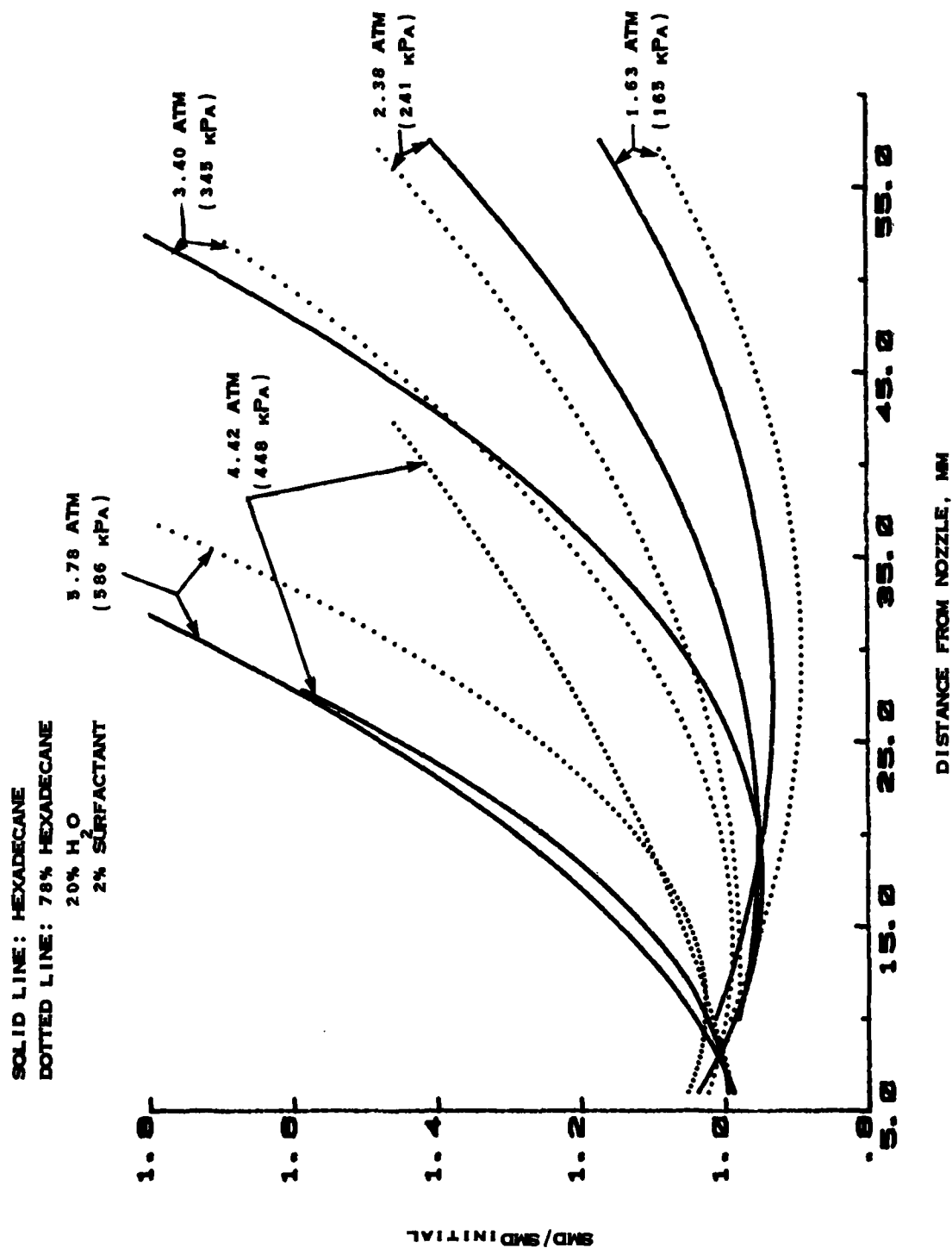


FIGURE 14. RESULTS OF FIGURES 12 AND 13 COMPARED

These trends correspond qualitatively to those expected if the emulsified fuel were undergoing microexplosions when the temperature and/or pressure were raised to a point where the drop temperature exceeded the spontaneous nucleation point of water. Below the spontaneous nucleation point the spray drop sizes should be similar for the two fuels, but as the drop temperature exceeds that condition the emulsified drop may be shattered into many smaller drops producing a smaller SMD than the neat fuel as distances from the nozzle increase.

In order to make this argument quantitative, it is necessary to know the drop temperature as a function of the air temperature and pressure. Presently there are no techniques to measure drop temperatures in a polydisperse spray where the small drops heat up rapidly while the large ones are much slower. This makes it necessary to predict the drop temperatures using the computer model to balance the heat conducted to the drop from the air with the heat used to vaporize the fuel. Some results from the model described earlier are shown in Tables 3 and 4 which indicate the increase in steady-state drop temperature with increasing air temperature or pressure. By comparing those tables with Figures 11 and 14, it may be seen that the drop size distributions for the emulsified and neat fuels diverge at a predicted steady state drop temperature of about 520 K. This may be compared with the limit of superheat of water of about 540 K (Ref. 12). The divergence of drop size distributions for emulsified and neat fuels at a drop temperature somewhat below the limit of superheat is consistent with the microexplosion hypothesis (Ref. 11). As mentioned previously, the limit of superheat is an upper limit where drop fragmentation must occur if water is present, while the probable temperature for spontaneous nucleation of water, and hence, microexplosions to occur is bounded by the normal boiling point (corrected for pressure) on the low end (~ 373 K) and the limit of superheat (~ 540 K) on the upper end. However, results from the model, which also predicts heat up times, would indicate

only the smaller diameter drops have reached the steady-state temperature at positions where the drop size distributions diverge.

Table 5 represents the computer predicted drop temperatures, (FTEMP) and the other drop information as explained previously for Table 2, for a location (X DROP) 26.4 mm from the nozzle for air conditions of 700 K and 448 kPa (4.42 atm). At these conditions, the results from Figure 11 indicate a considerable divergence between the emulsified and neat fuel SMD's. Although the steady-state temperature is close to the superheat limit of water (540 K) at these conditions, only the drops of initial size smaller than 28.0 μm exceed (approximately) 500 K and they represent about 34 percent of the original liquid volume of the spray. The drops equal to or larger than 177.6 μm represent less than three percent of the liquid volume of the initial spray and can be ignored. Thus, although the steady-state temperature is about 535 K, most of the drops are predicted to reach that temperature only late in their lifetime, and larger drops have only begun to heat up; e.g., the 141 μm drop has increased in "uniformly mixed" temperature from 311 K to 324K. Peak surface temperatures in the larger drops are higher, of course, than the uniformly mixed temperature would imply, but the result, nevertheless, is that the larger drops in the spray are, for the conditions of these experiments, much lower in temperature than the steady-state temperature. The variation of drop temperature with size coupled with the uncertainty of the temperature where spontaneous nucleation of the water microdrops should occur (as discussed earlier in the report) makes an exact condition where microexplosions should occur a meaningless exercise. What the model results do reveal is that the steady state drop temperature does increase with increasing air temperature and pressure to a range where spontaneous nucleation probably would occur if the water has not completely evaporated before reaching that condition. The model also indicates a considerable amount of the liquid spray volume which is contained in the larger drops is not at a temperature where microexplosions are expected.

Table 5. Computer Predicted Spray Characteristics for a Condition of

$T_{Air} = 700 \text{ K}$, $P_{Air} = 448 \text{ kPa}$
(4.42 atm), $V_{Air} = 8.54 \text{ m/s}$

R-R XBAR <UM>		R-R N		CORR.COEF.		SMD							
85.8		1.89		.974		45.53							
Initial	DIAM	TIME	X	DROP	Y	DROP	Z	DROP	U-VEL	V-VEL	W-VEL	FTEMP	RE
5.6	.9	.00020	.0069	.0021	0.0000	8.540			8.540	.000	0.000	534.7	.0
7.0	.9	.00031	.0080	.0022	0.0000	8.540			8.540	-.000	0.000	534.7	.0
8.8	.9	.00048	.0098	.0024	0.0000	8.540			8.540	-.000	0.000	534.7	.0
11.1	.9	.00073	.0123	.0028	0.0000	8.540			8.540	.000	0.000	534.7	.0
14.0	.9	.00111	.0162	.0033	0.0000	8.540			8.540	-.000	0.000	534.7	.0
17.6	.9	.00169	.0219	.0040	0.0000	8.540			8.540	.000	0.000	534.7	.0
22.2	12.7	.00205	.0264	.0051	0.0000	8.580			8.580	.030	0.000	534.7	.1
28.0	25.9	.00181	.0264	.0066	0.0000	9.145			9.145	.452	0.000	498.7	2.3
35.2	35.0	.00158	.0264	.0081	0.0000	10.629			10.629	1.560	0.000	444.8	10.2
44.4	44.4	.00142	.0264	.0091	0.0000	12.600			12.600	3.032	0.000	400.1	26.7
55.9	55.9	.00134	.0264	.0097	0.0000	14.200			14.200	4.226	0.000	370.7	49.9
70.5	70.5	.00130	.0264	.0099	0.0000	15.084			15.084	4.886	0.000	351.4	75.9
88.8	88.8	.00128	.0264	.0100	0.0000	15.533			15.533	5.221	0.000	338.6	105.3
111.9	111.9	.00126	.0265	.0102	0.0000	15.964			15.964	5.543	0.000	329.9	143.8
141.0	141.0	.00124	.0264	.0103	0.0000	16.369			16.369	5.846	0.000	324.0	193.9
177.6	177.6	.00122	.0264	.0104	0.0000	16.744			16.744	6.126	0.000	319.9	258.5
223.8	223.8	.00121	.0264	.0105	0.0000	17.072			17.072	6.370	0.000	317.2	340.9
282.0	282.0	.00120	.0265	.0106	0.0000	17.366			17.366	6.590	0.000	315.3	446.4
355.2	355.2	.00119	.0265	.0106	0.0000	17.629			17.629	6.786	0.000	314.0	581.0
447.6	447.6	.00118	.0264	.0107	0.0000	17.859			17.859	6.958	0.000	313.1	752.2
563.9	563.9	.00117	.0264	.0107	0.0000	18.061			18.061	7.109	0.000	312.4	969.6

The computer model is instructive in predicting and understanding some of the phenomena observed experimentally, but it is not sufficiently complete to compare precisely with the experimental results. The limitations of the current version of the computer code were mentioned earlier in this report and include: (1) no provision for inhomogeneities in drop size distribution along the line-of-sight, (2) secondary atomization of drops near the nozzle is ignored, and (3) the weighting factor associated with the laser beam location and size has been omitted. Because of the first two omissions, the model predicts an increase in SMD moving away from the nozzle while the experimental results show an initial decrease except at the highest temperatures. An effort was made to compare the trends for experimental and predicted SMD's by adjusting the initial Rosin-Rammler parameters ($\bar{x}$ and N) so that the predicted $\bar{x}$ and N at 11.4 mm and 16.4 mm were similar to the measured values with the results as shown in Figure 15. Experimentally measured SMD's at 6.4 mm were usually larger than at 11.4 mm while the predicted SMD's were significantly smaller. The fact that the atomization process was not complete at the 6.4 mm location as well as the other omissions from the model just mentioned probably account for that initial discrepancy. It should be noted that the upstream edge of the laser beam is only 2 mm from the nozzle at the 6.4 mm sampling location. There is a considerable discrepancy at the 21.4 mm location for the 700 K case. The discrepancy is probably partly due to an overestimate of the measured SMD due to beam steering problems, and points out the need to measure the amount of fuel vaporized at different locations to further check out the model. A more exact comparison of experimental and model results will require some additional sections to be added to the model to correct the deficiencies cited.

Drop Size Measurements in Flames

Drop size measurements in burning sprays have been attempted in several configurations including cases where the flame was stabilized in

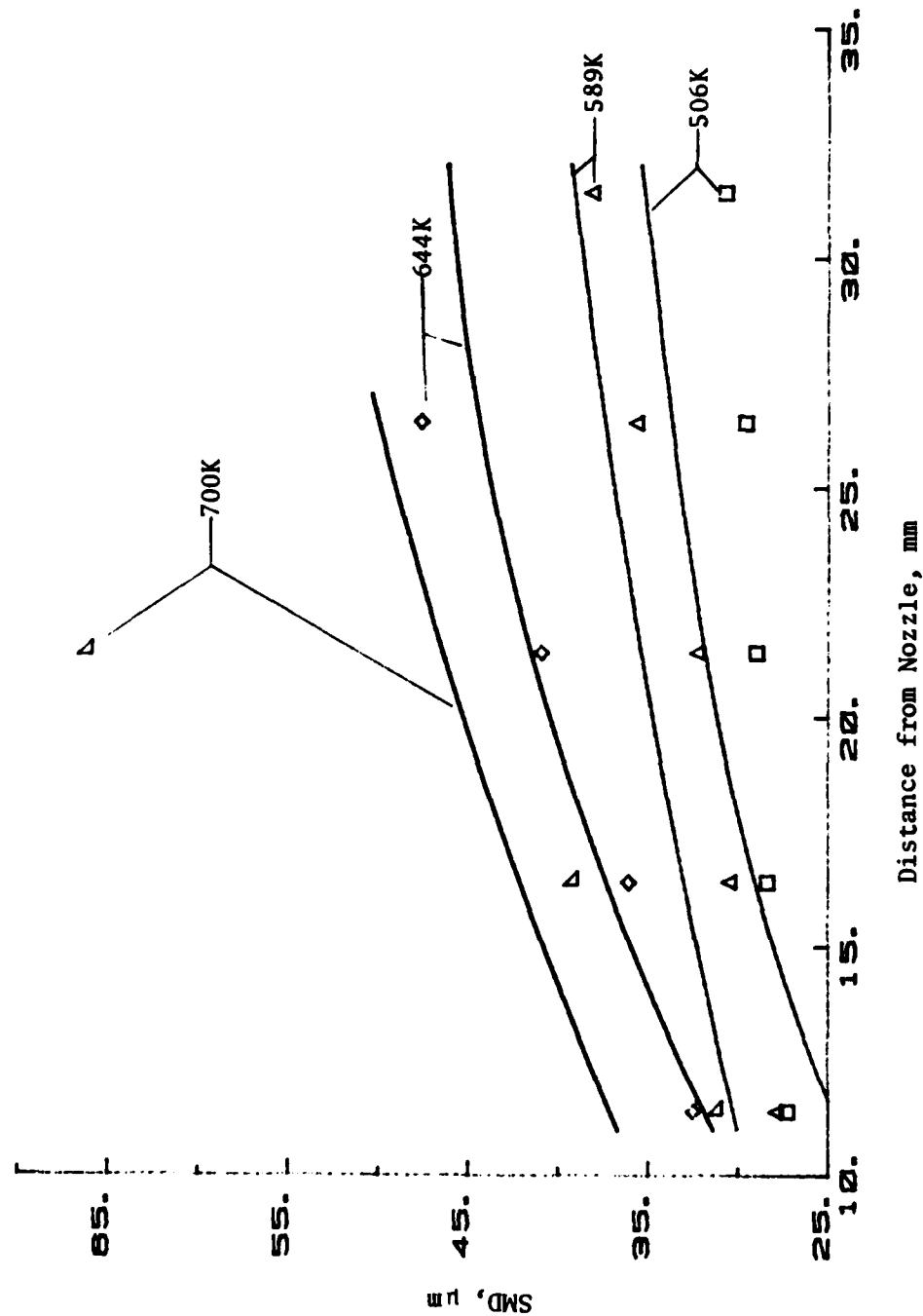


FIGURE 15. COMPARISON OF PREDICTED (LINES) AND MEASURED (SYMBOLS) SMD's AT DIFFERENT AIR TEMPERATURES ($P=4.42 \text{ atm}$) (448kPa)

a region downstream from the nozzle. Experiments to date have resulted in inadequate signal-to-noise ratios to determine reasonable drop size distributions. Generally, two types of problems are present when making size measurements with laser-diffraction instrumentation in burning sprays. First, the flame produces high levels of visible and near-infrared radiation (in the response range of the detectors) which is orders of magnitude higher in intensity than the desired scattered radiation from the HeNe laser. Secondly, the severe gradients in temperature and air/fuel vapor concentrations result in serious beam steering problems causing the laser beam to be directed onto areas of the detector other than the central ring. This produces signals which appear to be due to large drops scattering light onto the inner detector rings and thus represents a false signal.

The three modifications described in the EXPERIMENTAL APPARATUS section were sufficient to discriminate against the flame radiation for the cases examined. However, the severe refractive index gradients produced so much noise on the inner detector rings that the drop size data which were computed were judged to be unreasonable. Further consideration is being given to ways to circumvent this problem.

CONCLUSIONS

Techniques have been developed which allow for the determination of drop-size data in evaporating fuel sprays over a range of elevated pressures and temperatures important to gas-turbine combustion.

It has been determined that there are substantial differences in the evaporation characteristics of emulsified fuels when compared with neat fuels. The spray droplets of the evaporating emulsified fuel are, on the average, significantly smaller than the droplets of neat fuel at corresponding elevated temperature/pressure conditions. The differences are enhanced as the pressure increases for the range examined (to about 5.8 atm (590 kPa)). These findings are consistent with the microexplosion hypothesis but a thorough analysis of other possible effects has not been completed.

Limited experimental data would suggest that the size of drops at initial atomization depends strongly on the air pressure, with $SMD \propto P_{Air}^{-0.4}$.

RECOMMENDATIONS FOR NEXT YEAR

Results already described have indicated significant differences in drop sizes for evaporating sprays of emulsified and neat fuels. In order to understand the reasons for these differences, the following work is proposed for the next year of this program, although there may be insufficient time to pursue all of these suggestions.

1. Conduct similar atomization/evaporation experiments with single component fuels of lower boiling point than n-hexadecane. Fuels such as n-octane/water emulsions should not exhibit microexplosions but would still be subject to the "heat-sink" effect of water on the evaporation process. This will help to separate the microexplosion effect on drop size from the reduced evaporation rate due to the high heat of vaporization of water.
2. Develop method(s) for measuring fuel vapor concentration in sprays. Both optical and probe techniques have been used by other workers to measure fuel/air ratios in sprays and to differentiate between the liquid and vapor phases of the fuel. These would be useful in studying the evaporation of emulsified fuels, as microexplosions would enhance the evaporation rates while the "heat-sink" effect of water would slow down evaporation rates.
3. Modify computer model for 2-component fuels with various assumptions about relative evaporation rates. The effect of water emulsification with a single component fuel could be studied from a theoretical view to compare with the experimental results.
4. Modify computer model to include the inhomogeneity of spray, and laser beam location and intensity profile. This would lead to a better capability to compare experimental and computer predicted results.

5. Modify computer model to predict the concentration of fuel vapor as a function of axial distance from the nozzle. If the measurement techniques described in item (2.) are developed, they could be compared with the predicted results.

ACKNOWLEDGMENTS

This work has resulted from contributions of a large number of people, whose efforts we wish to acknowledge. The Office of Naval Research, with technical monitoring by M.K. Ellingsworth, provided funds for this program under Contract No. N0014-80-K-0460. Mr. R.C. Haufler performed much of the experimental work. Much of the computer model was based on work done by Professors J.S. Chin and A.H. Lefebvre at Purdue and W.H. Ayers, J. Swithenbank, and F. Boyson of the University of Sheffield. Assistance in the computer programming was provided by Mr. T.J. Callahan. Dr. B. Weiner of Malvern provided ideas in the use of the drop sizing instrument. Electronics necessary for this program were designed by S.A. Cerwin and constructed by H.F. Donoho, Jr. Dr. D.W. Naegeli at this laboratory and Dr. J.J. Sangiovanni of UTRC provided helpful ideas and Ms. S.J. Boyd and Mr. J.W. Pryor helped in manuscript preparation.

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APPENDIX A

FUEL SPRAY COMPUTER MODEL - MATHEMATICS

For purposes of discussion, the model is divided into three parts called (1) Thermodynamics, (2) Aerodynamics, and (3) Drop-Size Distribution. Each section is discussed in order. An overall flow chart is shown in Figure A-1.

Thermodynamics

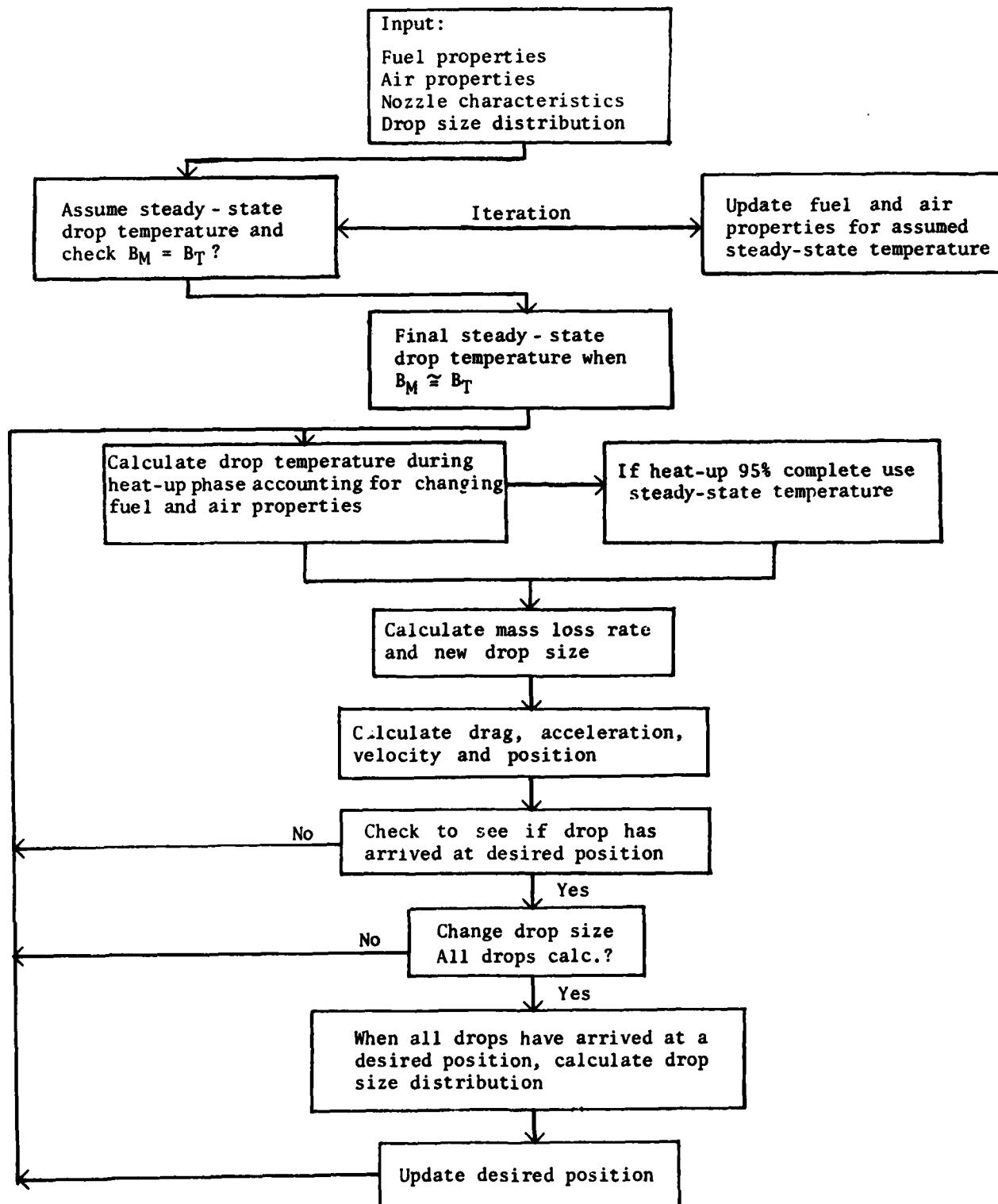
This part of the model computes the heat-up of the drop, the final steady-state temperature, and the fuel and air properties necessary for those calculations. This part of the model is identical to that described by Chin and Lefebvre (Ref. A1 and A2) except that some of the fuel property data were taken from the American Petroleum Institute Data Book (Ref. A3). The results from this model are very similar to those presented by Chin and Lefebvre when the model is used for quiescent fuel sprays. The integration of this part of the model with the other sections to be described allows the examination of sprays in situations where both spray and air are moving with a nonzero relative velocity. The mathematics are outlined below, but a more detailed derivation is given by Chin and Lefebvre (Ref. A1 and A2) which in turn is based on the theories described by Spalding (Ref. A4).

The steady-state temperature is determined as follows. The mass transfer rate, $\dot{m}$, from a drop is given by,

$$\dot{m}_F = 2\pi D (k_g/c_{p,g}) \ln (1+B) \quad (A1)$$

where D is the diameter, k_g is the thermal conductivity of the gas, $c_{p,g}$ is the specific heat at constant pressure, and B is either B_M , the mass diffusion transfer number if mass diffusion is controlling, or B_T , the

FIGURE A-1 FLOW CHART OF SPRAY MODEL



thermal diffusion transfer number if heat transfer is controlling and the Lewis number is assumed to be unity. B_M is defined as

$$B_M = (Y_{F,s} - Y_{F,\infty}) / (1 - Y_{F,s}) \quad (A2)$$

where $Y_{F,s}$ and $Y_{F,\infty}$ are the fuel mass fractions at the drop surface and in the ambient air, respectively, and $Y_{F,s}$ is

$$Y_{F,s} = P_{F,s} M_F / (P_{F,s} M_F + (P - P_{F,s}) M_A) \quad (A3)$$

where $P_{F,s}$ is the fuel vapor pressure at the drop surface, P is the ambient pressure, and M_F and M_A are the molecular weights of fuel and air, respectively. The vapor pressure was calculated using the method recommended by the American Petroleum Institute Data Book (Ref. A3) called Procedure 5A1.10, "Vapor Pressures of Pure Hydrocarbons."

The thermal diffusion transfer number B_T for an evaporating drop is

$$B_T = c_{p,g} (T_\infty - T_s) / L \quad (A4)$$

where T_∞ and T_s are the ambient air temperature and drop surface temperature and L is the latent heat of fuel vaporization corrected from the normal boiling point to the actual surface temperature.

The accuracy of Equation (A1) is very dependent on the choice of values for k_g and $c_{p,g}$. As recommended by Chin and Lefebvre (Ref. A1) a reference temperature was chosen as the drop surface temperature plus 1/3 of the difference between ambient air and surface temperatures. Similarly a reference value of the fuel vapor mass fraction was taken as the value just outside the surface plus 1/3 of the difference between the value at infinity and just outside the surface. Using these reference conditions denoted by "r" the specific heat of the gas is given by,

$$c_{p,g} = Y_{A,r} (c_{p,A} \text{ at } T_r) + Y_{F,r} (c_{p,V} \text{ at } T_r) \quad (\text{A5})$$

and the thermal conductivity by,

$$k_g = Y_{A,r} (k_A \text{ at } T_r) + Y_{F,r} (k_V \text{ at } T_r) \quad (\text{A6})$$

At steady-state conditions, $B_M = B_T$ or from Equations (A2) and (A4)

$$\frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}} = \frac{c_{p,g} (T_\infty - T_{s,st})}{L} \quad (\text{A7})$$

where $T_{s,st}$ is the desired surface temperature under steady-state conditions. Assuming that the fuel vapor concentration in the ambient air is zero ($Y_{F,\infty} = 0$) and substituting for $Y_{F,s}$ from Equation (A3) then (A7) becomes

$$\frac{P}{P_{F,s}} - \frac{M_F}{M_A} \frac{L}{c_{p,g} (T_\infty - T_{s,st})} - 1 = 0 \quad (\text{A8})$$

In solving Equation (A8) to determine the steady-state surface temperature $T_{s,st}$, some of the variables can be specified, P , M_F , M_A , and T_∞ but the remaining three variables are functions of temperature, with L being related to the heat of vaporization at the normal boiling point $L_{T,bn}$ by,

$$L = L_{T,bn} \left[(T_{Cr} - T_s) / (T_{Cr} - T_{bn}) \right]^{0.38} \quad (\text{A9})$$

where T_{Cr} is the critical temperature and T_{bn} is the normal boiling point of the fuel. In order to solve (A8) it is necessary to first assume a value for $T_{s,st}$. That temperature is used to calculate a reference temperature T_r which in turn is used to calculate those quantities specified in Equations (A5) and (A6) used to calculate $c_{p,g}$ and k_g , and to calculate L as specified in (A9). If the assumed value of $T_{s,st}$ is too low, the left side of Equation (A8) will be positive. An iterative procedure must be used to continue specifying $T_{s,st}$ until Equation (A8) is satisfied within the desired accuracy. That procedure results in a

determination of the steady state surface temperature $T_{s,st}$ and the transfer number $B=B_M=B_T$. The steady state quiescent evaporation constant $\lambda_{q,st}$ can then be determined from,

$$\lambda_{q,st} = 8 k_g \ln (1+B) / \rho_F c_{p,g} \quad (A10)$$

where ρ_F is the fuel density. Frossling (Ref. A5) has shown that convective effects can be accounted for in the case where heat transfer rates are controlling by,

$$\lambda_{c,st} = \lambda_{q,st} (1 + 0.276 Re_D^{0.5} Pr_g^{0.33}) \quad (A11)$$

where $\lambda_{c,st}$ is the steady-state evaporation constant corrected for convective effects, Pr_g is the Prandtl number for the gas, and Re_D is the Reynolds number using the relative velocity between the drop and the gas. This velocity should include a fluctuating component in the case of turbulent flow. Turbulence intensities were not measured in these experiments, but a value of 20 percent of the axial velocity was used as an estimate. The effective velocity used to calculate Re_D for the evaporation calculation was taken as the sum of the fluctuating component (20 percent of the air velocity) plus the difference between the drop and air velocities. These computations specify the steady-state properties of the drop.

The evaporation which occurs during the drop heat-up period is significant in many practical situations, with the drop being completely evaporated before reaching steady-state conditions in some instances. Chin and Lefebvre (Ref. A2) have predicted that high air pressures and convective effects, which are often absent in laboratory experiments, both tend to increase the relative importance of the heat-up period relative to the steady-state phase of drop evaporation. Because the experiments conducted in this study were of real sprays at high pressures and relative velocities, it was necessary to model the heat-up period in detail.

Chin and Lefebvre (Ref. A2) have shown that the rate of change of drop surface temperature is given by,

$$dT_s / dt = (\dot{m}_F L / c_{p,F} m) \{ (B_T / B_M) - 1 \} \quad (A12)$$

where $\dot{m}_F$ is specified by Equation (A1) with $B=B_M$ during the heat-up period, and m is the drop mass,

$$m = (\pi/6) \rho_F D^3 \quad (A13)$$

The change of drop size with time is given by (Ref. A2),

$$dD / dt = -4 k_g \ln (1+B_M) / \rho_F c_{p,g} D \quad (A14)$$

The drop temperature asymptotically approaches the steady-state temperature, and it was assumed that when the temperature had risen to 95 percent of the difference between the initial fuel temperature and the steady-state temperature, that the heat-up calculations could be terminated and steady-state properties used.

Aerodynamics

The approach used was a much more simplified version of the one developed at the University of Sheffield and described in several papers, e.g., Boyson and Swithenbank (Ref. A6). A cylindrical coordinate system was used where x is the axial distance, y the radial distance, and z the angular position, with corresponding velocities in the axial (u), radial (v), and tangential (w) directions. For this work, the tangential velocities were assumed zero.

The equations of motion of a particle (drop) neglecting all forces except drag, are,

$$\dot{u}_p = -F (u_p - u_\infty) \quad (A15)$$

$$\dot{v}_p = \frac{w_p^2}{y_p} - F (v_p - v_\infty) \quad (A16)$$

$$\dot{w}_p = \frac{v_p w_p}{y_p} - F (w_p - w_\infty) \quad (A17)$$

where the "p" subscripts refer to the particle and the " ∞ " subscript refers to the free stream, and F is given by,

$$F = (18 \mu_g / \rho_p D_p^2) (C_D Re / 24) \quad (A18)$$

where μ_g is the gas viscosity, ρ_p is the particle density, D_p is the particle diameter, C_D is the drag coefficient, and Re is the Reynolds number defined as,

$$Re = \frac{D_p \rho_g}{\mu_g} \left| \vec{u}_p - \vec{u}_\infty \right| \quad (A19)$$

The drag coefficient, C_D , is given by (Ref. A7),

$$C_D = 27 Re^{-0.84} \quad 0 < Re < 80 \quad (A20)$$

$$C_D = 0.271 Re^{0.217} \quad 80 < Re \leq 10^4 \quad (A21)$$

$$C_D = 2 \quad 10^4 > Re \quad (A22)$$

The equations of motion (A15 to A17) are solved numerically using a step size of 1 to 10 μ s, and the equations of trajectory are solved in a similar manner,

$$\dot{x}_p = u_p \quad (A23)$$

$$\dot{y}_p = v_p \quad (A24)$$

$$\dot{z}_p = \frac{w_p}{y_p} \quad (A25)$$

These equations describe the trajectory of a particle in a gas stream. For each iteration in the trajectory calculation, the drop size and temperature are updated using the procedure described in the Thermodynamics section.

At the end of each iteration through the trajectory calculations, the current calculated axial position of the particle is checked against a target value. When the particle reaches that target value for axial position, the position, transit time, size, temperature, and other parameters for that drop are frozen and the calculations are repeated for the next larger drop size. After all drops reach a targeted axial position, corresponding to a measurement location, the drop size distribution is calculated, important data are printed out, the target position is moved downstream, and the calculations are repeated.

Drop Size Distribution

The computer model makes all calculations on individual drops of certain sizes, but the instrumentation used to measure the spray works best in characterizing the drop sizes by two parameters which specify a size and width of the distribution. Three distributions may be selected: normal, log-normal, and Rosin-Rammler. The Rosin-Rammler distribution has provided the best fit of the sprays studied and has been used throughout this program. In order to compare the predictions from the computer model with the experimental results, it is necessary to convert the computer predicted drop sizes at a given location into an equivalent set of two parameters specifying the Rosin-Rammler distribution.

If R represents the fraction of the liquid being sprayed contained in drops larger than diameter D , then for the Rosin-Rammler distribution (Ref. A8),

$$R = \exp \left(-(D / \bar{x})^N \right) \quad (\text{A26})$$

where $\bar{x}$ represents a size, and N specifies the width of the distribution. It is convenient to specify a spray by a single parameter representing an "average" drop size. However, a straight numerical average is heavily weighted towards the smallest drops which are extremely plentiful but which contain a very small fraction of the total volume of the liquid. For combustion processes, the surface-to-volume ratio is important to evaporation, so an average drop size may be chosen which has a surface-to-volume ratio representative of the actual spray, and such an average is called the surface-volume mean diameter or Sauter mean diameter (SMD). The SMD is related to the Rosin-Rammler parameters by (Ref. A8),

$$\text{SMD} = \bar{x} / \Gamma(1-1/N) \quad N > 1 \quad (\text{A27})$$

Specifying $\bar{x}$ and N allows the calculation of the SMD, or specifying SMD and N determines $\bar{x}$.

An initial set of drop sizes distributed approximately exponentially in size (i.e., evenly spaced when plotted as $\ln D$) and covering the range of about $6\mu\text{m}$ to $560\mu\text{m}$ (corresponding to the response range of the drop sizing instrument) with 16 to 21 different sizes is used in the model. Assuming size classes bounded by these drops as end points, the initial fraction of liquid contained in drops larger than a certain size class is given by Equation (A26).

$$R_i = \exp \left(-(D_{0,i} / \bar{x})^N \right) \quad 1 \leq i \leq n \quad (\text{A28})$$

$$R_0 \equiv 1$$

$$R_{n+1} \equiv 0$$

where "n" is the number of drops, D_0 is the initial drop diameter, and the initial fraction of liquid in each size class is,

$$\begin{aligned} F_{0,i} &= R_i - R_{i+1} & 0 \leq i \leq n \\ F_{0,-1} &\equiv 0 \end{aligned} \quad (A29)$$

After evaporation begins, the small drops begin evaporating quickly while the large ones evaporate slowly, changing the fraction of liquid in the different size classes unevenly. Denoting the smallest nonevaporated drop size by "k", the fraction of liquid remaining in any size class is,

$$F_i = \frac{F_{0,i} \left\{ (D_i / D_{0,i})^3 / u_{p,i} + (D_{i+1} / D_{0,i+1})^3 / u_{p,i+1} \right\} / 2}{\sum_{j=k}^n F_{0,j} \left\{ (D_j / D_{0,j})^3 / u_{p,i} + (D_{j+1} / D_{0,j+1})^3 / u_{p,j+1} \right\} / 2} \quad (A30)$$

where

$$D_0 \equiv D_1$$

$$u_{p,0} \equiv u_{p,1}$$

$$D_{n+1} \equiv D_n$$

$$u_{p,n+1} \equiv u_{p,n}$$

$$\begin{aligned} k &\leq i \leq n \\ (0 &\leq k \leq n) \end{aligned}$$

and $u_{p,i}$ is the axial velocity of the i th drop, D_i is the instantaneous drop size, and $D_{0,i}$ is the initial drop size of the i th drop. Each size class is characterized by the drops making up the end points, and the initial fraction of liquid in a size class is modified by the average loss of volume of the end point drops. The velocity term is added to account for the fact that as the drops slow down they increase their relative concentration, and thus their weighting factor, in the sample volume.

The cumulative fraction of liquid in all size classes including and larger than the i th class is,

$$R_i = \sum_{j=i}^n F_j \quad k \leq i \leq n \quad (A31)$$

This instantaneous value of R_i is related to the drop sizes and Rosin-Rammler parameters by Equation (A28) with the initial drop size $D_{0,i}$ replaced by the instantaneous value D_i ,

$$R_i = \exp(-(D_i / \bar{x})^N) \quad k \leq i \leq n \quad (A32)$$

Taking the natural logarithm of both sides twice and excluding $i=k$ ($R_i=1$), Equation (A32) becomes,

$$\ln_e(\ln_e(1 / R_i)) = N \ln_e D_i - N \ln_e \bar{x} \quad k+1 \leq i \leq n \quad (A33)$$

This has the form of the equation of a straight line, $y=mx+b$, if the following definitions are used,

$$y = \ln_e(\ln_e(1/R))$$

$$m = N$$

$$x = \ln_e D$$

$$b = -N \ln_e \bar{x}$$

Thus, by determining a least squares fit of the straight line through the data $\ln_e(\ln_e(1/R_i))$ versus $\ln_e D_i$, the Rosin-Rammler parameters are given by,

$$N = m \text{ (the slope)} \quad (A35)$$

and

$$\bar{x} = \exp (-b / N)$$

A standard routine is used to perform the least squares operation and the Rosin-Rammler parameters and the SMD (from Equation (A27)) are determined at each target value of the axial location corresponding to the position where experimental data are obtained. Although the initial distribution at the nozzle is an ideal Rosin-Rammler distribution, the distribution downstream does not correspond exactly to the Rosin-Rammler equation due to the different evaporation rates for the different sized drops, and the degree of fit is determined by the correlation coefficient of the straight line through the computed data.

**APPENDIX A
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APPENDIX B

FUEL SPRAY COMPUTER MODEL - LISTING

&DROPP T=00004 IS ON CR TR USING 00068 BLKS R=0000

```
0001 FTH4,L,Q
0002 PROGRAM DROPP
0003 C THIS DROP EVAPORATION MODEL INCORPORATES MUCH OF THE HEAT TRANSFER
0004 C SUGGESTED BY CHIN AND LEFEBVRE IN AIAA-82-1176 - 8/30/82
0005 DIMENSION D(23),DIAM0(23),TIME(23),XP(23),YP(23),ZP(23),UP(23),
0006 C VP(23),WP(23),FF0(24),FF(24),R(24),FTEMP(23),RE(23),NU(23),
0007 C F(24),CB(23),CD(23),XDATA(23),YDATA(23),ZDATA(23),DMU(23),
0008 C XK(23),REN(25),
0009 & TSD(23),LAMBHU(23),LAMB(23)
0010 REAL L,LAMBST,NU,MUA,N,NNEW,M,LTBN,MWA,MWF,LEFT,KA,KV,KG,MUG,MUV,
0011 & LAMBHU,LAMBA,MASSD,MDOT
0012 C DROP DIAMETERS (M)
0013 DATA DIAM0/5.8,7.2,9.0,11.4,14.4,18.4,23.6,30.3,38.9,50.1,
0014 C 64.6,84.2,112.8,160.3,261.6,563.9/
0015 NDROP = 16
0016 DO 10 I=1,NDROP
0017 10 DIAM0(I) = DIAM0(I) / 1E6
0018 C ALTERNATE SET OF DROP DIAMETERS
0019 NDROP = 21
0020 DO 12 I = 1,NDROP
0021 QQ = (I-1)/3.0
0022 12 DIAM0(I) = 5.5505428 * (2.0**QQ) * 1.0E-6
0023 C STEP SIZE FOR TARGET VALUE AND FINAL TARGET VALUE (M)
0024 DATA XPT/.00500/
0025 DATA XPTT/.05635/
0026 DATA XPS/.00135/
0027 DATA II/0/
0028 DATA KK/0/
0029 C MASS FRACTION OF FUEL IN AMBIENT AIR SURROUNDING DROP
0030 DATA YFI/0.0/
0031 C FUEL INLET TEMPERATURE (K)
0032 DATA FTEMP0/311./
0033 C BOILING POINT OF FUEL (K)
0034 DATA TBN /560.0/
0035 C EXPANSION COEFF OF FUEL
0036 DATA CEX/0.00055/
0037 C CONE ANGLE OF SPRAY (DEGREES)
0038 DATA PHI/45./
0039 C DISTANCE FROM NOZZLE TO SHEET BREAKUP (M)
0040 DATA DBREAK/0.005/
0041 C SWIRL COMPONENT OF SPRAY (DEGREES)
0042 DATA FSWIRL/0.0/
0043 C INITIAL SPRAY VELOCITY (M/S)
0044 DATA VSPRAY/20.76/
0045 C MOLECULAR WEIGHT OF AIR
0046 DATA MWA/28.96/
0047 C INLET AIR VELOCITY, X,Y,Z COMP (M/SEC)
0048 DATA UA,VA,WA/08.54,0.,0./
0049 C STEP SIZE FOR TIME (SEC)
0050 DATA DELTAT/0.000010/
0051 C LATENT HEAT OF VAPORIZATION AT NORMAL BOILING POINT (KJ/KG)
0052 DATA LTBN/224./
0053 C FUEL DENSITY (KG/M**3)
0054 DATA RHOF0/776.6/
0055 C MOLECULAR WEIGHT OF FUEL
0056 DATA MWF/226.43/
0057 C NUMBER OF CARBON ATOMS IN FUEL MOLECULE
0058 DATA NOCARB/16/
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0059 C SURFACE TENSION OF FUEL (NT/M)
0060 DATA SIGMA/28.0E-3/
0061 C CRITICAL TEMP OF FUEL (K)
0062 DATA TCR/720.6/
0063 C CRITICAL PRESSURE OF FUEL (KPA)
0064 DATA PCR/1421./
0065 C CRITICAL DENSITY OF FUEL (KG/M**3)
0066 DATA RHOCR/239.0/
0067 C CRITICAL COMPRESSIBILITY OF FUEL
0068 DATA ZCR/0.225/
0069 C ACENTRIC FACTOR FOR FUEL (USED TO CALCULATE VAPOR PRESSURE)
0070 C SEE API DATA BOOK, CHAPTER 2
0071 DATA ACENTR/0.7418/
0072 WRITE (1,999)
0073 999 FORMAT ("ATEMP0(K) = , AIR PRESS(ATM) = ")
0074 READ (1,*) ATEMP0,P
0075 WRITE (1,990)
0076 990 FORMAT (" XBAR (MICRONS)=, N =, ")
0077 READ (1,*) XBAR,N
0078 XBAR = XBAR * 1.0E-6
0079 WRITE (6,996) ATEMP0,P
0080 996 FORMAT ("ATEMP0(K) = ",F6.0," AIR PRESS(ATM) = ",F6.2)
0081 C CONVERT PRESSURE TO KPA
0082 P = P * 101.325
0083 TAI= ATEMP0
0084 C CALCULATE QUANTITIES WHICH ARE INDEP OF DROP SIZE
0085 DO 14 I = 1,NDROP
0086 14 TIME(I) = 0.0
0087 C SET INITIAL DROP ARRAY VALUES
0088 XP0 = DBREAK * COS(PHI * 3.1415/360.)
0089 YP0 = DBREAK * SIN(PHI * 3.1415/360.)
0090 ZP0 = 0.
0091 C SPRAY VELOCITY COMPONENTS
0092 UP0 = VSPRAY * COS(PHI * 3.1415/360.) * COS(FSWIRL*2*3.1415/360.)
0093 VP0 = VSPRAY * SIN(PHI * 3.1415/360.) * COS(FSWIRL*2*3.1415/360.)
0094 WP0 = VSPRAY * SIN(FSWIRL * 2*3.1415/360.)
0095 DO 15 I = 1,NDROP
0096 D(I) = DIAM0(I)
0097 FTEMP(I) = FTEMP0
0098 UP(I) = UP0
0099 VP(I) = VP0
0100 WP(I) = WP0
0101 XP(I) = XP0
0102 YP(I) = YP0
0103 ZP(I) = ZP0
0104 15 R(I) = EXP(-((DIAM0(I)/XBAR)**N))
0105 R(0) = 1.0
0106 R(NDROP+1) = 0.0
0107 DO 90 I = 0,NDROP
0108 FF0(I) = R(I) - R(I+1)
0109 90 CONTINUE
0110 FF0(-1) = 0.0
0111 C OUTPUT INITIAL VALUES
0112 XBARMU = XBAR * 1E4
0113 WRITE (6,95) XBARMU,N,FTEMP0,TBN,PHI,VSPRAY,UP0,VP0,WP0
0114 95 FORMAT (F6.1,F5.2,2F6.0,F6.1,F7.0,3F7.1)
0115 WRITE (6,96) ATEMP0,UA,VA,WA
0116 96 FORMAT (4F12.1)
0117 WRITE (6,97) DELTAT,P,XP0,YP0,ZP0
0118 97 FORMAT (F8.5,F5.1,3F8.2)

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0119 C COMPUTE TSST, THE STEADY STATE DROPLET TEMPERATURE (K); ALSO LAMBST
0120 C THE STEADY STATE EVAPORATION CONSTANT (M**2/S)
0121 99 CONTINUE
0122     TSL = 200.
0123     TSH = TCR-1.
0124     IF (TSH.GT.TAI) TSH=TAI-1.
0125     DO 1000 I=1,100
0126     IF (I.EQ.1) GO TO 1010
0127     IF (I.EQ.2) GO TO 1020
0128     TS = (TSL + TSH) / 2.
0129     GO TO 1030
0130 1010 TS = TSL
0131     GO TO 1030
0132 1020 TS = TSH
0133 1030 CONTINUE
0134     TR = TS + (1./3.) * (TAI - TS)
0135     L = LBN * ((TCR-TS)/(TCR-TBN))**0.38
0136 C THIS EXPRESSION TO BE USED ONLY WHEN DATA FOR FOLLOWING EXPRESSION
0137 C NOT AVAILABLE
0138     PFS = 101.325*EXP(2.30259*(-16.188+32.124*TS/TBN-20.704*(TS/TBN)**2
0139     C +4.768*(TS/TBN)**3))
0140     TREDUC = TS/TCR
0141     A = 36/TREDUC - 35. - TREDUC**6 + 96.73*ALOG10(TREDUC)
0142     B = ALOG10(TREDUC) - 0.0364*A
0143     C = 7*ALOG10(TREDUC) - 0.118*A
0144     TERM1 = C - 1.192*B
0145     TERM2 = 4.93*B
0146     PREDUC = EXP(2.30259 * (TERM1 + ACENTR * TERM2))
0147     PFS = PREDUC * PCR
0148     PDIFF = P - PFS
0149     IF (PDIFF.LT.0.0) PDIFF = 0.0
0150     YFS = PFS*MWF / (PFS*MWF + PDIFF*MWA)
0151     YFR = YFS + (1./3.)*(YFI-YFS)
0152     YAR = 1. - YFR
0153     IF (TR.GT.600.) GO TO 1040
0154     CPA = 4.184 * (0.244388 - 4.20419E-5 * TR + 9.61128E-8 * TR**2
0155     & - 1.16383E-11 * TR**3)
0156     GO TO 1050
0157 1040 CPA = 4.184 * (0.208831 + 7.71027E-5 * TR - 8.56726E-9 * TR**2 -
0158     & 4.75772E-12 * TR**3)
0159 1050 CONTINUE
0160     CPV = (0.363 + 0.000467*TR) * (5. - 0.001*RHOF0)
0161     CPG = YAR * CPA + YFR * CPV
0162     LEFT = (P/PFS) - (MWF/MWA)*L/(CPG*(TAI-TS)) -1.
0163     IF (I.LT.3) GO TO 1060
0164     IF (ABS(LEFT).LT.0.005) GO TO 1083
0165     IF (LEFT.LT.0.0) GO TO 1080
0166     TSL = TS
0167     GO TO 1000
0168 1080 TSH = TS
0169 1060 IF (I.EQ.1.AND.LEFT.LT.0.0) GO TO 1099
0170     IF (I.EQ.2.AND.LEFT.GT.0.0) GO TO 1099
0171 1000 CONTINUE
0172 1083 WRITE(6,1081)
0173 1081 FORMAT(" TS, TSL, TSH, LEFT, P, PFS, L, CPG ")
0174     WRITE(6,*) TS,TSL,TSH,LEFT,P,PFS,L,CPG
0175 1070 TSST = TS
0176     WRITE(1,1075) TSST,LEFT
0177 1075 FORMAT(F10.2,F15.3)
0178     IF (TR.GT.850.) GO TO 1100

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0179      KA = 1.E-4 * (1.13841E-3 + 1.01789E-3*TR - 5.82577E-7*TR**2 +
0180      & 2.46855E-10*TR**3)
0181      GO TO 1110
0182 1100 KA = 1.E-4 * (-.0999992 + 1.19034E-3*TR - 5.29096E-7*TR**2 +
0183      & 1.11208E-10*TR**3)
0184 1110 CONTINUE
0185      E = 2. - 0.0372*(TR/TBN)**2
0186      KV = 1.E-6 * (13.2 - 0.0313 *(TBN-273.)) * (TR/273.))**E
0187      KG = YAR * KA + YFR * KV
0188      WRITE(1,1111)
0189 1111 FORMAT(" KG,KA,KV,YAR,YFR,E,TR ")
0190      WRITE(1,*) KG,KA,KV,YAR,YFR,E,TR
0191      BM = (YFS - YFI) / (1 - YFS)
0192      BT = CPG * (TAI - TSST) / L
0193      RHOFT = RHOF0 * (1 - 1.8*CEX*(TS-288.6) - (0.090*(TS-288.6))**2
0194      & / (TCR - 288.6)**2))
0195      LAMBST = 8 * ALOG(1+BM) / (RHOFT * (CPG/KG))
0196 C DENSITY OF AIR (KG/M**3)
0197      ZAIR = 1.0
0198 101 H = (0.003103/TR) * P / ZAIR
0199      ZAIRN = (1./(1.-H)) - (7349./TR**1.5) * (H/(1.+H))
0200      IF (ABS((ZAIRN-ZAIR)/ZAIRN).LT.0.0005) GOTO 102
0201      ZAIR = ZAIRN
0202      GOTO 101
0203 102 CONTINUE
0204      RHOA = MWA / ZAIR * (P/(8.314*TR))
0205 C DENSITY OF FUEL VAPOR (KG/M**3)
0206      CALL VPRDN (TCR,PCR,MWF,TR,P,RHOV)
0207 C VISCOSITY OF AIR (KG/M*S) SUTHERLAND CORRELATION
0208      MUA = 1.425E-6 * SQRT(TR) / (1 + (100/TR))
0209 C VISCOSITY OF THE FUEL VAPOR AND MIXTURE WITH AIR (KG/M*S)
0210      CALL VPRVS(TR,TCR,ZCR,MUA,MUV,MUG,MWA,MWF,YAR,YFR)
0211      RHOG = 1. / (YAR/RHOA + YFR/RHOV)
0212      WRITE(1,1112)
0213 1112 FORMAT(" LAMBST,BM,BT,RHOFT,CPG,KG ")
0214      WRITE(1,*) LAMBST,BM,BT,RHOFT,CPG,KG
0215 C
0216 C
0217 C
0218 C COMPUTE DROP HEAT-UP PARAMETERS
0219 C COMPUTE QUANTITIES WHICH DEPEND ON DROP SIZE
0220 C
0221 98 CONTINUE
0222 C
0223      DO 155 I=1,NDROP
0224      IF (TIME(I).LT.DELTAT) TSD(I) = FTEMP0
0225 100 IF ((TSD(I)-FTEMP0).GE.(0.95*(TSST-FTEMP0))) GOTO 3060
0226      TR = TSD(I) + (1./3.) * (TAI - TSD(I))
0227 C DENSITY OF AIR (KG/M**3)
0228      ZAIR = 1.0
0229 103 H = (0.003103/TR) * P / ZAIR
0230      ZAIRN = (1./(1.-H)) - (7349./TR**1.5) * (H/(1.+H))
0231      IF (ABS((ZAIRN-ZAIR)/ZAIRN).LT.0.0005) GOTO 105
0232      ZAIR = ZAIRN
0233      GOTO 103
0234 105 CONTINUE
0235      RHOA = MWA / ZAIR * (P/(8.314*TR))
0236 C DENSITY OF FUEL VAPOR (KG/M**3)
0237      CALL VPRDN (TCR,PCR,MWF,TR,P,RHOV)
0238 C VISCOSITY OF AIR (KG/M*S) SUTHERLAND CORRELATION

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0239      MUA = 1.425E-6 * SQRT( TR ) / ( 1 + ( 100 / TR ) )
0240 C   VISCOSITY OF THE FUEL VAPOR AND MIXTURE WITH AIR (KG/M* S)
0241      CALL VPRVS( TR, TCR, ZCR, MUA, MUV, MUG, MWA, MWF, YAR, YFR )
0242      TREDUC = TSD( I ) / TCR
0243      A = 36 / TREDUC - 35. - TREDUC**6 + 96.73 * ALOG10( TREDUC )
0244      B = ALOG10( TREDUC ) - 0.0364 * A
0245      C = 7 * ALOG10( TREDUC ) - 0.118 * A
0246      TERM1 = C - 1.192 * B
0247      TERM2 = 4.93 * B
0248      PREDUC = EXP( 2.30259 * ( TERM1 + ACENTR * TERM2 ) )
0249      PFS = PREDUC * PCR
0250      PDIFF = P - PFS
0251      IF ( PDIFF .LT. 0.0 ) PDIFF = 0.0
0252      YFS = PFS * MWF / ( PFS * MWF + PDIFF * MWA )
0253      YFR = YFS + ( 1. / 3. ) * ( YFI - YFS )
0254      YAR = 1. - YFR
0255      IF ( TR .GT. 600. ) GO TO 3040
0256      CPA = 4.184 * ( 0.244368 - 4.20419E-5 * TR + 9.61128E-8 * TR**2
0257      & - 1.16383E-11 * TR**3 )
0258      GO TO 3050
0259 3040 CPA = 4.184 * ( 0.208831 + 7.71027E-5 * TR - 8.56726E-9 * TR**2 -
0260      & 4.75772E-12 * TR**3 )
0261 3050 CONTINUE
0262      CPV = ( 0.363 + 0.000467 * TR ) * ( 5. - 0.001 * RHOF0 )
0263      CPG = YAR * CPA + YFR * CPV
0264      IF ( TR .GT. 850. ) GO TO 3100
0265      KA = 1.E-4 * ( 1.13841E-3 + 1.01789E-3 * TR - 5.82577E-7 * TR**2 +
0266      & 2.46855E-10 * TR**3 )
0267      GO TO 3110
0268 3100 KA = 1.E-4 * ( -.0999992 + 1.19034E-3 * TR - 5.29096E-7 * TR**2 +
0269      & 1.11208E-10 * TR**3 )
0270 3110 CONTINUE
0271      E = 2. - 0.0372 * ( TR / TBN )**2
0272      KV = 1.E-6 * ( 13.2 - 0.0313 * ( TBN - 273. ) ) * ( TR / 273. )**E
0273      KG = YAR * KA + YFR * KV
0274      L = LBN * ( ( TCR - TSD( I ) ) / ( TCR - TBN ) )**0.38
0275      BT = CPG * ( TAI - TSST ) / L
0276      BM = ( YFS - YFI ) / ( 1 - YFS )
0277      RHOG = 1. / ( YAR / RHOA + YFR / RHOF )
0278      RHOF0 = RHOF * ( 1 - 1.8 * CEX * ( TSD( I ) - 288.6 ) - ( 0.090 * ( TSD( I ) - 288.6 )**2
0279      & / ( TCR - 288.6 )**2 ) )
0280      LAMBHU( I ) = 8 * ALOG( 1 + BM ) / ( RHOF * ( CPG / KG ) )
0281 C   PRANDTL NO.
0282      3060 PRNDT = CPG * MUG / KG
0283 C   REYNOLDS NO.
0284      RE( I ) = D( I ) * RHOG * SQRT( ( UP( I ) - UA )**2 + ( VP( I ) - VA )**2 +
0285      & ( WP( I ) - WA )**2 ) / MUG
0286 C   MODIFY REYNOLDS NO. USED TO CALCULATE MASS LOSS TO INCLUDE A
0287 C   TERM FOR TURBULENCE INTENSITY EQUAL TO 20 PERCENT OF X-AXIS VEL
0288      REM( I ) = D( I ) * RHOG * ( SQRT( ( UP( I ) - UA )**2 + ( VP( I ) - VA )**2 +
0289      & ( WP( I ) - WA )**2 ) + 0.2 * UA ) / MUG
0290      IF ( ( TSD( I ) - FTEMP0 ) .GE. ( 0.95 * ( TSST - FTEMP0 ) ) ) GO TO 3070
0291      LAMBA( I ) = LAMBHU( I ) * ( 1 + 0.276 * REM( I )**0.5 * PRNDT**0.33 )
0292      GO TO 3080
0293 3070 CONTINUE
0294      LAMBA( I ) = LAMBST * ( 1 + 0.276 * REM( I )**0.5 * PRNDT**0.33 )
0295 3080 CONTINUE
0296      MASSD = ( 3.141596 / 6 ) * RHOF * D( I )**3
0297      MDOT = ( 3.141596 / 4. ) * RHOF * LAMBA( I ) * D( I )
0298      T = TSD( I ) / TBN

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0299      CPF = 3.52390-6.15627*T+6.99895*T**2-2.47850*T**3+NOCARB*(-0.016019
0300      & -0.003128*T+0.172186*T**2-0.058406*T**3)
0301      TSD(I)=TSD(I)+(MDOT * L /(CPF * MASSD) * ((BT/BM) - 1.) * DELTAT)
0302      IF ((TSD(I)-FTEMP0).GE.(0.95*(TSST-FTEMP0))) TSD(I)=TSST
0303      D(I) = D(I) - (LAMBA(I)/(2.*D(I))) * DELTAT
0304      IF (D(I).LE.0.9E-6) D(I)=0.899E-6
0305      C DRAG COEFFICIENT, CD
0306      IF (RE(I).GT.80.) GO TO 110
0307      CD(I) = 27. * RE(I)**(-0.84)
0308      GO TO 130
0309      110 IF (RE(I).GT.10000) GO TO 120
0310      CD(I) = 0.271 * RE(I)**0.217
0311      GO TO 130
0312      120 CD(I) = 2.
0313      130 CONTINUE
0314      C DRAG FACTOR, F
0315      F(I) = 18. * MUG*CD(I) * RE(I) /(RHOFT * D(I)**2 * 24.)
0316      C NEW DROPLET VELOCITY AND POSITION
0317      UP(I) = -F(I) * (UP(I) - UA) * DELTAT + UP(I)
0318      VP(I) = -F(I) * VP(I) * DELTAT + VP(I)
0319      WP(I) = 0.
0320      XP(I) = UP(I) * DELTAT + XP(I)
0321      YP(I) = VP(I) * DELTAT + YP(I)
0322      ZP(I) = 0.
0323      150 CONTINUE
0324      IF (D(I).LE.0.9E-6) GO TO 152
0325      TIME(I) = TIME(I) + DELTAT
0326      GO TO 153
0327      152 D(I) = 0.9E-6
0328      KK = I
0329      GO TO 155
0330      153 CONTINUE
0331      IF (XP(I).LT.XPS) GO TO 100
0332      155 CONTINUE
0333      C
0334      C
0335      C
0336      DO 211 I = 1,NDROP
0337      211 DMU(I) = D(I) * 1.0E6
0338      GOTO 312
0339      DO 312 I=1,NDROP
0340      WRITE (6,310) I,TIME(I),DMU(I),XP(I),FF0(I)
0341      310 FORMAT (1X,I3,F10.5,F8.2,F8.2,F9.6)
0342      312 CONTINUE
0343      C COMPUTE ROSIN-RAMMLER PARAMETERS OF NEW DISTRIBUTION
0344      D(KK) = 0.9E-6
0345      D(0) = D(1)
0346      DIAM0(0) = DIAM0(1)
0347      UP(0) = UP(1)
0348      D(NDROP+1) = D(NDROP)
0349      DIAM0(NDROP+1) = DIAM0(NDROP)
0350      UP(NDROP+1) = UP(NDROP)
0351      SUMFF = 0.0
0352      DO 160 I=KK,NDROP
0353      160 SUMFF = SUMFF + FF0(I) * ((D(I) / DIAM0(I))**3 / UP(I) + (D(I+1)
0354      & /DIAM0(I+1))**3 / UP(I+1)) / 2
0355      DO 170 I=KK,NDROP
0356      170 FF(I) = FF0(I) * ((D(I)/DIAM0(I))**3 / UP(I) + (D(I+1)/DIAM0(I+
0357      & 1))**3 / UP(I+1)) / 2 /SUMFF
0358      DO 175 I=KK,NDROP

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0359 175 R(I) = 0.0
0360 DO 180 I=KK,NDROP
0361 DO 180 J=I,NDROP
0362 180 R(I) = R(I) + FF(J)
0363 K = NDROP
0364 DO 181 I=NDROP, KK+2, -1
0365 181 IF (R(I).LT.0.001) K = I-1
0366 KL = KK + 1
0367 DO 190 I=KL,K
0368 ZDATA(I) = ALOG(1/R(I))
0369 YDATA(I) = ALOG(ZDATA(I))
0370 190 XDATA(I) = ALOG(D(I))
0371 SUMX = 0.
0372 SUMY = 0.
0373 SUMX2 = 0.
0374 SUMY2 = 0.
0375 SUMXY = 0.
0376 DO 200 I=KL,K
0377 SUMX = SUMX + XDATA(I)
0378 SUMY = SUMY + YDATA(I)
0379 SUMXY = SUMXY + (XDATA(I) * YDATA(I))
0380 SUMX2 = SUMX2 + XDATA(I)**2
0381 200 SUMY2 = SUMY2 + YDATA(I)**2
0382 KD = K - KL + 1
0383 M = (SUMXY - (SUMX*SUMY/KD)) / (SUMX2 - (SUMX**2/KD))
0384 B = (SUMY - M * SUMX)/KD
0385 SIGMAX = SQRT((SUMX2 - (SUMX**2)/KD) / (KD-1))
0386 SIGMA = SQRT((SUMY2 - (SUMY**2)/KD) / (KD-1))
0387 CC = M * SIGMAX / SIGMA
0388 NNEW = M
0389 XBARNW = EXP(-B/NNEW)
0390 XBRNUM = XBARNW * 1.0E6
0391 IF (NNEW.LT.1.0) GOTO 202
0392 Y=2.-1./NNEW
0393 G = Y**Y*EXP(-Y)*SQRT(2.*3.1415/Y)*(1.+1./((12.*Y)+1./((288.*Y**2)
0394 & -139./((51840.*Y**3))-571./((2488320.*Y**4)))
0395 SMD = XBRNUM * (1.-1./NNEW) / G
0396 GOTO 204
0397 202 WRITE(1,203)
0398 203 FORMAT (" VALUE OF N LESS THAN 1.0 ")
0399 204 CONTINUE
0400 C OUTPUT STATEMENTS
0401 WRITE (6,205)
0402 205 FORMAT (//, ' R-R XBAR (UM) ', ' R-R N ', ' CORR.COEF.',
0403 & ' SMD ')
0404 WRITE (6,210) XBRNUM,NNEW,CC,SMD
0405 210 FORMAT (F15.1,F15.2,F15.3,F15.2)
0406 WRITE (6,215)
0407 215 FORMAT (1X,/,7H DIAM ,8H TIME ,7H X DROP,7H Y DROP,7H Z DROP,
0408 C 8H U-VEL,8H V-VEL,8H W-VEL,6H FTEMP,6H RE)
0409 WRITE (6,220) (DMU(I),TIME(I),XP(I),YP(I),ZP(I),UP(I),VP(I),WP(I),
0410 C TSD(I),RE(I), I=1,NDROP)
0411 220 FORMAT (F7.1,F8.5,3F7.4,3F8.3,F6.1,F7.1)
0412 223 CONTINUE
0413 GOTO 2402
0414 WRITE (1,2400)
0415 2400 FORMAT(" LAMBHU(I), LAMBA(I), TSD(I) ")
0416 WRITE (1,2401) (LAMBHU(I),LAMBA(I),TSD(I), I=1,NDROP)
0417 2401 FORMAT (2E15.5,F15.3)
0418 2402 CONTINUE

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0419      IF (XPS.LE.XPTT) GO TO 230
0420      GO TO 240
0421 230   XPS = XPS + XPT
0422      GO TO 98
0423 1099  WRITE(1,1099)
0424 1098  FORMAT(" PROBLEM IN EVALUATING TSST AT ORIG LIMIT VALUES ")
0425      WRITE(1,*)LEFT,P,PFS,MWF,MWA,L,CPG,TAI,TS
0426 240   CONTINUE
0427      STOP
0428      END
0429      SUBROUTINE VPRDN (TCR,PCR,MWF,TR,P,RHOV)
0430      REAL MWF
0431      R = 8.314
0432      A = 0.4278 * R**2 * TCR**2.5 / PCR
0433      C = 0.0867 * R * TCR / PCR
0434      BB = B / (R*TR)
0435      AB = A / (B*R*TR**1.5)
0436      Z = 1.0
0437 2210   H = BB * P / Z
0438      ZN = (1./(1.-H)) - AB*(H/(1.+H))
0439      IF (((ZN-Z)/ZN).LT..0005) GO TO 2200
0440      Z = ZN
0441      GOTO 2210
0442 2200   Z = ZN
0443      RHOV = (MWF/Z) * (P/(R*TR))
0444      RETURN
0445      END
0446      SUBROUTINE VPRYS (TR,TCR,ZCR,MUA,MUV,MUG,MWA,MWF,YAR,YFR)
0447      DIMENSION A(7)
0448      REAL MUA,MUV,MUG,MWA,MWF,OMEG,OMGINV
0449      EK = 65.3*TCR*ZCR**3.6
0450      SIG = 0.01866*(MWF/(RHOV/1000.))**0.333 / ZCR**1.2
0451      A(1)=9.1426362E-1
0452      A(2)=-1.0689360
0453      A(3)=6.8077797E-1
0454      A(4)=-2.1208677E-1
0455      A(5)=3.4487186E-2
0456      A(6)=-2.8188225E-3
0457      A(7)=9.1590342E-5
0458      OMGINV = 0.
0459      DO 2300 I=1,7
0460 2300   OMGINV = OMGINV + A(I)* (ALOG10(TR/EK))**I
0461      OMEG = 1./OMGINV
0462  C VISCOSITY OF FUEL VAPOR (PA*SEC OR KG/(M*SEC))
0463      MUV = 2.669E-8 *(MWF*TR)**0.5 / (SIG**2 * OMEG)
0464  C CALCULATE VISCOSITY OF MIXTURE
0465      PHI12=(1.+(MUA/MUV)**0.5*(MUV/MWA)**0.25)**2/(8.*(1.+MWA/MUV))**
0466      & 0.5
0467      PHI21=(1.+(MUV/MUA)**0.5*(MWA/MUV)**0.25)**2/(8.*(1.+MUV/MWA))**
0468      & 0.5
0469      MUG=MUA/(1.+PHI12*(YFR/MWF/(YAR/MWA))) + MUV/(1.+PHI21*(YAR/MWA/
0470      & (YFR/MWF)))
0471      RETURN
0472      END

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