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AN INVESTIGATION OF THE COMBUSTION CHARACTERISTICS OF FUEL
DROPLET ARRAYS

Final Technical Report

By
J. J. Sangiovanni

June 1980

Work Performed Under Contract No. AC22-78ET13334

United Technologies Research Center
East Hartford, Connecticut

U. S. DEPARTMENT OF ENERGY

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ABSTRACT

The combustion characteristics of fuel droplet sprays were investigated in support of national efforts to develop efficient combustion systems for alternative liquid fuels. Through a combination of experimental and theoretical research, an improved understanding of the dominant physical and chemical processes associated with the combustion of liquid fuels in spray flames was sought. Specifically, the program was directed at establishing the nature and extent of droplet/droplet interaction and the multicomponent nature of real fuels on the ignition and combustion characteristics of spray flames. Since experimental investigations of full-scale combustors and furnaces are expensive and complex, a unique free-droplet combustion experiment provided the present investigation with a well-controlled simulation of spray combustion. As a complement to the experimental observations, various theoretical models were used to identify the dominant processes responsible for the effects of droplet/droplet interaction and the multicomponent nature of liquid fuels. One of these theoretical models was developed specifically for the present program to describe the nonsteady ignition and combustion of a multicomponent fuel droplet. The effect of droplet/droplet interaction on ignition and combustion of continuous monodispersed droplet streams was evaluated experimentally for droplet spacings ranging from a few droplet diameters to about forty diameters. The influence of fuel properties was assessed for the pure hydrocarbons, isooctane and hexadecane, binary mixtures of isooctane and hexadecane in various proportions, and No. 2 fuel oil.

Experimental observations indicate that ignition delay times increase sharply by about three-fold when droplet spacings are reduced to less than five droplet diameters. Results of theoretical predictions indicate that as droplet spacing is made smaller, the effect of droplet/droplet interaction on ignition delay becomes increasingly more pronounced for small droplets, low gas phase temperatures, and fuels of low volatility. Although this result suggests that ignition of heavy grades of alternative liquid fuels will be inhibited in dense sprays, other theoretical and experimental results indicate that the addition of a small quantity of a volatile component to a heavy fuel shortens ignition times substantially. Observed burning times show a gradual, but substantial, increase as a result of droplet/droplet interaction; as droplet spacing is decreased from 40 to 5 diameters, burning times increase by about 60%. A compilation of data for an extensive range of experimental parameters show universally that the amount by which droplet/droplet interaction increases burning times depends only on droplet spacing and not on the fuel type or the ambient conditions. Burning times of multicomponent fuel droplets are found to be weighted heavily toward the burning time for the least volatile component. Theoretical predictions demonstrate that this independence of burning times on the initial fuel mixture proportions can be ascribed to liquid phase mass diffusion limitations.

FOREWORD

The work reported herein was performed by the United Technologies Research Center for the U. S. Department of Energy under Contract No. DE-AC22-78ET13334 (formerly ET-78-C-03-2054) which was initiated September 25, 1978.

The Principal Investigator wishes to acknowledge the skillful and cooperative assistance of Mr. Raymond J. Michaud who designed, developed, and operated the droplet combustion experiment. The assistance provided by Mrs. Cynthia G. Egolf and Ms. Barbara M. Shayer with the development of the computer program for evaluating the theoretical model which describes the ignition and combustion of multi-component fuel droplets is gratefully acknowledged.

This work was performed under program management of the Pittsburgh Energy Technology Center of the U. S. Department of Energy, Pittsburgh, PA, and the Technical Manager was Mr. James D. Hickerson, Combustion Project Management Division. The Technical Monitor for the program was Dr. Jack Fisher, Chemical Engineering Division, Argonne National Laboratory, Argonne, IL.

SUMMARY

In support of national efforts to reduce dependence of the United States on petroleum imports by utilizing alternative liquid fuels for power generation and transportation applications, the United Technologies Research Center under Contract No. DE-AC22-78ET13334 (formerly (ET-78-C-03-2054) with the U. S. Department of Energy has conducted an investigation of the combustion characteristics of fuel droplet sprays. Through a combination of experimental and theoretical research, an improved understanding of the dominant physical and chemical processes associated with the combustion of liquid fuels in spray flames has been sought. Specifically, the program was directed at establishing the nature and extent of the effects of droplet/droplet interaction and the multicomponent nature of real fuels on the ignition and combustion characteristics of spray combustion flames.

INTRODUCTION

Increased emphasis on the use of alternative synthetic fuels derived from coal and oil shale to reduce dependence of the United States on petroleum imports from other nations* has brought about the need for improved technology for the effective combustion of such broad-specification fuels. Liquid fuels produced from coal, oil shale, and heavy petroleum crude are expected to be significantly different from traditional, highly-refined, petroleum-based liquid fuels. These alternative liquid fuels, especially those produced from coal, are likely to have a higher aromatic content and thus have less hydrogen content, have a higher organically-bound nitrogen content, and contain trace-metal contaminants. Although these undesirable fuel characteristics can be remedied to some extent by extensive refining, this approach is neither technically or economically feasible at the present time. Hence, with currently available combustion technology, the use of alternative liquid fuels can be expected to result in increased soot formation, increased deposit and particulate formation, and increased emissions of nitrogen oxides (NO_x). These combustion characteristics would in turn result in increased equipment plugging, fouling, and corrosion and increased health hazards. Furthermore, the alternative liquid fuels are composed of a multitude of hydrocarbon components with widely varying volatilities and states of mixedness which pose additional problems of vaporization, ignition delay, unsteady combustion, droplet swelling, disruptive liquid phase boiling, and liquid phase pyrolysis.

In support of national efforts to utilize alternative liquid fuels for power generation and transportation applications, the program reported herein addresses the need for an improved understanding of the dominant physical and chemical processes associated with the combustion of droplet sprays. Through a combination of experimental and theoretical research, this program seeks to provide sufficient fundamental understanding of spray combustion for the optimal design of liquid-fueled combustion systems. Specifically, the program was directed at establishing the nature and extent of the effects of droplet/droplet interaction and the multicomponent nature of real liquid fuels on the ignition and combustion characteristics of spray combustion flames.

Since fuel sprays are composed of numerous individual droplets which range in size from about 2 to 200 μm , literally hundreds of theoretical and experimental investigations of the combustion characteristics of single, isolated droplets have been performed over the past twenty-five years. In practical liquid-fueled combustors, however, the fuel sprays consist of a system of fuel droplets which are usually composed of many liquid components. And, as for most complicated systems, the behavior of a fuel spray cannot be understood completely by the behavior of its isolated parts without also accounting for how those parts inter-

*Presidential Import Reduction Program (July 16, 1979)

act. Inasmuch as dense sprays prevail in practical combustors where droplet spacings range from less than a droplet diameter near the injector to about thirty diameters further downstream, droplet/droplet interactions modify substantially the gas phase transport of heat and mass from corresponding conditions for a single, isolated fuel droplet. The multicomponent nature of real fuels complicates the spray combustion system further with finite rate transport of fuel components in the liquid phase and preferential vaporization of certain components.

DROPLET COMBUSTION EXPERIMENT

The experimental system used previously at UTRC for investigations of the ignition and combustion characteristics of continuous monodispersed fuel droplet streams (Refs. 1-3) was modified to facilitate the investigation of multicomponent, real fuels which are generally nonpolar. The various models of the UTRC free-droplet combustion experiment provide a well-controlled simulation of spray combustion consisting of monodispersed fuel droplet streams which are injected into a hot combustion gas stream. Precise time and spatial control of the monodispersed droplet streams has permitted the use of high-speed photographic and spectroscopic techniques for measurements of ignition delay times, combustion rates, flame structure development and flame temperature.

A schematic diagram of the UTRC free-droplet combustion experiment developed for the present investigation is shown in Fig. 1. While the basic features of this model of the experiment are essentially the same as earlier models, the latest experiment includes the capability of changing the spacing between droplets of nonpolar fuels; the ability to change droplet spacing is necessary because of the importance of droplet/droplet interactions on ignition and combustion in droplet sprays. In general, each of the various models of the droplet combustion experiment provide a continuous stream of fuel droplets of a known size, spacing, and speed which are injected on a precise trajectory in a uniform, stable and long-path combustion ambient.

The hot gas environment for droplet combustion is provided by the post-combustion zone of lean, premixed, laminar, gaseous, fuel-air flames stabilized on a flat-flame burner. A quartz duct attached to the burner prevents mixing of the hot combustion gases with the surrounding air and serves to maintain laminar flow in the post-combustion gas stream. Methane, hydrogen, air, and nitrogen, metered through critical flow orifices, are mixed external to the burner. The premixed gases are introduced into the base of the burner whereupon they flow through a series of stainless steel screens and a packed bed of glass beads to provide a uniform velocity profile. The burner flame is stabilized on a 10 cm square hastelloy honeycomb structure comprised of 1.5 mm wide hexagonal cells. A somewhat larger hole of 3 mm diameter is provided in the center of the burner for injection of the droplets into the combustion region.

In the latest model of the experiment, a stream of polar droplets (e.g. alcohol) travel horizontally and the nonpolar fuel droplets travel vertically upward such that the paths of the two streams cross as shown in the photograph in Fig. 2a. A matched pair of vibrated capillary jets provide the two separate monodispersed streams of polar and nonpolar droplets at the same frequency and with essentially the same droplet velocity and droplet size. The selected nonpolar fuel droplets travel ultimately into the combustion region where they become entrained by the hot gases, vaporize, and burn as they are carried upward.

To generate the droplet streams, jets of the two liquids are forced from capillary orifices at constant pressure while the capillaries are vibrated mechanically along their major axes by electromagnetic transducers. The periodic mechanical disturbance of the liquid jets, which when superimposed at a precise frequency on the surface tension (Rayleigh) instability of the liquid jets, causes the jets to break up into streams of uniformly sized and spaced droplets with one droplet being produced from each jet for each vibration cycle.

The trajectory of the horizontally oriented stream of polar liquid droplets is controlled by an electrostatic charging and deflection mechanism which causes selected polar liquid droplets to collide with corresponding nonpolar fuel droplets. In this manner, the spacing in a monodispersed stream of nonpolar fuel droplets is controlled simply by bumping out unwanted droplets. This is accomplished in part by ensuring that the polar droplets are charged by a low voltage potential applied to the polar liquid orifice of approximately 100 VDC if they are not charged adequately by fluid friction within the capillary orifice. As the charged polar droplets pass through an electrostatic field produced between two pairs of deflection plates their trajectory can be controlled precisely by regulating the voltages applied across each pair of plates (0 to ± 1500 VDC) to effect collisions with each of the nonpolar droplets as shown in the photograph in Fig. 2b. To permit every n th ($1 \leq n \leq 100$) selected nonpolar fuel droplet to pass into the combustion region for investigation, a low voltage positive pulse of approximately 200 VDC is applied to a charge repulsion ring located immediately downstream of the polar liquid capillary jet during the time when corresponding polar droplets are being formed. The resultant trajectory of these selected polar droplets is sufficiently different from the other polar droplets that they do not collide with the corresponding nonpolar fuel droplets. Hence, selected nonpolar fuel droplets are permitted to pass undisturbed into the combustion region. The photographs in Figs. 2c and 2d show two typical operating modes with one droplet and two droplets being selected from every five nonpolar fuel droplets, respectively. Several of the selected polar droplets which did not collide with the corresponding nonpolar fuel droplets can be seen in the lower right corner of these photographs.

Flame flashback into the droplet generator chamber is avoided by purging the chamber with nitrogen (gas) while evacuating any liquid or vapor which collects in the chamber. To prevent premature ignition of the droplet streams, the rejected droplets are extracted by a suction tube which is located immediately adjacent to the point of collision of the two droplet streams.

Temperature measurements in the droplet combustion region are obtained using a silica coated 0.08 mm diameter, Pt-Pt/10 percent Rh thermocouple. By comparing temperatures measured using the thermocouple probe with comparable measurements using a modified sodium line reversal technique, thermocouple radiation and conduction corrections are determined. The ambient gas stream velocities are computed from the measured combustion region temperatures and the measured total flowrate of gases supplied to the flat flame burner with the ambient pressure taken as one atmosphere.

Using high-speed photographic techniques, the history of the droplets is recorded from the time the droplets enter the combustion region. Illumination of the droplets for stroboscopic observation of droplet streams and single flash photographs is provided by a General Radio type 1538-A stroboscope equipped with a type 1538-P4 auxiliary flash capacitor. A ground glass diffuser is placed in front of the stroboscope to provide uniform back-lighting for single flash photographs of the droplets. Both single flash, stop-action slide photographs of drops and time exposure slide photographs of droplet flame development are provided by a single lens reflex Nikon F2 Photomic 35 mm camera equipped with a 200 mm telephoto lens, various plus-lenses, and a bellows focusing attachment. The droplet combustion experiment is equipped with a vertical traversing mechanism to permit a series of photographs of the droplet stream and flame front history throughout the combustion region. A typical set of photographic slides made to determine droplet ignition delay times are shown in Fig. 3. The frequency of droplets entering the combustion region is provided independently by the droplet generator system and a magnification factor is provided by a calibration photographic slide. Droplet spacing and velocity as functions of position and time in the combustion region are determined for a given droplet frequency from photographic slides such as the one shown in Fig. 3a. A typical droplet history within the combustion region is shown in Fig. 4. Figure 4 also shows that the velocity of the droplets is influenced by gravity and aerodynamic forces as they traverse the combustion region. The instantaneous droplet velocity is obtained from the product of the droplet frequency and the droplet spacing measured from the photographic slides. Integrating the droplet velocity history then provides the residence time for droplets in the combustion region as a function of position. The ignition delay time is then computed from the droplet history and the position along the droplet trajectory where visible light is first emitted by the combustion process as shown in a time-averaged photographic slide such as shown in Fig. 3b. The variation in droplet size with time, used to determine evaporation and burning rates, is provided by a series of magnified photographic slides at various vertical positions; these slides are similar to the one shown in Fig. 3b but the total magnification factor on a large screen is approximately 100 times. A typical droplet burning characteristic made from photographic slides is shown in Fig. 5 as the temporal variation of the normalized droplet surface area for several droplet spacings. The slight nonlinear behavior of the normalized droplet surface area during the initial period of droplet combustion has been shown by a theoretical model to be a result of nonsteady droplet heating (Ref. 4). Using experimental data similar to that shown in Fig. 5, the total burning time has been determined as a function of spray configuration or droplet spacing and combustor ambient temperature and oxygen content.

THEORETICAL MODELS

Several theoretical models, one of which was developed especially for the present investigation, have been used to provide insight into the fundamental physical and chemical processes associated with the ignition and combustion of fuel droplets and droplet arrays. Specifically, the theoretical models have been used to assess the effects of both droplet/droplet interaction and the multicomponent nature of real fuels on ignition and combustion of droplets and droplet arrays in addition to the usual combustor parameters such as ambient temperature and oxygen content. By using these theoretical models to complement the experimental observations, the nature and extent of the various fundamental processes have been evaluated and the dominant processes have been identified.

The first of these theoretical models, which has served as the basis for the other more comprehensive models, describes the nonsteady heating, vaporization, and subsequent self-ignition and combustion of a single-component fuel droplet which is moving relative to a hot combustion gas stream. A schematic diagram of this somewhat idealized combustion model for a single, isolated fuel droplet is shown in Fig. 6 and a detailed description and an evaluation of this model is available in Ref. 4. In this theoretical model, gas phase heat and mass transfer are regarded as quasi-steady processes and transient heat conduction is assumed to be the only transport mechanism within the droplet. Since movement of the droplet relative to the gas stream enhances the transfer of heat and mass by forced convection in the region immediately surrounding the droplet, gas phase transport processes are presumed in this model to take place within a gas film whose thickness is a function of the droplet relative velocity. An ignition criterion which was developed originally by Faeth and Olson (Ref. 5) is used in this model. Ignition is hypothesized by this criterion, and combustion is assumed to be self-sustaining, when the concentration of a crucial chain-branching, intermediate, chemical species reaches a critical level at some point in the gas phase. Although this theoretical model was formulated with the capability of representing finite gas phase reaction rates, the thin-flame approximation has been utilized exclusively for combustion modeling because suitable reaction kinetics data is not available.

An extension of the theoretical model for droplet ignition and combustion to the limiting droplet spacing represented by a continuous cylindrical filament of liquid has provided a means of evaluating the full potential of droplet/droplet interaction for inhibiting droplet ignition and combustion. Specifically, the potential influence of droplet/droplet interaction in monodispersed droplet streams has been illustrated by the ratio of ignition times and burning times for cylindrical filaments and isolated spherical droplets. The theoretical model for describing the ignition of a continuous cylindrical filament of liquid fuel is presented in Ref. 3.

To provide a means for evaluating the effects of the multicomponent nature of real fuels on ignition and combustion, a theoretical model which describes such behavior for single isolated droplets has been developed for the present investigation. A detailed description of this latest theoretical model for describing the nonsteady ignition and combustion of multicomponent fuel droplets is presented in Appendix I of this report.

RESULTS AND DISCUSSION

Since an earlier investigation of the effect of droplet/droplet interaction on ignition and combustion in droplet arrays had been restricted to alcohol fuels because of experimental limitations (Ref. 1), further study of this effect was warranted to assess this important effect for both pure and multicomponent hydrocarbon fuels. Using the droplet combustion experiment and measurement techniques described in the previous section, ignition delay times and burning times were measured for continuous monodispersed streams of $260\text{ }\mu\text{m}$ fuel droplets (initial nominal diameter). The influence of fuel properties was assessed for two pure fuels, isooctane and hexadecane, binary mixtures of isooctane and hexadecane in various proportions, and No. 2 fuel oil. The effect of droplet/droplet interaction was evaluated by varying droplet spacing from a few droplet diameters to approximately forty droplet diameters. The potential importance of combustor operating parameters was assessed for variations of ambient temperature ($1242\text{ K} \leq T_{\infty} \leq 1578\text{ K}$) and ambient oxygen mass fraction ($0.0766 \leq (\omega_o)_{\infty} \leq 0.1556$) at one atmosphere pressure.

Effects of Droplet Interaction

The results of experiments to determine the effect of droplet/droplet interaction on the ignition delay time of monodispersed streams of hexadecane droplets are shown in Fig. 7. Similar data, however, were not obtainable for pure isooctane because of the extremely short ignition delay times ($<1\text{ msec}$) for this relatively volatile fuel. Unfortunately, the technique for determining ignition by the appearance of visible emission is inaccurate when either the ignition delay time is very short or when the initial flame is rather nonluminous. Not unlike earlier observations for alcohols and in agreement with theoretical predictions for a wide range of typical fuel characteristics (Refs. 1 and 3), the data in Fig. 7 show that ignition delay times for hexadecane increase sharply by approximately three-fold as droplet spacing is reduced to less than five droplet diameters. The ignition delay time for a given droplet spacing is shown to increase significantly as the ambient temperature is decreased while the ambient oxygen content is held nearly constant. The slight decrease in ignition delay times shown in Fig. 7 at higher droplet spacings is associated with enhanced convective heating of the droplets as a result of an increase in the droplet/gas relative velocity as droplet spacing is decreased; droplet velocities increase monotonically with decreasing droplet spacing because the aerodynamic drag force is reduced when each droplet travels in the wake of a preceding droplet. For very small droplet spacings, however, when the effect of droplet/droplet interaction on ignition delay time is strongest, convective heating does not appear to be important.

Based on the results shown in Fig. 7, the conclusions of the earlier investigations (Refs. 1 and 3) as to the nature and extent of droplet/droplet interaction on ignition delay in droplet arrays can be extended to all fuel types. The theoretical models developed for the earlier investigation to describe ignition for the

limiting droplet spacings represented by an isolated droplet and a continuous cylindrical filament of liquid provide an understanding of the extent of potential droplet interaction effects on ignition delay time. Predictions from these models indicate that as droplet spacing is made smaller, the effect of droplet/droplet interaction on ignition becomes increasingly more pronounced for small droplets, low gas phase temperatures, and fuels of low volatility. The latter of these criteria suggests that ignition of droplet sprays of heavy grades of alternative liquid fuels could be inhibited substantially by droplet/droplet interaction. Results to be presented in the following section will show that the addition of a volatile component to a fuel composed mainly of heavy components will substantially shorten ignition delay times. The theoretical models also suggest that the phenomenon of increased ignition delay time as a result of droplet/droplet interaction can be ascribed to a reduction in the droplet heating rate; specifically as droplet number density is increased, more droplets must be heated by a reduced volume of hot gas in the neighborhood of the droplets.

A set of preignition rate constants have been determined for use in theoretical investigations of the ignition delay characteristics of isooctane, hexadecane, and mixtures of these two hydrocarbons. The rate constants shown in Table I for hexadecane were determined by selectively matching the observed ignition delay times shown in Fig. 7 for isolated droplet spacings to the theoretical model presented in Ref. 2. This procedure for extracting the preignition rate constants for the ignition criterion from Faeth and Olson (Ref. 5) consisted of first determining the activation energy, E , by matching predicted ignition delay times with the measured ignition times shown in Fig. 7 to obtain the correct trend with temperature. Appropriate values of K_1 and K_3 for hexadecane were then selected to obtain an acceptable correlation of the predicted and measured ignition delay times. Since the droplet ignition experiments were conducted at an ambient pressure of one atmosphere, the functional dependence of ignition delay time on pressure was not established for hexadecane, hence, the value of K_2 was taken arbitrarily as unity. Because droplet ignition delay times could not be measured for isooctane for the reasons cited above, the preignition rate constants shown in Table I for isooctane were taken from the work by Faeth and Olson (Ref. 5) which they in turn derived from the experimental work by Burwell and Olson for a steady flow reactor (Ref. 6).

The results of experiments which were conducted to establish the effect of droplet/droplet interaction on the combustion of continuous monodispersed streams of hydrocarbon droplets are summarized in Figs. 8-11. These data have been correlated as the variation in total burning time with relative droplet spacing as a function of ambient temperature, ambient oxygen weight fraction, and fuel type. As was observed for alcohol fuels in an earlier investigation (Ref. 1), these data show universally that droplet burning times increase substantially with decreasing droplet spacing. Burning times for small initial droplet spacings of the order of five droplet diameters are shown to be as much as 60% higher than comparable times for isolated fuel droplets. While the effect of droplet/droplet interaction on ignition delay is shown above to be important only for very small droplet spacings (of the order of a few droplet diameters), the influence of droplet/droplet interaction on combustion times is shown by these results to be important for considerably larger droplet spacings. This evidence of an increase in burning times due to droplet/droplet interaction at large droplet spacings of the order of

TABLE I

RATE CONSTANTS FOR IGNITION CRITERION
FROM FAETH AND OLSON (REF. 5)

	$K_1\text{-sec}^{-1}$	K_2	K_3	E-Kcal/g-mole
hexadecane	5.0×10^7	1.0*	1.0	17.9
isooctane ⁺	1.09×10^{15}	2.57	1.0	64.4

*The effect of pressure was not evaluated.

⁺From Faeth and Olson (Ref. 5)

20 to 40 droplet diameters is somewhat unexpected since flame positions for single droplet combustion are usually located at 6 to 12 droplet diameters (Refs. 7 and 8).

Although changes in the ambient oxygen concentration does not appear to alter the general effect of droplet/droplet interaction on droplet combustion, as shown in Figs. 8-11, increasing the ambient oxygen concentration has the expected effect of reducing the burning time for a given droplet spacing. However, at very small droplet spacings where the effect of droplet/droplet interaction is most intense, the effect of droplet/droplet interaction appears to become independent of both ambient temperature and oxygen mass fraction. This observed trend with ambient oxygen mass fraction lends support to the theory that the effect of droplet/droplet interaction on the combustion of droplet arrays is due primarily to local oxygen depletion in the neighborhood of individual droplets. The theoretical models by Chiu and Liu (Ref. 9), Labowsky and Rosner (Ref. 10) and Labowsky (Ref. 11) which describe the combustion of simple droplet arrays also show that the burning rate depends only on the droplet spacing; as droplet spacing is made smaller the burning rate becomes limited by the rate of oxygen diffusion from the ambient surrounding the droplet array. To further illustrate this observation, all of the available experimental data on the combustion of monodispersed droplet streams from the present investigation with hydrocarbon fuels (Fig. 8-11) and the earlier investigation with alcohol fuels (Ref. 1) have been replotted as the increase in burning time relative to the burning time for a single, isolated droplet. These data in Fig. 12 show an essentially universal dependence of the burning time for monodispersed droplet streams on the droplet spacing. In view of the extensive range of the experimental parameters which are represented by the data in Fig. 12, the increase in burning time as a result of droplet/droplet interaction can be said to depend only on the geometry of the droplet array. In other words, droplet spacing and the overall size of the droplet array govern the burning rate of a droplet array by controlling the rate of oxygen diffusion into the array.

Multicomponent Effects

By way of introduction to the subject of multicomponent effects in droplet ignition and combustion, results of the theoretical model described in Appendix I are presented in Figs. 13-16 for the case of a 260 μm droplet composed initially of equal parts by mass of isooctane and hexadecane. The predictions shown here correspond to a typical experimental case having the following conditions: 295°K initial droplet temperature, 1400°K ambient temperature, 0.1355 ambient oxygen mass fraction, and 30 cm/sec droplet relative velocity. Since circulation within fuel droplets is not expected to be particularly important in the experiments conducted for this investigation, heat and mass transport within the droplets is assumed to be entirely by molecular conduction and diffusion, respectively. Accordingly, the liquid phase heat and mass diffusion coefficients are taken in the computations as $0.8 \times 10^{-3} \text{ cm}^2/\text{sec}$ and $1 \times 10^{-4} \text{ cm}^2/\text{sec}$, respectively, hence, the Lewis number is representative of alkane mixtures. The preignition rate constants used for computation of the ignition criterion are given in Table I.

Figure 13 shows the development of mass fraction profiles for isooctane and hexadecane at selected times throughout ignition and combustion of the droplet. Immediately upon exposure of the droplet to the combustion ambient, large mass

fraction gradients develop rapidly in a thin layer near the surface of the droplet as the more volatile isooctane vaporized preferentially. Because mass diffusion within the droplet is rate limited and isooctane is very volatile, isooctane becomes depleted at the droplet surface in approximately 10% of the droplet lifetime whereupon the mass fraction profiles appear to take on a quasi-steady state characteristic until the droplet is consumed. Actually, as will be shown below, transient mass transfer processes persist in the liquid phase throughout the entire droplet lifetime. The simultaneous development of droplet temperature profiles is shown in Fig. 14. Since liquid phase heat conduction is a very efficient process compared to mass diffusion (Lewis number equals 80), temperature gradients within the droplet are shown to be quite modest throughout the entire droplet lifetime with the possible exception of the initial period. As the droplet heats up, after slightly more than half of the droplet lifetime has elapsed, the temperature profile does indeed take on a quasi-steady state characteristic at which time the droplet temperature is nearly uniform.

The above observations are further illustrated in Fig. 15 where the temporal variation of the surface and center values of mass fractions and temperature are shown for the binary fuel droplet. This detailed representation for the variation of mass fractions reveals that the surface mass fraction for the more volatile component (isooctane) changes appreciably throughout the entire droplet lifetime. As a result of liquid phase mass diffusion limitations, the droplet combustion process is shown here to consist of three regimes; a rapid initial transient period, a short, almost quasi-steady, intermediate period, and a long, final transient period. During the initial transient period, the isooctane mass fraction is depleted rapidly at the droplet surface due to its volatility, while in the core of the droplet the mass fraction is essentially unchanged from the initial value. Subsequently, a short, almost quasi-steady, intermediate period exists during which the mass fractions at the droplet surface as well as the droplet center remain essentially constant. For this condition to exist, it is necessary that the rate of transport of species to the droplet surface by diffusion be essentially equal to the rate of vaporization. As the droplet shrinks in size during the final transient period, liquid phase mass diffusion is no longer limiting the transport of isooctane, hence, the mass fraction of isooctane at the droplet surface increases. Since the droplet surface temperature during this final transient period is considerably higher than the normal boiling temperature for isooctane, this increase in the mass fraction of isooctane at the droplet surface, albeit small, is reflected as a substantial increase in the rate of vaporization for isooctane. It should be noted that these detailed predictions for the temporal variation of the isooctane mass fraction at the droplet surface required the extremely accurate numerical integration techniques which are described in Appendix I. To ensure the required accuracy for these detailed predictions, both the radial mesh size near the droplet surface and the dimensionless time interval were taken as 10^{-4} .

The resultant temporal variation of the fractional rates of vaporization for the two components of the binary droplet are shown in Fig. 16. Initially, when the

mass fractions of the two components are still equal at the droplet surface and the droplet temperature is low, the more volatile isooctane is vaporized at a considerably faster rate than is hexadecane. As the isooctane becomes depleted at the droplet surface and the droplet temperature begins to rise, the rates of vaporization of the two components rapidly approach equal values. Subsequently, the rates of vaporization of hexadecane and isooctane reach local maximum and minimum values, respectively, as the mass fractions at the droplet surface remain temporarily constant during the intermediate quasi-steady period. During the final transient period of the droplet lifetime, the rates of vaporization of the two components begin to approach equal values as the droplet shrinks in size and the mass fraction of isooctane at the droplet surface increases due to the enhanced rate of diffusion from within the droplet. In the limit of time, as the droplet becomes infinitesimally small and liquid phase mass diffusion is no longer rate limiting, the mass fractions of the two components should become equal to the initial values which have existed in the core of the droplet. The theoretical model is incapable of predicting this result, however, because such a prediction requires an infinitesimally small diffusion time.

The effect of the multicomponent nature of real fuels on droplet ignition delay times is illustrated in Fig. 17. Since droplet/droplet interaction can produce significant increases in ignition delay times at close droplet spacings, the experimental data shown in Fig. 17 were obtained for large droplet spacings of about 30 to 40 droplet diameters. To provide insight into the physical and chemical processes which dominate the ignition of multicomponent fuel droplets, Fig. 17 also includes a theoretical prediction of droplet ignition delay times as a function of fuel composition for a typical experimental condition. Both the theoretical and experimental results in Fig. 17 show a pronounced nonlinear decrease in ignition delay time with increased isooctane mass fraction. Apparently, isooctane is so much more volatile than hexadecane that the ignition process is enhanced greatly by even a small amount of isooctane in the mixture. The theoretical predictions presented above for a binary fuel droplet clearly illustrate that the rate of vaporization of isooctane is substantially higher than the rate for hexadecane during the ignition period. The predicted ignition criterion profiles shown in Fig. 18 for the instant when ignition occurs (i.e. $\sum \psi_i = 1.0$) serve as evidence that the ignition delay time of a multicomponent droplet is controlled by the most volatile component(s). Despite the fact that Table I shows that hexadecane is more reactive than isooctane during ignition, hexadecane simply does not vaporize at a rate anywhere near the rate for isooctane so it does not contribute much to the ignition process.

Although both the experimental data and the theoretical prediction shown in Fig. 17 illustrate the same trend with fuel droplet composition, poor quantitative agreement of ignition delay times is shown. In an attempt to explain this discrepancy, at least two reasons for the poor quantitative agreement were identified. First, as was mentioned in the previous section, the technique for measuring ignition delay times, by the first appearance of visible emission from the flame, is inaccurate when either the ignition delay time is very short or when the initial flame is rather nonluminous. Since both of these experimental difficulties exist for ignition delay measurements for isooctane, the actual ignition delay times

should be somewhat shorter than indicated and in better agreement with the theoretical predictions. Second, the rate constants used in the ignition criterion for isooctane (Table I) may not be applicable to the comparison shown in Fig. 17 because they were derived from flow reactor data taken for a temperature range which is much lower than ambient temperatures for the present investigation.

Figure 19 shows experimental data and a theoretical prediction which together serve to illustrate the effect of the multicomponent nature of real fuels on droplet burning times. These same experimental data are used in Fig. 10 to illustrate the effect of droplet/droplet interaction on droplet burning times for isooctane/hexadecane mixtures. Since the theoretical model is representative of an isolated droplet, only the experimental data for large spacings can be compared quantitatively with the theoretical prediction. The results presented in Fig. 19 clearly indicate a nonlinear, variation of droplet burning times with initial fuel mixture proportions; as the initial mass fraction of the more volatile component (isooctane) is increased, the burning times are relatively unaffected. More specifically, the burning times for binary fuel droplets are shown here to be weighted heavily toward the burning time for the least volatile component (hexadecane).

By referring to the theoretical predictions presented in Figs. 13-16 for the combustion of a binary fuel droplet, this observed trend for burning times with initial fuel mixture proportions can be interpreted physically. As discussed above, isooctane is rapidly depleted at the droplet surface during the initial period of combustion because liquid phase mass diffusion is a very slow process compared to isooctane vaporization. Even though isooctane is very volatile at the droplet surface temperature associated with combustion, the isooctane becomes "trapped" within the core of the droplet. Hence, the rate of vaporization of the binary droplet is limited essentially by the rate of vaporization for hexadecane.

Although much theoretical and experimental evidence has been reported to substantiate the theory that multicomponent fuel droplets can undergo fragmentation during combustion (Refs. 12 and 13), the phenomenon was not observed with the isooctane/hexadecane mixtures used in the experimental phase of the present investigation. These earlier investigations show clearly that fragmentation of a multicomponent droplet during vaporization can be induced by homogeneous nucleation of the mixture within the droplet. As a multicomponent droplet vaporizes, in the absence of appreciable internal circulation, the more volatile components are vaporized preferentially at the droplet surface while the mixture proportions in the interior of the droplet remain relatively unchanged. Subsequently, the surface temperature of the droplet will rise to accommodate the vaporization temperature of the mixture and, by thermal conduction, the temperature of the droplet interior also will begin to rise. If the temperature somewhere in the interior of the droplet reaches the superheat limit for the local mixture composition, homogeneous nucleation will occur at that location and the resultant vaporization will cause the droplet to fragment. The subjects of homogeneous nucleation and superheat limits for hydrocarbon liquids are discussed more thoroughly in Refs. 14-16.

To better understand why droplet fragmentation was not observed in the present investigation, Fig. 20 was constructed using the theoretical model for multicomponent droplet combustion to illustrate the tendency for homogeneous nucleation within a binary fuel droplet. The plot shows that as the initial proportion of isooctane to hexadecane is increased the minimum difference between the superheat limit temperature, T_L , and the droplet temperature, T_d , decreases. Hence, homogeneous nucleation of fuel droplets should not have been expected during the present experimental investigation since the initial proportions of isooctane were too low. Even for higher initial proportions of isooctane, unless the superheat limit correlation or the theoretical model are slightly in error, homogeneous nucleation should not be expected. It is interesting to note that, for a pressure of 10 atmospheres, the theoretical model predicts that homogeneous nucleation will occur for essentially all mixture proportions of isooctane and hexadecane. The tendency for homogeneous nucleation increases with higher ambient pressures because the droplet vaporization temperature increases substantially while the superheat limit temperature increases only slightly (see Appendix I).

CONCLUSIONS AND RECOMMENDATIONS

The important conclusions from the present theoretical and experimental investigations regarding the combustion characteristics of liquid fuels in spray flames are as follows:

- (1) Droplet ignition delay times for small droplet spacings of less than five droplet diameters can be three or more times longer than the ignition times for isolated droplets.
- (2) The effect of droplet/droplet interaction on ignition becomes increasingly more inhibiting for small droplets, low gas phase temperatures, and fuels of low volatility.
- (3) The addition of a small quantity of a volatile hydrocarbon component to a liquid fuel which has a high boiling point will shorten ignition delay times substantially.
- (4) Burning times of droplet arrays increase gradually, but substantially, by about 60% as droplet spacing is decreased from 40 to 5 droplet diameters.
- (5) The amount by which droplet/droplet interaction increases burning times of monodispersed droplet streams depends only on droplet spacing and not on the fuel type or ambient conditions.
- (6) In the absence of significant internal droplet circulation, the burning times of multicomponent fuel droplets are nearly independent of the initial fuel mixture proportions; the burning times for mixtures are weighted heavily toward the burning time for the least volatile component.

Although traditional liquid fuels have been tailored for their intended combustion applications, enhancement of the quality of synthetic liquid fuels by the usual method of hydrogenation should be avoided because production costs will increase substantially. In view of the above conclusions, however, some judicious modifications of synthetic liquid fuels can increase the combustion performance of such fuels at only a nominal cost. For example, ignition delay times and combustion times could be reduced by the addition of small quantities of volatile hydrocarbon components to the synthetic fuel which would vaporize readily and promote droplet fragmentation by homogeneous nucleation. Because droplet size and droplet spacing have been shown to have a pronounced effect on ignition and combustion times, research should be undertaken to develop techniques for achieving acceptable droplet spray injection and atomization characteristics with alternative liquid fuels. Finally, analytical models for describing the combustion of liquid fuels in spray flames should incorporate the present theoretical and experimental results on the effects of droplet/droplet interaction and the multicomponent nature of real fuels on ignition and combustion times.

A THEORETICAL MODEL FOR THE NONSTEADY IGNITION AND COMBUSTION OF A MULTICOMPONENT FUEL DROPLET

Introduction

An existing theoretical model (Ref. 4) for describing the nonsteady heating, vaporization, and subsequent self-ignition and combustion of a single, isolated fuel droplet which is moving relative to a hot, oxidizing ambient has been extended to permit examination of such characteristics for multicomponent fuel droplets. Figure 6 shows a schematic representation of the fuel droplet system during combustion including typical profiles for temperature, mass fraction of fuel components, and oxidizer mass fraction. The system is considered to be spherically-symmetric, isobaric, and at low pressure (typically less than one-tenth of the fuel critical pressure). Heat and mass transport within the droplet is assumed to be by molecular conduction and diffusion, respectively, such that temperature and mass fractions of fuel components are permitted to vary both spatially and temporally. Although the mathematical complexities imposed by this last consideration could be avoided by assuming that rapid circulation exists within the droplet of the strength postulated by El Wakil et al. (Ref. 17) and Law et al. (Ref. 18), such circulation would be unlikely within the fuel droplets of typical liquid-fueled combustors because droplet diameters are small ($< 200 \mu\text{m}$) and fuel viscosities are relatively high ($> 2 \text{ cs}$). Heat and mass transfer throughout the gas phase are considered to occur by conduction and diffusion as well as by radial convective transport of mass which results from droplet vaporization. Since movement of the droplet relative to the ambient gas enhances the transfer of heat and mass by convection in the region immediately surrounding the droplet, gas phase transport processes are presumed to take place within a gas film whose thickness is a function of the droplet relative velocity. This latter assumption, being somewhat inconsistent with the restriction of spherical symmetry, limits the model to either moderate relative velocities of perhaps less than 1 m/sec or the forward stagnation region of the droplet.

For the subcritical pressure range of interest, gas phase heat and mass diffusion rates are of the order of 10^{-1} to $1 \text{ cm}^2/\text{sec}$, while liquid phase heat and mass transfer rates are of the order of $10^{-3} \text{ cm}^2/\text{sec}$ and $10^{-5} \text{ cm}^2/\text{sec}$, respectively, and the liquid surface regression rate is of the order of 10^{-4} to $10^{-3} \text{ cm}^2/\text{sec}$. Inasmuch as gas phase transfer rates are much faster than all of the liquid phase transfer rates, gas phase heat and mass transfer can be represented as quasi-steady processes. The validity of this quasi-steady approximation has been substantiated by the numerical analysis of Hubbard et al, (Ref. 19). Furthermore, Law and Sirignano (Ref. 20) have demonstrated that effects due to liquid surface regression during the droplet heating period are negligible relative to the liquid phase heat conduction rate.

Formulation of Governing Equations

Based on the foregone physical model, the nonsteady liquid phase temperature, T_l , and mass fraction of each component, ω_{il} , are governed by the following heat and

mass diffusion equations:

$$\frac{1}{x^2} \frac{\partial}{\partial x} \left(x^2 \frac{\partial T_l}{\partial x} \right) = \frac{\partial T_l}{\partial \tau} \quad (1)$$

$$\frac{1}{x^2} \frac{\partial}{\partial x} \left(x^2 \frac{\partial \omega_{il}}{\partial x} \right) = \lambda_{il} \frac{\partial \omega_{il}}{\partial \tau} \quad (2)$$

where λ_{il} is the Lewis number of the liquid components and x and τ are nondimensional radial position and time, respectively.

If spatial variations in the products of mass density and diffusivities (i.e. ρa and ρD) within the gas film surrounding the droplet are small compared to variations in temperature and chemical species, the quasi-steady gas phase temperature, T_g , mass fraction of each fuel component, ω_{ig} , and mass fraction of oxygen, ω_o , are governed by the following conservation equations:

$$\frac{\partial}{\partial x} \left(x^2 \frac{\partial T_g}{\partial x} \right) - \theta_{Tg} \frac{\partial T_g}{\partial x} = \sum_i \frac{H_i}{C_g} \xi_i \quad (3)$$

$$\frac{\partial}{\partial x} \left(x^2 \frac{\partial \omega_{ig}}{\partial x} \right) - \theta_{ig} \frac{\partial \omega_{ig}}{\partial x} = \xi_i \quad (4)$$

$$\frac{\partial}{\partial x} \left(x^2 \frac{\partial \omega_o}{\partial x} \right) - \theta_{og} \frac{\partial \omega_o}{\partial x} = \sum_i \gamma_i \xi_o \quad (5)$$

where the nondimensional rates of vaporization and reaction are defined as

$$\theta_{Tg} = \frac{\dot{m}_f}{4\pi a \rho_g a_g} \quad \xi_T = \frac{a^2 x^2 R_i}{\rho_g a_g}$$

$$\theta_{ig} = \frac{\dot{m}_f}{4\pi a \rho_g D_{ig}} \quad \xi_i = \frac{a^2 x^2 R_i}{\rho_g D_{ig}}$$

$$\theta_{og} = \frac{\dot{m}_f}{4\pi a \rho_g D_{og}} \quad \xi_o = \frac{a^2 x^2 R_i}{\rho_g D_{og}}$$

$$\text{and} \quad \dot{m}_f = \sum_i \dot{m}_i$$

For continuity of temperature, chemical species, heat, and mass at the droplet and gas film boundaries, the solution of these governing differential equations must satisfy the following boundary conditions:

$$\frac{\partial T_\ell}{\partial x} (0, \tau) = 0 \quad (6)$$

$$T_\ell (1, \tau) = T_g (1, \tau) = T_s (\tau) \quad (7)$$

$$\frac{\partial T_\ell}{\partial x} (1, \tau) = \frac{1}{c_\ell} \left[K \frac{\partial T_g}{\partial x} (1, \tau) - \theta_{T_\ell} L \right] \quad (8)$$

$$T_g (x_\delta, \tau) = T_\infty \quad (9)$$

$$\frac{\partial \omega_{i\ell}}{\partial x} (1, \tau) = \left[\omega_{i\ell} (1, \tau) - \epsilon_i \right] \theta_{i\ell} \quad (10)$$

$$\omega_{ig} (1, \tau) = \omega_{igs} (\tau) \quad (11)$$

$$\omega_{ig} (x_\delta, \tau) = 0 \quad (12)$$

$$\frac{\partial \omega_{ig}}{\partial x} (1, \tau) = \left[\omega_{ig} (1, \tau) - \epsilon_i \right] \theta_{ig} \quad (13)$$

$$\frac{\partial \omega_o}{\partial x} (1, \tau) = \theta_{og} \omega_o (1, \tau) \quad (14)$$

$$\omega_o (x_\delta, \tau) = (\omega_o)_\infty \quad (15)$$

Initial conditions for the dependent variables are taken to be arbitrary.

Phase Change Description

Since the phase change processes for volatile liquids occurs at a much faster rate than the gas phase transport processes, the vapor concentration at the droplet surface can be assumed to be saturated. By further assuming that the liquid behaves

as an ideal mixture, Raoult's law and the Clausius - Claperyron equation provide the following relationship for the mass fraction of each fuel vapor component at the droplet surface as a function of the mass fractions of the various fuel components and the temperature at the droplet surface:

$$\omega_{igs} = \omega_{ils} \cdot \frac{\sum_j (\omega_{jgs} / M_j)}{\sum_j (\omega_{jls} / M_j)} \cdot \left(\frac{P_{bi}}{P_\infty} \right) \cdot \exp \left[\frac{L_i M_i}{R} \left(\frac{1}{T_{bi}} - \frac{1}{T_s} \right) \right] \quad (16)$$

Ignition Criterion

An ignition criterion, which was developed originally by Faeth and Olson (Ref. 5) for single-component hydrocarbon fuels, is used in the present model because this criterion could be extended easily to ignition of multicomponent vapor mixtures. This ignition criterion is based on the premise that ignition occurs, and combustion is self-sustaining, when the concentration of a crucial chain-branching, intermediate, chemical species reaches a critical level at some point in the gas phase. The rate of formation of this crucial intermediate species, which is unidentified, was shown by Faeth and Olson to depend on the gas phase history for pressure, temperature, and fuel and oxidizer concentrations. The buildup of the crucial intermediate species in the gas phase from each fuel component, when normalized relative to the critical concentration of the intermediate species necessary for ignition, is given by the expression

$$\psi_i(x, \tau) = \frac{a^2}{a_L} \int_0^\tau K_{i1} \rho^{K_{i2}} \phi_i^{K_{i3}}(x, \tau) \exp \left[- \frac{E_i}{R T_g(x, \tau)} \right] d\tau \quad (17)$$

where the rate constants, K_{i1} , K_{i2} , K_{i3} and E_i , are to be determined empirically for each fuel component and the local equivalence ratio is defined as

$$\phi_i(x, \tau) = \gamma_i \frac{\omega_{ig}(x, \tau)}{\omega_o(x, \tau)}$$

Since the same chain-branching, intermediate, chemical species are produced in varying amounts during oxidation of the various hydrocarbons, the buildup of a crucial intermediate species can be treated as the cumulative contribution from each of the components of a fuel mixture. Hence, the analog of the ignition criterion for a multi-component fuel is the sum

$$\bar{\Psi}(x, \tau) = \sum_i \psi_i(x, \tau) \quad (18)$$

The variation of $\Psi(x, \tau)$ then describes the tendency for ignition as a function of fuel composition and associated kinetic rate constants. When Ψ reaches unity at some time and location in the gas phase, ignition is predicted.

Rates of Combustion

Because gas phase reaction rates of typical fuels at normal combustion temperatures are extremely fast as compared to gas phase transport processes, theoretical models for the combustion of single component fuel droplets have customarily used the thin-flame approximation, which states that the outwardly diffusing fuel vapor reacts stoichiometrically and completely with the inwardly diffusing oxidizer at an infinitesimally thin flame front. For multicomponent fuels, this assumption should be equally valid because the volatile hydrocarbon species comprising typical liquid fuels have reaction rates which are very fast compared to gas phase transport processes. Hence, if the multicomponent fuel vapor is assumed to react collectively at a thin flame front located at a nondimensional radius x_b , the rate of reaction of each component can be expressed as

$$R_i(x_b) = \frac{\dot{m}_i}{4\pi b^2} \frac{\delta(x - x_b)}{a} \quad (19)$$

where the delta function is defined as

$$\delta(x - x_b) = \begin{cases} 0 & \text{for } x \neq x_b \\ \infty & \text{for } x = x_b \end{cases} \text{ and } \int_0^\infty \delta(x - x_b) \cdot F(x) dx = F(x_b)$$

For complete and stoichiometric reaction of fuel and oxidizer at the flame position, the thin-flame approximation also requires that

$$\omega_o(x_b, \tau) = 0 \quad (20)$$

During combustion, all of the fuel components in the gas phase can be treated collectively, and Eq. (4) can be summed over all components to obtain the total fuel conservation equation

$$\frac{\partial}{\partial x} \left(x^2 \frac{\partial \omega_f}{\partial x} \right) - \theta_f \frac{\partial \omega_f}{\partial x} = \xi_f \quad (21)$$

where the gas phase diffusion coefficients for all fuel species have been assumed to be equal to D_f , $\omega_f = \sum_i \omega_{i,g}$ and $\xi_f = \sum_i \xi_i$. The boundary conditions to be satisfied by ω_f , obtained by summing Eqs. (11) and (12) for all fuel components,

are

$$\omega_f(l, \tau) = \omega_{fs}(\tau) \quad (22)$$

$$\omega_f(x_s, \tau) = 0 \quad (23)$$

and the total rate of fuel vaporization, obtained by summing Eq. (13) similarly, is

$$\theta_f = \frac{-\frac{\partial \omega_f}{\partial x}(l, \tau)}{1 - \omega_{fs}(\tau)} \quad (24)$$

where

$$\omega_{fs}(\tau) = \omega_{fs}(l, \tau)$$

Superheat Limits

For a vaporizing multicomponent droplet, in the absence of appreciable internal circulation, the rate of mass diffusion within the droplet is very slow in comparison with that for thermal diffusion. Under these conditions, the more volatile components of the mixture are preferentially vaporized at the droplet surface and they are not replenished by mass diffusion from the interior of the droplet. Eventually, only the least volatile components will remain at the droplet surface while the composition of the droplet interior will be nearly constant and unchanged from the initial composition. As these changes in mass composition take place, the surface temperature of the droplet will rise to accommodate the vaporization temperature of the mixture, approaching the boiling temperature of the heaviest component. Simultaneously, thermal conduction of heat from the droplet surface will cause the temperature of the droplet interior to also increase. If liquid phase mass diffusion is rate limiting in comparison to thermal conduction, the temperature somewhere in the interior of the droplet may eventually exceed the limit of superheat for the local mixture composition, causing homogeneous nucleation within the droplet. The resultant vaporization within the droplet will cause internal pressure to increase followed by fragmentation of the droplet.

The limits of superheat have been measured by Skripov (Ref. 14) and Apfel (Ref. 15) for a variety of pure hydrocarbons as a function of pressure. Law (Ref. 12) has since shown that the available data can be correlated satisfactorily by the explicit relationship

$$\left(1 - \frac{T_{Li}}{T_{ci}}\right) = 0.111 \left(1 - \frac{P}{P_{ci}}\right)^{0.858} \quad (25)$$

where T_{Li} is the superheat limit temperature and the subscript ci represents the critical constants for the pure hydrocarbon. Measurements by Blander and Katz (Ref. 16) of the limits of superheat for hydrocarbon mixtures which exhibit ideal solution behavior show an approximately linear variation of the superheat limit temperature with liquid mole fraction; namely

$$T_L(x, \tau) = \sum_i T_{Li} X_i(x, \tau) \quad (26)$$

Integral Equation Solutions

As a consequence of the quasi-steady approximation for gas phase transport processes, a rigorous simultaneous solution of the governing differential equations is not required. Because of this mathematical simplification, each of the ordinary and partial differential equations can be solved independently for selected boundary conditions. The remaining boundary conditions can then be matched at selected times throughout the ignition and combustion process by an iterative numerical analysis of the solutions to these governing differential equations. The solutions to the differential equations and the numerical analysis, which are discussed below, follow directly from the single component droplet combustion model in Ref. 4.

Using Green's function techniques, Eqs. (1) and (2) for the nonsteady, diffusion of heat and mass within the fuel droplet can be transformed to implicit integral equations which are amenable to numerical solution. Similar techniques have been used to model both steady state and transient diffusion processes (Refs. 2, 4, and 21-24), and a detailed discussion of the procedures for transforming ordinary and partial differential equations to integralequations can be found in Ref. 25. The integral equations for temperature and the mass fraction of each component within the fuel droplet as functions of position and time, obtained by transforming Eqs. (1) and (2) for time dependent gradients at the droplet surface, are

$$\begin{aligned} T_\ell(x, \tau) = & \int_0^\tau \frac{\partial T_\ell}{\partial x_0}(1, \tau_0) \cdot G_T(x, \tau / 1, \tau_0) d\tau_0 \\ & + \int_0^1 x_0^2 \cdot T_\ell(x_0, 0) \cdot G_T(x, \tau / x_0, 0) dx_0 \end{aligned} \quad (27)$$

and

$$\begin{aligned} \omega_{i\ell}(x, \tau) = & \int_0^\tau \frac{\partial \omega_{i\ell}}{\partial x_0}(l, \tau_0) \cdot G_i(x, \tau/l, \tau_0) d\tau_0 \\ & + \int_0^l x_0^2 \cdot \omega_{i\ell}(x_0, 0) \cdot G_i(x, \tau/x_0, 0) dx_0 \end{aligned} \quad (28)$$

The Green's function, for small values of $\tau \ll 1$ obtained by Laplace transform techniques is

$$\begin{aligned} G_i(x, \tau/x_0, \tau_0) = & \frac{1}{2\pi x_0} \left\{ (\pi\Delta)^{-1/2} \left[\exp\left(-\frac{\nu_1^2}{4\Delta}\right) - \exp\left(-\frac{\nu_2^2}{4\Delta}\right) \right. \right. \\ & + \exp\left(-\frac{\nu_3^2}{4\Delta}\right) - \exp\left(-\frac{\nu_4^2}{4\Delta}\right) - \exp\left(-\frac{\nu_5^2}{4\Delta}\right) + \exp\left(-\frac{\nu_6^2}{4\Delta}\right) \Big] \\ & + 2 \left[\exp(-\nu_3 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_3}{2\Delta^{1/2}} - \Delta^{1/2}\right) - \exp(-\nu_4 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_4}{2\Delta^{1/2}} - \Delta^{1/2}\right) \right. \\ & - \exp(-\nu_5 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_5}{2\Delta^{1/2}} - \Delta^{1/2}\right) + \exp(-\nu_6 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_6}{2\Delta^{1/2}} - \Delta^{1/2}\right) \Big] \\ & - \left[8(\Delta/\pi)^{1/2} + (\pi\Delta)^{-1/2} \right] \left[\exp\left(-\frac{\nu_7^2}{4\Delta}\right) - \exp\left(-\frac{\nu_8^2}{4\Delta}\right) - \exp\left(-\frac{\nu_9^2}{4\Delta}\right) + \exp\left(-\frac{\nu_{10}^2}{4\Delta}\right) \right] \\ & + 4 \left[(1 + \nu_3 + 2\Delta) \cdot \exp(-\nu_3 - 2 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_3 + 2}{2\Delta^{1/2}} - \Delta^{1/2}\right) - \Delta^{1/2} \right. \\ & - (1 + \nu_4 + 2\Delta) \cdot \exp(-\nu_4 - 2 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_4 + 2}{2\Delta^{1/2}} - \Delta^{1/2}\right) \\ & - (1 + \nu_5 + 2\Delta) \cdot \exp(-\nu_5 - 2 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_5 + 2}{2\Delta^{1/2}} - \Delta^{1/2}\right) \\ & \left. \left. + (1 + \nu_6 + 2\Delta) \cdot \exp(-\nu_6 - 2 + \Delta) \cdot \operatorname{erfc}\left(\frac{\nu_6 + 2}{2\Delta^{1/2}} - \Delta^{1/2}\right) \right] \right\} \end{aligned} \quad (29)$$

where

$$\begin{aligned} \nu_1 &= x - x_0, \quad \nu_2 = x + x_0, \quad \nu_3 = -x - x_0 + 2, \quad \nu_4 = -x + x_0 + 2, \quad \nu_5 = x - x_0 + 2 \\ \nu_6 &= x + x_0 + 2, \end{aligned}$$

$$\Delta = \frac{\kappa_j(\tau - \tau_0)}{a^2},$$

and κ_j is the appropriate heat or mass diffusivity for the liquid phase.

It is of interest to note that in Eqs. (27) and (28), the first integral with respect to time represents the effect of a time dependent gradient at the droplet surface and the second integral with respect to position represents the effect of initial profiles. As a result of the form of these integral equations, a versatile numerical procedure can be performed by expressing the transient processes as a series of successive short time intervals using suitable time-averaged gradients at the droplet surface. In this manner, the temperature and mass fraction profiles computed at each value of time become the initial conditions for computations at the subsequent time. The time-averaged gradients required to evaluate the first integral in Eqs. (27) and (28) for each successive time interval are given by the boundary conditions stated in Eqs. (8) and (10). The rates of vaporization and the gas phase temperature gradient needed, in turn, to evaluate Eqs. (8) and (10) are to be obtained from solutions of Eqs. (3) - (5) for the quasi-steady gas phase transport processes.

The methods for transforming the quasi-steady differential equations for gas phase conservation to integral equation solutions using Green's function techniques are presented in Ref. 4. Upon applying these methods to Eqs. (3), (4), (5), and (21), subject to the boundary conditions given in Eqs. (7), (9), (11), (12), (14), (15), (22), and (23) and the rate of reaction for the thin-flame approximation in Eq. (19), the following solutions are obtained for the quasi-steady gas phase temperature and mass fraction profiles, respectively, during ignition and combustion:

$$\begin{aligned}
 T_g(x, \tau) = & T_\infty \left[\frac{e^{-\theta_{Tg}/x} - e^{-\theta_{Tg}}}{e^{-\theta_{Tg}/x_\delta} - e^{-\theta_{Tg}}} \right] + T_s \left[\frac{e^{-\theta_{Tg}/x_\delta} - e^{-\theta_{Tg}/x}}{e^{-\theta_{Tg}/x_\delta} - e^{-\theta_{Tg}}} \right] \\
 & + \frac{\bar{H}}{C_g} \left\{ \begin{aligned} & \left[\frac{e^{-\theta_{Tg}/x} - e^{-\theta_{Tg}}}{e^{-\theta_{Tg}/x_\delta} - e^{-\theta_{Tg}}} \right] \cdot \left[1 - e^{(\theta_{Tg}/x_b - \theta_{Tg}/x_\delta)} \right] & \text{for } 1 \leq x \leq x_b \\ & \left[\frac{e^{-\theta_{Tg}/x} - e^{-\theta_{Tg}/x_\delta}}{e^{-\theta_{Tg}/x_\delta} - e^{-\theta_{Tg}}} \right] \cdot \left[1 - e^{(\theta_{Tg}/x_b - \theta_{Tg})} \right] & \text{for } x_b \leq x \leq x_\delta \end{aligned} \right.
 \end{aligned} \tag{30}$$

$$\omega_{ig}(x, \tau) = \omega_{igs} \left[\frac{e^{-\theta_{ig}/x_b} - e^{-\theta_{ig}/x}}{e^{-\theta_{ig}/x_b} - e^{-\theta_{ig}}} \right] + \epsilon_i \begin{cases} \left[\frac{e^{-\theta_{ig}/x} - e^{-\theta_{ig}}}{e^{-\theta_{ig}/x_b} - e^{-\theta_{ig}}} \right] \cdot [1 - e^{(\theta_{ig}/x_b - \theta_{ig}/x_b)}] & \text{for } 1 \leq x \leq x_b \\ \left[\frac{e^{-\theta_{ig}/x} - e^{-\theta_{ig}/x_b}}{e^{-\theta_{ig}/x_b} - e^{-\theta_{ig}}} \right] \cdot [1 - e^{(\theta_{ig}/x_b - \theta_{ig})}] & \text{for } x_b \leq x \leq x_b \end{cases} \quad (31)$$

$$\omega_o(x, \tau) = \omega_{o\infty} \cdot e^{(\theta_{og}/x_b - \theta_{og}/x)}$$

$$-\bar{\gamma} \begin{cases} e^{-\theta_{og}/x} [e^{\theta_{og}/x_b} - e^{\theta_{og}/x_b}] & \text{for } 1 \leq x \leq x_b \\ [1 - e^{(\theta_{og}/x_b - \theta_{og}/x)}] & \text{for } x_b \leq x \leq x_b \end{cases} \quad (32)$$

$$\omega_f(x, \tau) = \omega_{fs} \left[\frac{e^{-\theta_f/x_b} - e^{-\theta_f/x}}{e^{-\theta_f/x_b} - e^{-\theta_f}} \right] + \begin{cases} \left[\frac{e^{-\theta_f/x} - e^{-\theta_f}}{e^{-\theta_f/x_b} - e^{-\theta_f}} \right] \cdot [1 - e^{(\theta_f/x_b - \theta_f/x_b)}] & \text{for } 1 \leq x \leq x_b \\ \left[\frac{e^{-\theta_f/x} - e^{-\theta_f/x_b}}{e^{-\theta_f/x_b} - e^{-\theta_f}} \right] \cdot [1 - e^{(\theta_f/x_b - \theta_f)}] & \text{for } x_b \leq x \leq x_b \end{cases} \quad (33)$$

Note that when using the equations above for the temperature and mass fraction profiles in the gas phase during ignition or pure vaporization, the terms which represent the effects of reaction and involve the flame position, x_b , are to be taken as zero.

The temperature gradient in the gas phase at the droplet surface is given by Eq. (30) as

$$\frac{\partial T_g}{\partial x}(1, \tau) = \frac{\theta_{Tg} e^{-\theta_{Tg}} \left\{ T_{\infty} - T_s + \frac{\bar{H}}{c_g} [1 - e^{(\theta_{Tg}/x_b - \theta_{Tg}/x_b)}] \right\}}{e^{-\theta_{Tg}/x_b} - e^{-\theta_{Tg}}} \quad (34)$$

The nondimensional flame position obtained from Eq. (32) for the thin-flame approximation in Eq. (20) is

$$x_b = - \frac{\theta_{og}}{\theta_{og}/x_g - \ln\left(\frac{\bar{\gamma}}{\omega_{o\infty} + \gamma}\right)} \quad (35)$$

Then by using Eqs. (33) and (35) to evaluate Eq. (24), the total nondimensional rate of vaporization is

$$\theta_f = - \left(\frac{x_g}{x_g - 1} \right) \left[\frac{D_f}{D_{og}} \ln(1 - \omega_{fs}) + \ln\left(\frac{\gamma}{\omega_{o\infty} + \gamma}\right) \right] \quad (36)$$

The nondimensional rate of vaporization for each fuel component, θ_{ig} , can be obtained in a similar manner by using Eqs. (31) and (35) to evaluate Eq. (13). A comparison of this result with Eq. (36) for the total rate of vaporization shows that the fractional rate of vaporization is linearly proportional to the fractional fuel mass fraction at the droplet surface; namely

$$\epsilon_i = \frac{\dot{m}_i}{\dot{m}_f} = \frac{\omega_{igs}}{\omega_{fs}} \quad (37)$$

Boundary Layer Thickness

Estimates of the film thickness, δ , needed to determine the gas phase temperature and weight fraction profiles are based on the empirical Nusselt number correlations developed by Ranz and Marshall (Ref. 26) for simultaneous heat and mass transfer during droplet vaporization. A detailed derivation of the equations for the gas phase film thickness is available in Ref. 2. This derivation consists of equating the heat and mass fluxes at the droplet surface, based on the profiles given by Eqs. (30 - 33), to the corresponding fluxes expressed in terms of the Nusselt numbers for free or forced convection. By properly accounting for the effects of droplet vaporization, unidirectional mass transfer, and chemical reaction, the expression obtained for the gas phase film thickness is

$$\frac{\delta}{a} = \frac{2}{Nu - 2} \quad (38)$$

The empirical correlations developed by Ranz and Marshall (Ref. 26) for the Nusselt numbers for simultaneous heat and mass transfer during droplet vaporization are as follows:

For forced convection of heat and mass

$$Nu_h = 2 + 0.6 Re^{1/2} Pr^{1/3} \quad (39a)$$

$$Nu_m = 2 + 0.6 Re^{1/2} Sc^{1/3} \quad (39b)$$

and for free convection of heat and mass

$$Nu_h = 2 + 0.6 Gr^{1/4} Pr^{1/3} \quad (40a)$$

$$Nu_m = 2 + 0.6 Gr^{1/4} Sc^{1/3} \quad (40b)$$

where

$$Nu_h = 2 a h_c / k_g, Nu_m = 2 a k_c / \rho_g D_i$$

$$Re = 2 a \rho_g V_r / \mu_g, Pr = \mu_g c_g / k_g$$

$$Gr = (2a)^3 \rho_g^2 g \beta \Delta T / \mu_g, Sc = \mu_g / \rho_g D_i$$

For the present investigation the characteristic temperature difference for free convection, ΔT , is taken as $|T_\infty - T_s|$ and the gas phase properties are evaluated at the mean temperature $T_g = \frac{1}{2} (T_\infty + T_s)$. The thermal coefficient of volumetric expansion of the gas, β , which appears in the Grashof number is taken as $1/T_g$. Note that Eqs. (38) - (40) state that the gas film thickness which surrounds the droplet is infinite when the droplet is motionless relative to the gas stream and gravity is absent. As the relative velocity increases, the film thickness becomes smaller.

Droplet Size Variation

The instantaneous mass of a multicomponent fuel droplet is given by

$$m_d(t) = 4\pi \int_0^{a(t)} \rho_\ell(r,t) r^2 dr \quad (41)$$

where, if the liquid is assumed to be an ideal mixture, the liquid density depends on the mass fractions and the liquid densities of the individual components in the manner

$$\rho_\ell(r,t) = \frac{1}{\sum_j \frac{\omega_j(r,t)}{\rho_{j\ell}}} \quad (42)$$

The rate of change of droplet mass with respect to time is then related to the total rate of vaporization by the expression

$$\begin{aligned} \dot{m}_f(t) = -\frac{dm_d}{dt} = & -4\pi \left\{ \rho_\ell(a,t) a^2(t) \frac{da}{dt} \right. \\ & \left. + \int_0^{a(t)} \frac{\partial}{\partial t} [\rho_\ell(r,t)] r^2 dr \right\} \end{aligned} \quad (43)$$

And since the term in Eq. (43) which involves the rate of change of liquid density with respect to time is small compared to the other term, integrating Eq. (43) gives an approximate expression for the instantaneous droplet radius

$$a^2(t) \approx a_0^2 - \frac{1}{2\pi} \int_0^t \frac{\dot{m}_f(t)}{\rho_\ell(a,t) a(t)} dt \quad (44)$$

Numerical Procedure

An examination of Eqs. (30) - (37) indicates that the gas phase profiles and gradients at the droplet surface for temperature and mass fractions, flame position, and rates of vaporization depend only on the temperature and the fuel mass fractions in this liquid at the droplet surface. Hence, the main function of the numerical procedure is to match or couple the analytical solutions for temperature and mass fractions at the liquid-gas interface for a series of successive, short, time intervals which cover the transient ignition and combustion process. The numerical procedure for each successive time consists of the following steps:

1. Assume the temperature and fuel mass fractions in the liquid phase at the droplet surface; corresponding values for the previous time or iteration can be used to select the assumed values.
2. Compute the gas phase film thickness, δ , for the selected mode of gas phase heat and mass transfer using Eqs. (38) - (40).
3. Using a set of linear, simultaneous equations based on Eq. (16), compute the mass fraction of each fuel component in the gas phase at the droplet surface.
4. Compute the total and individual rates of vaporization, $\dot{m}_f$ and $\dot{m}_i$, respectively, using Eqs. (36) and (37).
5. If ignition has been established, compute the nondimensional flame position, x_b , using Eq. (35).
6. Compute the gas phase temperature gradient at the droplet surface $\frac{\partial T_g}{\partial x}(1, \tau)$, using Eq. (34).
7. Compute the liquid phase temperature gradient at the droplet surface $\frac{\partial T_\ell}{\partial x}(1, \tau)$, using Eq. (8).
8. Compute the mass fraction gradient for each fuel component in the liquid phase at the droplet surface, $\frac{\partial \omega_{i\ell}}{\partial x}(1, \tau)$, Eq. (10).
9. Compute the droplet surface temperature, $T_s = T_\ell(1, \tau)$, using Eq. (27) and the numerical average of the liquid phase temperature gradient at the droplet surface for this and the previous time.
10. Compute the fuel mass fractions in the liquid phase at the droplet surface, $\omega_{i\ell s} = \omega_{i\ell}(1, \tau)$, Eq. (28) and the numerical average of the mass fraction gradients in the liquid phase at the droplet surface for this and the previous time.
11. Compare the assumed and computed values for T_s and $\omega_{i\ell s}$ from Steps 1, 9, 10 and repeat the above procedure until a satisfactory accuracy is obtained.

12. After determining the temperature and fuel mass fractions at the droplet surface for this time compute the temperature and mass fraction profiles in both the liquid and gas phases using Eqs. (27) - (33).
13. Establish self-ignition, if ignition has not yet occurred, by computing the profile for the ignition criterion, $\bar{\Psi}(x, \tau)$, using Eqs. (17) and (18) and compare the result with unity.
14. Verify whether homogeneous nucleation within the droplet and subsequent fragmentation of the droplet has taken place, by computing the temperature profile for the liquid phase superheat limit, $T_L(x, \tau)$, using Eqs. (25) and (26) and compare the result with the actual temperature profile in the liquid phase, $T_g(x, \tau)$. The instant at which $T_g(x, \tau) = T_L(x, \tau)$ signifies vaporization within the droplet due to homogeneous nucleation and can be identified approximately as the state when fragmentation of the droplet has occurred.
15. Determine the droplet size at the end of the time interval by numerical integration of Eq. (44).

APPENDIX II

TABULATIONS OF EXPERIMENTAL DATA

TABLE II-1

EFFECT OF DROPLET SPACING ON IGNITION DELAY TIME FOR

260 μm DIAMETER n-HEXADECANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

$(\Delta/d)_\infty$	$(\omega_\infty)_\infty$	$T_\infty \sim \text{K}$	$t_i \sim \text{msec}$
31.679	0.1355	1452	9.205
17.04	0.1355	1452	6.711
9.377	0.1355	1452	7.318
7.776	0.1355	1452	6.469
5.718	0.1355	1452	6.00
2.194	0.1355	1452	16.00
31.266	0.1438	1363	10.454
22.878	0.1438	1363	10.896
16.068	0.1438	1363	10.340
8.966	0.1438	1363	10.025
7.441	0.1438	1363	9.078
4.118	0.1438	1363	17.184
2.091	0.1438	1363	27.441
43.992	0.1212	1578	6.328
34.950	0.1212	1578	6.1530
24.586	0.1212	1578	5.9418
13.693	0.1212	1578	5.9583
11.5785	0.1212	1578	5.8087
8.5210	0.1212	1578	5.7258
6.042	0.1212	1578	5.8392
3.306	0.1212	1578	7.8821
30.689	0.1556	1242	16.9849
22.9402	0.1556	1242	16.2947
17.052	0.1556	1242	14.8808
8.7251	0.1556	1242	14.7546
7.577	0.1556	1242	14.1215
5.6932	0.1556	1242	14.1710
3.3307	0.1556	1242	24.3714
1.4343	0.1556	1242	71.1653

TABLE II-2

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME FOR

260 μm DIAMETER n-HEXADECANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

$(\Delta/d)_o$	$(\omega_o)_\infty$	$T_\infty \sim K$	$(t_b - t_i) \sim \text{msec}$
36.8	0.1355	1452	126
30.7	0.1355	1452	134
20.9	0.1355	1452	146
12.5	0.1355	1452	150
7.2	0.1355	1452	158
6.3	0.1355	1452	180
4.7	0.1355	1452	216
2.8	0.1355	1452	244
29.3	0.1438	1363	123
25.3	0.1438	1363	121
19.4	0.1438	1363	138
10.5	0.1438	1363	150
7.0	0.1438	1363	165
6.1	0.1438	1363	175
4.7	0.1438	1363	207
2.8	0.1438	1363	205
27.5	0.1556	1242	117
23.7	0.1556	1242	119
17.3	0.1556	1242	127
10.0	0.1556	1242	145
7.2	0.1556	1242	156
5.7	0.1556	1242	169
4.4	0.1556	1242	228
2.4	0.1556	1242	208
23.9	0.0766	1473	129
21.1	0.0766	1473	148
17.2	0.0766	1473	156
10.1	0.0766	1473	167
7.1	0.0766	1473	188
6.2	0.0766	1473	206
4.7	0.0766	1473	221
2.7	0.0766	1473	223

TABLE II-3

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME FOR

260 μm DIAMETER ISOCTANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

$(\Delta/d)_o$	$(\omega_o)_\infty$	$T_\infty \sim K$	$(t_b - t_i) \sim \text{msec}$
27.3	0.1355	1452	78
10.7	0.1355	1452	104
7.6	0.1355	1452	112
3.2	0.1355	1452	152
15.2	0.1438	1363	83
6.2	0.1438	1363	104
4.5	0.1438	1363	113
2.0	0.1438	1363	165
16.0	0.1556	1242	77
7.1	0.1556	1242	96
4.4	0.1556	1242	109
1.9	0.1556	1242	162
15.5	0.0766	1473	98
7.0	0.0766	1473	123
4.3	0.0766	1473	134
2.0	0.0766	1473	195

TABLE II-4

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME FOR
 260 μm DIAMETER DROPLETS WITH $T_{\infty} = 1452 \text{ K}$ AND $(\omega_o)_{\infty} = 0.1355$ AS A FUNCTION
 OF FUEL COMPOSITION (BY VOLUME)

<u>$(\Delta/d)_o$</u>	<u>$(t_b - t_i) \sim \text{msec}$</u>
90% Hexadecane/10% Isooctane	
23.5	121
19.9	125
14.2	127
8.2	146
6.2	159
5.1	172
3.9	205
2.4	278
70% Hexadecane/30% Isooctane	
34.2	123
27.3	118
19.5	120
10.5	133
7.9	151
6.6	170
4.9	191
2.9	217
50% Hexadecane/50% Isooctane	
31.7	108
23.1	108
15.8	115
9.4	132
7.7	144
6.1	163
4.7	173
2.7	255

- continued -

- continued -

TABLE II-4

<u>$(\Delta/d)_0$</u>	<u>$(t_b - t_i) \sim \text{msec}$</u>
100% Hexadecane/0% Isooctane	
36.8	126
30.7	134
20.9	146
12.5	150
7.2	158
6.3	180
4.7	216
2.8	244
0% Hexadecane/100% Isooctane	
27.3	78
10.7	104
7.6	112
3.2	152

TABLE II-5

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME FOR

260 μm DIAMETER NO. 2 FUEL OIL DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

$(\Delta/d)_0$	$(\omega_o)_\infty$	$T_\infty \sim K$	$(t_b - t_i) \sim \text{msec}$
34.6	0.1355	1452	117
25.1	0.1355	1452	131
14.8	0.1355	1452	145
8.7	0.1355	1452	159
5.2	0.1355	1452	219
2.5	0.1355	1452	258
21.3	0.1438	1363	127
19.1	0.1438	1363	129
15.5	0.1438	1363	137
9.6	0.1438	1363	155
5.5	0.1438	1363	188
2.3	0.1438	1363	268
23.5	0.1556	1242	122
20.6	0.1556	1242	130
16.4	0.1556	1242	127
9.7	0.1556	1242	151
6.1	0.1556	1242	168
2.4	0.1556	1242	251
19.8	0.0766	1473	145
17.2	0.0766	1473	143
12.0	0.0766	1473	157
8.0	0.0766	1473	177
4.0	0.0766	1473	221
2.6	0.0766	1473	271

TABLE II-6

EFFECT OF FUEL DROPLET COMPOSITION (BY VOLUME)

ON IGNITION DELAY TIME WITH $(\Delta/d)_0 \approx 40$

$(\omega_o)_\infty$	$T_\infty \sim K$	$t_i \sim \text{msec}$
100% Hexadecane/0% Isooctane		
0.1355	1452	9.0
0.1438	1363	11.0
0.1212	1578	6.5
0.1556	1242	12.0
95% Hexadecane/5% Isooctane		
0.1355	1452	7.0
0.1438	1363	8.0
0.1212	1578	6.5
0.1556	1242	9.0
90% Hexadecane/10% Isooctane		
0.1355	1452	7.0
0.1438	1363	6.8
0.1212	1578	6.5
0.1556	1242	8.2
50% Hexadecane/50% Isooctane		
0.1556	1242	4.0

TABLE II-7

EFFECT OF FUEL DROPLET COMPOSITION ON COMBUSTION TIME FOR

260 μm DIAMETER DROPLETS WITH $T_{\infty} = 1452 \text{ K}$, $(\omega_o)_{\infty} = 0.1355$, and $(\Delta/d)_o \approx 40$

INITIAL MASS FRACTIONS

<u>Hexadecane</u>	<u>Isooctane</u>	<u>$t_b \sim \text{msec}$</u>
1.00	0.00	126
0.91	0.09	116
0.72	0.28	114
0.53	0.47	109
0.00	1.00	80

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NOMENCLATURE

a	Radius of spherical fuel droplet, cm
b	Radius of flame surface position, cm
c	Specific heat at constant pressure, cal/g-deg K
d	Diameter of fuel droplet, μm
D	Mass diffusion coefficient, cm^2/sec
E	Activation energy for ignition criterion, cal/g-mole
F	General function
g	Acceleration of gravity, equals 980.665 cm/sec^2
G	Green's function
Gr	Grashof number for heat or mass convection
h_c	Heat convection coefficient, $\text{cal/cm}^2\text{-sec-deg K}$
H	Heat of reaction per unit mass of fuel (negative for exothermic reaction), cal/g
k	Thermal conductivity, cal/cm-sec-deg K
k_c	Mass convection coefficient, cm/sec
K_1	Rate constant in ignition criterion, sec^{-1}
K_2	Constant in ignition criterion denoting order of pressure dependence
K_3	Constant in ignition criterion denoting order of equivalence ratio dependence
L	Latent heat of vaporization, cal/g
m	Mass of fuel droplet, g
$\dot{m}$	Rate of vaporization, g/sec

NOMENCLATURE (CONT'D)

M	Molecular weight
n	Integer values, 1, 2, 3, - - - etc.
Nu	Nusselt number for heat or mass convection
P	Pressure, atm
Pr	Prandtl number
r	Radial position measured from center of fuel droplet, cm
R	Rate of reaction, g/cm ³ -sec
R	Perfect gas law constant, equals 1.987 cal/g-mole-deg K
Re	Reynolds number
Sc	Schmidt number
t	Time, sec
T	Temperature, deg K
V	Velocity, cm/sec
x	Normalized radial position, equals r/a

Greek Symbols

α	Thermal diffusivity, equals $k/\rho c$, cm ² /sec
β	Thermal coefficient of volumetric expansion of the gas phase
γ	Mass of oxygen per mass of a fuel component for stoichiometric reaction
δ	Gas phase film thickness for heat or mass convection, cm, or delta function
Δ	General dimensionless time interval used in Green's function, or center to center space between droplets

NOMENCLATURE (CONT'D)

- Fractional rate of vaporization of a fuel component, equals $\dot{m}_i / \sum_j \dot{m}_j$
- θ Dimensionless rate of vaporization, defined in text
- κ Appropriate heat or mass diffusion coefficient used in Green's function
- K Ratio of thermal conductivities, equals k_g/k_ℓ
- λ Lewis number of liquid phase, equals α_ℓ/D_ℓ
- μ Dynamic viscosity, poises
- ξ General reaction rate function, defined in text
- ρ Mass density, g/cm³
- τ Dimensionless time, equals $\alpha_\ell t/a^2$
- ϕ Equivalence ratio, defined in text
- X Mole fraction
- ψ Ignition criterion, defined by Eqs. (17) and (18)
- ω Mass fraction

Subscripts

- b** Refers to the normal boiling point of a liquid component at one atmosphere, or dimensionless flame position
- c** Refers to heat or mass convection, critical value of intermediate species, or critical conditions for a liquid component
- d** Refers to fuel droplet
- f** Refers to all fuel vapor components considered collectively
- g** Refers to gas phase
- h** Refers to gas phase heat transfer

NOMENCLATURE (CONT'D)

- i Refers to a general fuel component i, or ignition state
- j Refers to a general fuel component j
- L Refers to the superheat limit temperature of a liquid component or mixture
- l Refers to liquid phase
- m Refers to gas phase mass transfer
- o Refers to oxygen, or the source coordinate system of the Green's function
- r Refers to droplet velocity relative to the ambient gas
- s Refers to droplet surface
- T Refers to gas phase temperature profile
- ∞ Refers to ambient conditions in the gas phase
- δ Refers to the outer boundary of the gas phase film thickness

Overlines

- Indicates an average quantity which is weighted with respect to the instantaneous fractional rate of vaporization; e.g., $\bar{H} = \sum_i \epsilon_i H_i$

DROPLET COMBUSTION EXPERIMENT

DROPLET SPACING BY STEAM INTERACTION

FIG. 2

FIGURE 3a. HIGH-SPEED PHOTOGRAPH OF DROPLET STREAM USED TO DETERMINE DROPLET SPACING AND DROPLET VELOCITY

FIGURE 3b. DIRECT TIME-AVERAGED PHOTOGRAPH OF FLAT FLAME AND DROPLET FLAME USED TO DETERMINE IGNITION TIME

TYPICAL DROPLET HISTORY DURING COMBUSTION OF MONODISPERSED DROPLET STREAM

TYPICAL VARIATION OF NORMALIZED DROPLET SURFACE AREA DURING COMBUSTION OF A MONODISPERSED DROPLET STREAM

DROPLET COMBUSTION MODEL

EFFECT OF DROPLET SPACING ON IGNITION DELAY TIME

260 μm n-HEXADECANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

CONDITION	$T_{\infty} - \text{K}$	$(\omega_o)_{\infty}$
◇	1242	0.1556
△	1363	0.1438
○	1452	0.1355
□	1578	0.1212

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME

260 μm DIAMETER, n-HEXADECANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME

260 μm DIAMETER, ISOCTANE DROPLETS AS A FUNCTION OF AMBIENT CONDITIONS

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME

260 μm DIAMETER DROPLETS WITH $T_\infty = 1452 \text{ K}$ AND $(\omega_o)_\infty = 0.1355$ AS A FUNCTION OF FUEL COMPOSITION

EFFECT OF DROPLET SPACING ON TOTAL BURNING TIME

260 μm DIAMETER, NO. 2 FUEL OIL DROPLETS AS A FUNCTION OF AMBIENT CONDITONS

RELATIVE INCREASE IN DROPLET BURNING TIME DUE TO DROPLET INTERACTION

MASS FRACTION PROFILES WITHIN A BINARY FUEL DROPLET DURING IGNITION AND COMBUSTION

260 μm ISOCTANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)

IN AIR AT 1400K 0.1355 g O_2/g AIR AND 1 ATM

TEMPERATURE PROFILES WITHIN A BINARY FUEL DROPLET DURING COMBUSTION

260 μm ISOCTANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)
IN AIR AT 1400K 0.1355 g O_2/g AIR AND 1 ATM

VARIATION OF MASS FRACTIONS AND TEMPERATURE AT THE SURFACE AND CENTER OF A BINARY FUEL DROPLET DURING IGNITION AND COMBUSTION

260 μm ISOCTANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)

IN AIR AT 1400K 0.1355 g O_2/g AIR AND 1 ATM

VARIAION OF FRACTIONAL RATES OF VAPORIZATION DURING IGNITION AND COMBUJSTION OF A BINARY FUEL DROPLET

260 μm ISOOCOTANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)

IN AIR AT 1400K 0.1355 g O_2/g AIR AND 1 ATM

EFFECT OF FUEL DROPLET COMPOSITION ON IGNITION DELAY — COMPARISON OF EXPERIMENT AND THEORY

EXPERIMENTAL CONDITION	T_{∞} — K	$(\omega_O)_{\infty}$
□	1242	0.1556
△	1363	0.1438
○	1452	0.1355
◇	1578	0.1212
— THEORETICAL PREDICTION FOR A 260 μ m DROPLET IN AIR AT 1400K 0.1355 g O_2 /g AIR AND 1 ATM

IGNITION CRITERION PROFILES FOR A BINARY FUEL DROPLET AT IGNITION260 μm ISOCTANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)IN AIR AT 1400K 0.1355 g O_2/g AIR AND 1 ATM

EFFECT OF FUEL DROPLET COMPOSITION ON COMBUSTION TIME-COMPARISON OF EXPERIMENT AND THEORY

TENDENCY FOR HOMOGENEOUS NUCLEATION WITHIN A BINARY FUEL DROPLET DURING COMBUSTION

260 μm ISOOCANE/HEXADECANE DROPLET (50/50 MIXTURE INITIALLY BY MASS)

IN AIR AT 1400K 0.1355 g O_2/g AIR and 1 ATM