IGNITION OF FUEL SPRAYS

FINAL TECHNICAL REPORT

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by

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A theoretical-experimental program has been conducted to investigate the ignition of combustible sprays. One-dimensional unsteady calculations to study the spray ignition process were performed first for a monodisperse fuel-air spray in front of a planar heated wall and later for polydisperse single-component fuel sprays. The effect of different droplet heating models was investigated and it is found that at certain equivalence ratios ignition delay time and energies can be smaller in the heterogeneous case than in the limiting gaseous premixed case. Because of the critical dependency of ignition upon the distance of the heat source to the nearest droplet, spray ignition criteria are not precisely defined by fuel type, droplet size distribution and equivalence ratio but a range of ignition delay times and ignition energies is found due to the probabilistic effect of the droplet ignition. For polydisperse sprays it was found that not the Sauter-mean-diameter characteristics but polydisperse spray ignition can be well correlated with an equivalent monodisperse spray by using a mean diameter based on the total surface area.
of the spray
The experimental part of the program was designed to verify the theoretical spray ignition description and should help in understanding the physics and chemistry of the process. The experiment focused on the importance of transport mechanisms on individual fuel droplet ignition. An electrically heated flat plate was positioned in front of a vertical stream of Decane droplets. The geometry and dynamic of the arrangement was photographically recorded to obtain time and space resolved information. As expected from theoretical results, the ignition event depends on the temperature of the hot surface, the geometry of the arrangement, the properties of the fuel spray, the residence time of the droplet in the thermal boundary layer and the fuel vapor concentration of the carrier gas at room temperature. Comparisons of ignition delay times translated into ignition delay distances show discrepancy with predicted values. The lack of radiation heat transfer and the enhanced convective heat transfer of the experiment are most likely the reasons the mismatch between theory and experiment.
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ABSTRACT

A theoretical-experimental program has been conducted to investigate the ignition of combustible sprays. One-dimensional unsteady calculations to study the spray ignition process were performed first for a monodisperse fuel-air spray in front of a planar heated wall and later for polydisperse single-component fuel sprays. The effect of different droplet heating models was investigated and it is found that at certain equivalence ratios ignition delay time and energies can be smaller in the heterogeneous case than in the limiting gaseous premixed case. Because of the critical dependency of ignition upon the distance of the heat source to the nearest droplet, spray ignition criteria are not precisely defined by fuel type, droplet size distribution and equivalence ratio but a range of ignition delay times and ignition energies is found due to the probabilistic effect of droplet ignition. For polydisperse sprays it was found that ignition can be well correlated with an equivalent monodisperse spray by using a mean diameter based on the total surface area of the spray and not the Sauter-mean-diameter.

The experimental part of the program was designed to verify the theoretical spray ignition description and should help in understanding the physics and chemistry of the process. The experiment focused on the importance of transport mechanisms on individual fuel droplet ignition. An electrically heated flat plate was positioned in front of a vertical stream of decane droplets. The geometry and dynamic of the arrangement was photographed to obtain time and space resolved information. As expected from theoretical results, the ignition event depends on the temperature of the hot surface, the geometry of the arrangement, the properties of the fuel spray, the residence time of the droplet in the thermal boundary layer and the fuel vapor concentration of the carrier gas at room temperature. Comparisons of ignition delay times translated into ignition delay distances show discrepancy with predicted values. The lack of radiation heat transfer and the enhanced convective heat transfer of the experiment are most likely the reasons the mismatch between theory and experiment.

SUMMARY OF EFFORT

The program has concentrated on the ignition of combustible mixtures by hot surfaces. The early part of the program concentrated on single-phase gaseous systems while the later part of the program emphasized ignition of sprays. The effort has included both experiment and theory. Many research papers (1-3,7-13), seminars, conference presentations (4-6,14,15) and informal transfer of information has resulted from the successful effort.

The early experiments involved laser energy heating a metal sphere that, in turn, ignited a surrounding combustible mixture of air and hydrogen. Sometimes the metal itself ignited. Theory and experiment showed that ignition time delay increased as sphere radius decreased or as deposited laser energy decreased (1-6). The theory accounted for time-dependent behavior and predicted both the point in time when the temperature begins to “run away” and the establishment of a flame.

Later the ignition of sprays and the establishment of sprays was carefully studied and reported extensively (7-15). Both theory and experiment indicated that ignition delays decreased as source temperature decreased. The more interesting result was that normally, ignition delay decreased as droplet initial size decreased until a certain optimal size below which
ignition delay increased. Therefore, the minimum ignition delay off-stoichiometric mixture ratios did not occur at the zero diameter or premixed condition. The great importance of spacing between droplets and distance of droplets from the ignition source has been clearly demonstrated. The effect of the random variation of droplet spacing has been carefully analyzed.

References


RESEARCH OBJECTIVES

This research program was initiated to investigate the governing processes leading to the ignition of a fuel spray in air. In order to interpret and describe experimental ignition studies a theoretical model of increasing complexity was adopted. Theoretical and experimental efforts complemented each other. The theory provides guidance during the design and specification of the experimental facilities, and experiments supplied data to check the theory and identify weaknesses. The main objective of the program was to understand heterogeneous ignition and to derive from the model which developed during the progress of the program practical guidelines on how to ignite sprays or how to avoid fuel spray ignition. Work Statement

The following describes briefly the approach to come to a consistent conclusion of the research program. Two parallel sub-programs were conducted with strong interaction between the groups.

Theory Development and Numerical Modeling* (W.A. Sirignano, S.K. Aggarwal)

Experiment and Material Properties (H.T. Sommer)

Theory: One dimensional unsteady Eulerian-Lagrangian description. Spray simulated by described size distribution.
Heat transfer: Conduction, convection perpendicular to heat source.
Chemistry: single steps kinetics.
Droplet: describe size distribution, internal temperature field, mass and heat transfer.

The Spray Ignition Model was developed in three phases:

Phase 1: One dimensional unsteady heat transfer calculations, heated surface - droplet, conduction, convection, no mass transfer, no chemistry.
Phase 2: As mass transfer and chemistry, monodisperse spray simulation.
Phase 3: Polydisperse spray simulation.

*(left to be included: two-dimensional description, transverse natural convection, radiation heat transfer, relative droplet motion)
**Experiment:** Compare measurements with modeling results Phase 2 and 3. Two dimensional steady natural convection boundary layer flow (vertical flat plate) one dimensional unsteady a droplet connected system. Observation of heat source temperature, droplet velocity, size and distance to heat source, ignition location. (Ignition is characterized by optical radiation effect.)

The Experiment development went through 3 Phases:

- **Phase 1:** Design and specification of experimental apparatus (constraint: as close as possible resemble geometry and conditions of theory)
- **Phase 2:** Construction of experimental apparatus (provide flexibility for future geometry changes)
- **Phase 3:** Conduct experiments (the Ignition "delay distance" was investigated as function of heat source temperature, droplet size and distance of the droplet from the heat source.)

**STATUS OF THE RESEARCH**

**Overview**

A theoretical-experimental program has been initiated at Carnegie-Mellon University with emphasis on the ignition of combustible sprays. Although the principal investigator and an associate investigator have relocated recently, the program has continued as a cooperative effort. This program has involved the examination of a broad range of phenomena but this abstract will discuss primarily the recent progress on the study of a stream of droplets moving past a heated flat plate. The purpose of the program is to understand the mechanisms that are dominant, in various portions of the parameter range, in the ignition of hydrocarbon fuel sprays. The phenomenon is studied on the fine scale (smaller than the average spacing between droplets) and the random variation of some key parameters will be taken into account.

The starting point for the theoretical study is the set of equations for a chemically reacting flow in a unsteady compressible boundary layer. The source terms are due to the chemical reactions and the vaporization of droplets. Self similar solutions of the steady-state form of these equations are used as the initial conditions for calculating the vaporization and trajectories of droplets. A Howarth transformation is employed to reduce the steady-state compressible equations to the incompressible form. The result is the Blasius equation and the corresponding energy equation. The solution of the energy equation is easily found for a unity Prandtl number as a function of the solution of the Blasius equation.
The Blasius equation is solved by a fourth order Runge-Kutta scheme in conjunction with a shooting method. This yields $U, \Theta$, and $\rho$ (as given by)

$$U = U_0 f$$

$$\Theta = 1 - f = \frac{T - T_0}{T_p - T_0}$$

$$\rho = S_0 \frac{T_0}{T}$$

$T_0$ = Free stream Temperature

$T_p$ = Hot plate Temperature

Hyperbolic liquid-phase equations for a droplet (or a group of droplets) can be solved. Initial values are specified. The value of the Blasius coordinate is obtained giving droplet location. The gas-phase properties are then calculated at this location by an interpolation method. The droplet equations are solved by a second-order Runge-Kutta method. The droplet surface temperature is obtained by using a conduction-limit transient heating model. This yields new values of the droplet properties. At the new location, the gas-phase properties are calculated, which are then employed to advance the droplet properties. This procedure is repeated for a specified time period.

For the purpose of debugging the numerical code, the problem of droplet ignition in the thermal boundary of a hot plate has been solved. The ignition criterion is based on the critical Damkohler number. The ignition length (the axial length traversed by the droplet) is calculated as a function of plate temperature and the initial droplet location with respect to the plate. A few representative results are shown below:

Dynamics, vaporization and ignition of a single droplet in a boundary layer:

Effect of $Y_{in}$ (distance of droplet from plate) $T_p$ = 1500 K

<table>
<thead>
<tr>
<th>$Y_{in}$ cm</th>
<th>$X_{ign}$ (length to ignite) cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.03</td>
<td>0.340</td>
</tr>
<tr>
<td>0.05</td>
<td>0.581</td>
</tr>
<tr>
<td>0.08</td>
<td>0.489</td>
</tr>
<tr>
<td>0.10</td>
<td>0.618</td>
</tr>
<tr>
<td>0.115</td>
<td>0.793</td>
</tr>
<tr>
<td>0.12</td>
<td>does not ignite</td>
</tr>
</tbody>
</table>

Effect of $T_p$ (plate Temperature) $Y_{in}$ = 0.05 cm

<table>
<thead>
<tr>
<th>$T_p$ K</th>
<th>$X_{ign}$ (length to ignite) cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>falls to ignite</td>
</tr>
<tr>
<td>1300</td>
<td>0.53</td>
</tr>
<tr>
<td>1400</td>
<td>0.437</td>
</tr>
<tr>
<td>1500</td>
<td>0.381</td>
</tr>
<tr>
<td>1700</td>
<td>0.319</td>
</tr>
</tbody>
</table>

These results are preliminary and do not show that a minimum occurs in ignition delay as distance from the ignition source varies. In non-flowing spray calculations already published in the Proceedings of the Twentieth Symposium (International) on Combustion, it has been shown that in a certain parameter range, a minimum occurs in ignition delay as distance
from the ignition source varies. Also, a minimum can be found as initial size varies. Since the basic physics of the flowing and non-flowing systems are identical, we expect a minimum can occur in the flowing system as we extend the parameter survey.

Based on the theoretical considerations an experiment was designed to determine the dependency of fuel droplet ignition on each major system variable enhancing or reducing a particular physical effect. The droplet size was identified as one of the important variables of the process. The following experiments have been conducted to identify the influence of the above quantities on fuel ignition. An electrically heated flat plate was positioned in front of a single droplet stream of Toluene generated by TSI model 3450 vibrating orifice aerosol generator. The distance between the hot plate and the droplet stream was measured through a microscope. The droplet generator produces a single stream of droplets of uniform size when tuned appropriately. Droplet velocity and spacing of droplets were determined through double-flash photography. The following quantitative results were observed: the event of ignition is strongly affected by the temperature of the hot surface, the distance of the droplet to the wall, and the residence time of the droplet in front of the hot surface.

It was observed that with increasing wall temperature the ignition delay time (residence time in front of hot surface) was reduced. Due to enhanced radiative and conductive heat transfer evaporation of the fuel is stimulated and a vapor-air mixture of optimum ignition condition was reached earlier. For constant wall temperature, a minimal ignition time delay was observed for a specific distance from the hot surface. During this experiment the wall temperature was kept constant, the stream of 110 μm diameter droplets was brought closer to the surface, and the location of ignition relative to the leading edge of the hot surface was measured. It was observed that once a flame had developed after ignition of the first droplet, the point of ignition moved further down the droplet stream indicating that radiative and conductive heat transfer from the flame enhanced the ignition of approaching droplets. For very small droplets (below 30 μm diameter) a stable flame remained even after the hot surface was removed.

Currently, we can only compare the experimental and theoretical results on a qualitative basis. It is observed in experiments that ignition occurs earlier than the model predicts. The reason for this may be that the radiation heat transfer is not included in the model. A comparison of predicted decane ignition delay times and Toluene delay times calculated from experimental data indicates a qualitative agreement considering the difference in material properties.

THEORETICAL WORK

Ignition studies of combustible fuel-air mixtures are motivated by numerous engineering applications. Fire-safety of aircraft as reported by Campbell [9], explosions in mines, discussed by Blickensderfer et al. [8], and design of incendiary weapons, discussed by Manheim [11], and of ignition systems for internal combustion engines are some typical examples. There is also scientific relevance of such studies, since the underlying phenomena such as the droplet and spray processes, the oxidation mechanism, and fluid-mechanical and heat-transfer processes, are not well understood. While the ignition of gaseous fuel-air mixtures has been extensively studied, the literature on spray ignition is quite scant. The experimental works are due to Miyasaka and Mizutani [12,13] who used shock tube techniques to study the ignition of premixed spray column, to
Ballal and Lefebvre [6,7] who studied the spark ignition of homogeneous fuel-air mixtures, and to Chan and Polymeropoulos [10] who also used electric sparks for the ignition of laminar tetrel-air monodisperse spray. The only theoretical studies reported are by Ballal and Lefebvre [6,7] who used dimensional analysis to express ignition delay time and ignition energy as functions of various parameters, by Peters and Mellor [14] who also employed dimensional analysis, and by Aggarwal and Sirignano [2] who reported a numerical study on the ignition of monodisperse spray by a planar hot wall.

There are two major motivations for this study. First, it is important to consider the ignition of a polydisperse spray, since a monodisperse spray is a highly idealized situation which can be realized only in a laboratory by using some special experimental techniques. See, for example, the experimental study of Ashgrizzadeh and Yao [5]. The second is to examine if the ignition of a polydisperse spray can be simulated by an equivalent monodisperse spray represented by an appropriate mean diameter. Contrary to what has often been reported in the literature, the present results, discussed later, indicate that the Sauter mean diameter does not correlate the polydisperse sprays for predicting the ignition delays and ignition energies. Instead, the polydisperse results correlate to those of an equivalent monodisperse spray represented by a mean diameter based on the total spray surface area.

The physical model and the governing equations along with the boundary and initial conditions are discussed in Section 2. The numerical method to solve the two-phase equations is also described there. The results and the conclusions are presented in Sections 3 and 4, respectively.

The Physical Model

The physical model considered here is that of spray-air mixture contained in a tube. The mist of air and fuel droplets is quiescent initially. Since the computations are one dimensional (but unsteady), only the tube length is important; the tube cross-section is immaterial. The spray consists of polydisperse single-component fuel droplets. As is the case in any numerical computations, a discrete size distribution is considered. The left end of the tube is enclosed by an adiabatic surface. The present calculations are for the latter case.

The governing equations used to predict the gas-phase and liquid-phase properties, the droplet heating model, and the fuel-oxidation mechanism are described in the earlier papers of Aggarwal and Sirignano [2] and of Aggarwal et al. [4]. The boundary conditions and the initial conditions for the gas phase are the same as those in the study of Aggarwal and Sirignano [3]. The initial conditions for the liquid phase are described below. A hybrid Eulerian-Lagrangian method is used to solve the governing equations for the two phases. An Eulerian approach is employed to solve the gas-phase equations. The unsteady solution of the gas and liquid properties is continued until the ignition is detected. The state of ignition is defined by the zero heat-flux condition at the ignition source. The numerical procedure and the justification for using this procedure have been discussed by Aggarwal et al. [1], Sirignano [16], and Aggarwal and Sirignano [2].
Initial Conditions for Spray

The amount of liquid-fuel mass which is initially present can be expressed as

\[ m_f = \frac{0.21 E_r M_f \rho_c L (1 - Y_{fl})}{\Psi M_0} - Y_{fl} \rho_c L \]  

(1)

where \( E_r \) is the overall equivalence ratio based on the total liquid and vapor fuel initially present, \( \rho_c \) the initial gas density, \( L \) the tube length, \( \Psi \) the molar stoichiometric ratio of oxygen and fuel, \( Y_{fl} \) the initial fuel vapor mass fraction, and \( M_f \) and \( M_O \) the molecular weights of fuel and oxygen respectively. Note that the mass fraction of oxygen in air is assumed to be 0.21. For single-component fuel droplets, the total liquid-fuel mass can also be written as

\[ m_f = \sum_{k} m_k \]  

(2)

and

\[ m_k = \frac{4}{3} \pi L \rho_l n_k r_k^3 \]  

(3)

Here \( n \) is the number of droplets per unit area, \( r \) is the droplet radius, and \( d \) is the droplet spacing in the axial direction. \( k \) represents the number of droplet sizes used to represent the initial size distribution. For example, \( k = 1 \) for a monodisperse spray, whereas for a bidisperse distribution, \( k = 2 \). For a continuous size distribution such as Rosin-Rammler distribution [15], \( k \) will be infinite and the summation in Eq. (2) will be replaced by an integral. It should be emphasized, however, that in numerical computations, only a discrete and finite size distribution can be employed.

The initial gas-phase properties, the tube length and the initial fuel vapor mass fraction are specified first. Then, for given fuel type and overall equivalence ratio, Eq. (1) yields the total liquid-fuel mass. The liquid mass for any \( k \)th droplet-size group is obtained from

\[ m_k = \xi_k m_f \]  

(4)

where \( \xi_k \), which is the ratio of mass in \( k \)th size group to the total liquid-fuel mass, also needs to be specified initially. Then, for a given value of \( r_k \), \( n_k \) (or \( d_k \)) can be calculated if some relation is given between \( n_k \) and \( d_k \). For an isotropic droplet spacing, the square of \( d_k \) varies inversely with \( n_k \) since the inverse of the square root of \( n_k \) represents the droplet spacing in the transverse direction. This yields the values of \( n_k \) and \( d_k \) for each size group. To complete the specification of initial spray properties, we still need to provide, for each \( k \)th group, the location of the droplet nearest to the ignition source. For the monodisperse case, it was established by Aggarwal and Sirignano [2] that this is an important parameter and underscores the statistical character of spray ignition. The influence of this parameter for each \( k \)th group is discussed in the next section.
Fig. 1 Variation of ignition delay time with the location of nearest droplets in each size group for a bidisperse spray. Initial drop diameters $d_0 = 50$ and 100 microns with equal mass distribution, $E_r = 1.0$, decane, (a) location of smaller droplets varied, (b) location of larger droplets varied.

Results

For the results presented here, the computation domain, or the tube length is 2 cm, initial pressure and gas temperature are one atmosphere and 310K respectively, initial fuel vapor mass fraction is 0.001 everywhere in the tube, and hot wall temperature is 1500K. The spatial and temporal step sizes for numerical integrations are 0.02 cm and 5 microseconds, respectively. The step sizes have been taken in a range where step-size independence occurs within a reasonable approximation. Figure 1 gives the dependence of ignition delay time, normalized with the time-step size of numerical computations, upon the distance of the nearest droplet to the hot wall. The first set of results is for a bidisperse spray with initial droplet diameters of 50 and 100 microns. The liquid mass is equally distributed in the two sizes. The fuel is decane and the overall equivalence is unity. Note that for polydisperse spray, location of each drop-size group is an independent parameter. Thus, in a parametric study, location of one group is varied while keeping the location of others fixed. The results indicate that the ignition delay times have much stronger sensitivity to the location of smaller size-group droplets. Because of the faster vaporization rates due to the larger surface area, the smaller droplets participate more significantly in the ignition process. A minimum value in ignition delay and ignition energy (not shown) is found as the distance of smaller droplets is varied. The reaction rate maximizes at the optimum distance which can be expected since gas temperature and fuel vapor concentration decrease with increasing distance from the wall. If the droplets are too near the hot wall, then the gas mixture becomes locally fuel rich and the ignition delay increases. There is also some influence of the isothermal boundary condition at the hot wall. For example, if the droplets were at the wall, then the fuel vapor would be consumed without participating in the ignition process, since the heat release from the exothermic reaction would be lost due to the constant temperature condition there. Perhaps a more important observation from Figure 1 is that the spray ignition process has a statistical character. In practice the droplet locations are not precisely...
known; either the probability of having droplets at a given location or a range of locations can be specified. This means that for a given droplet size distribution, fuel type, and equivalence ratio, only a range of ignition delays or ignition energies can be predicted.

![Image](image_url)

**Fig. 2** Ignition delay time versus overall equivalence ratio for (A) bidisperse spray with mass equally distributed to 50 and 100 micron diameters, (B) monodisperse with $d_{20}$, (C) monodisperse with $d_{32}$, and (D) monodisperse with $d_0 = 50$ microns.

In Figure 2, the ignition time delays are plotted versus the overall equivalence ratios for decane fuel. Note that for the following results (Figures 2-8) the distance of the nearest droplets from the hot wall is 0.02 cm.

Four different cases are shown in Fig. 2. Curve A shows the results for a bidisperse spray 50 and 100 microns, with equal mass for each diameter. Curve B represents an equivalent monodisperse spray with droplet diameter equal to $d_{20}$ which is the diameter based on the total surface area of bidisperse spray, i.e., the total surface area of this monodisperse spray and the bidisperse spray are the same. Curve C represents a monodisperse spray with droplet diameter equal to the Sauter mean diameter ($d_{32}$), whereas curve D is for a monodisperse spray of diameter 50 microns. Definitions of $d_{20}$ and $d_{32}$ are given in Appendix A. It is clearly seen that the Sauter mean diameter (SMD) is incapable of predicting the ignition characteristics of a polydisperse spray. This not only yields different ignition delays at a given equivalence ratio but also different values of the optimum equivalence ratio. For example, the optimum equivalence ratios for the minimum ignition delay are, respectively 1.5 and 2.5 for the bidisperse spray and the equivalent monodisperse spray represented by SMD. (As a matter of fact, the monodisperse spray with initial drop diameter of 50 microns yields better predictions than that with SMD.) The bidisperse results can, however, be well correlated with an equivalent monodisperse spray by using $d_{20}$ which represents the effect
Fig. 3 Ignition delay time versus overall equivalence ratio for (A) bidisperse spray with initial diameters of 100 and 200 microns, each with equal mass, (B) monodisperse with $d_{20}$, (C) monodisperse with $d_{32}$, and (D) monodisperse with $d_0 = 100$ microns.

Fig. 4 Ignition delay time versus overall equivalence ratio for (1) polydisperse spray with three initial drop sizes with equal mass distribution, (2) monodisperse with $d_{20}$, and (3) monodisperse with SMD ($d_{32}$) of surface area which is important in spray ignition. This implicitly conforms with the results of Aggarwal and Sirignano (1985) where the spray surface area was found to be a key parameter. Since, for a fixed equivalence ratio, smaller droplets provide a larger surface area, they play a much more active role in the spray ignition process. The most important observation here is that by using a droplet diameter based on the total surface area of the spray, one can accurately correlate the ignition behavior of a polydisperse spray to an equivalent monodisperse spray. Any generalization of this statement requires that the above observation be
validated over a wide range of various gas-phase and liquid-phase and liquid-phase parameters. This is discussed next.

The difference in the results of Figure 3 and Figure 2 is that the initial droplet diameters are different. Again, the use of \( d_{20} \) rather than \( d_{32} \), can reasonably correlate the bidisperse ignition data. Results for a polydisperse spray with three initial droplet sizes are shown in Figure 4. Each size group has the same amount of liquid mass. The corresponding results for equivalent monodisperse spray with droplet diameters of \( d_{20} \) and \( d_{32} \) are also given in Figure 4. It is again clearly demonstrated that the surface area mean diameter provides a much better correlation to the polydisperse results than provided by the Sauter mean diameter. These conclusions remain unchanged when the liquid mass to various drop-size groups is non-uniformly distributed. For example, with uniform mass distribution (Figure 4) at unity overall equivalence ratio, \( d_{20} \) and \( d_{32} \) overpredict the ignition time delay by 15 and 4.8 percent, respectively. With non-uniform mass distribution (100, 150 and 200 micron size groups carrying 25, 50 and 25 percent liquid mass, respectively), the corresponding overpredictions are 10 and 1.7 percent. It is also worth mentioning that in addition to ignition-delay plots in Figures 1-4, we could have plotted ignition energies, but the conclusions would be the same.

![Figure 5](image)

**Fig 5** Ignition energy versus equivalence ratio for three cases. Curve (A), bidisperse spray with initial diameters of 100 and 200 microns, each with equal mass; curve (B), monodisperse spray with \( d_{20} \) and curve (C), monodisperse with \( d_{32} \) : decane.

One typical result is shown in Figure 5, where ignition energy \( Q \) in millijoules is plotted versus the overall equivalence ratio for a bidisperse and two corresponding monodisperse sprays with \( d_{20} \) and \( d_{32} \).

Figure 6 gives the variation of ignition delay time with the overall equivalence ratio for a bidisperse hexane spray with initial droplet diameters of 50 and 100 microns. The results for the corresponding monodisperse sprays with diameters \( d_{20} \) and \( d_{32} \) are also shown. The observations are essentially the same as for the decane fuel, i.e., the polydisperse spray ignition behavior can be reasonably simulated by an equivalent monodisperse spray if one uses the surface area mean diameter.
Fig. 6 Ignition delay time versus overall equivalence ratio for a bidisperse spray with initial droplet diameters of 50 and 100 microns, and two equivalent monodisperse sprays.

Figures 2 and 6 also indicate the existence of an optimum overall equivalence ratio where the ignition delay time minimizes. The occurrence of optimum equivalence ratio and its dependence upon initial drop size and fuel volatility for the monodisperse have been discussed by Aggarwal and Sirignano [2]. The general conclusion was that the occurrence of optimum overall equivalence is related to the maximization of the gas-phase reaction rate. As initial drop size is increased or as the fuel volatility is decreased larger overall equivalence ratios are required to provide the optimal gas-phase mixture for minimizing the ignition delay and ignition energy. The behavior of polydisperse sprays is expected to be the same but with one major difference. In addition to fuel volatility and initial drop sizes, the optimum equivalence ratio will also depend on the droplet size distribution.

The dependence of ignition delay times upon initial drop sizes of a polydisperse spray is examined next. For the fixed ratios of droplet diameters and for fixed distribution of liquid mass to various size groups, the ignition delay time can be plotted versus any one of the initial diameters. Here, the results are presented in terms of ignition delay time versus the diameter of the smaller-size group. For example, the diameter of the larger group in a bi-disperse spray calculation (displayed in Fig. 7 and 8) is taken as two times that of the smaller size group and the liquid mass is equally distributed into the two groups. Note that the Sauter mean diameter \(d_{32}\) and the surface-area mean diameter \(d_{20}\) will scale linearly with \(d_S\). Figures 7 and 8 give the ignition delays versus the diameter of the smaller size group for decane and hexane. The results are qualitatively similar to those for monodisperse sprays, discussed by Aggarwal and Sirignano [2]; for polydisperse sprays also, minimum values of ignition delay are found as initial droplet sizes vary at fixed overall equivalence ratio. Generally the minimum value occurs at larger droplet sizes as overall equivalence ratio increases or fuel volatility increases. The same droplet surface area effect as discussed by Aggarwal and Sirignano [3] is present for the polydisperse sprays. As overall equivalence ratio increases or as fuel volatility increases, larger initial drop sizes are required in order to provide the optimum gas-phase mixture for maximizing the gas-phase reaction rate and minimizing the ignition delay.
Fig. 7 Ignition delay time versus the smaller droplet diameter for a bidisperse spray at different overall equivalence ratios: decane.

Fig. 8 Ignition delay time versus the smaller droplet diameter for a bidisperse spray at different overall equivalence ratios: hexane.

and ignition energy. For polydisperse sprays, the values of optimum droplet sizes for given equivalence ratio and fuel volatility would, of course, depend upon the initial size distribution. The existence of optimum droplet sizes also means that the use of Sauter mean diameter would lead to overpredictions or underpredictions of ignition delays depending upon the overall equivalence ratio and the initial droplet sizes. In the range of initial droplet sizes, where ignition delay time increases with increase in $d_S$ (see Figures 7 and 8), $d_{32}$ would overpredict the ignition delays. For droplet sizes where $t_{ig}$ decreases when $d_S$ increases, $d_{32}$ would underpredict the ignition delays and ignition energies.

The effects of some other parameters such as ignition source temperature, cold mixture temperature, initial fuel vapor mass fraction, and droplet heating models have already been examined for a monodisperse spray by Aggarwal and Sirignano [2]. Since it is quite reasonable to expect the same qualitative behavior for polydisperse sprays, these types of calculations are not repeated in this paper.
Conclusions

Following the approach used by Aggarwal and Sirignano [2], ignition of a polydisperse spray has been studied. The ignition delay time and ignition energy have been obtained as functions of initial droplet sizes, size distribution, overall equivalence ratio and fuel volatility. The major conclusion here is that the ignition behavior of polydisperse spray cannot be simulated by an equivalence monodisperse spray of Sauter mean diameter. Depending upon the range of initial droplet sizes and overall equivalence ratios, this may overpredict or underpredict the ignition delays and the ignition energies. The polydisperse results can, however, be well correlated to an equivalent monodisperse spray of surface-mean diameters. Thus the total surface area of the polydisperse and the equivalent monodisperse sprays should be the same.

The critical dependence of ignition upon distance of the ignition source to the nearest smaller-size droplets indicates that the spray ignition has a statistical character. The results also indicate that for a given overall equivalence ratio, fuel volatility and size distribution, there are optimum initial drop sizes where the ignition delay and the ignition energy minimize. Similarly for given droplet sizes, fuel volatility and size distribution, the optimal overall equivalence ratios are also obtained. Similar results were also obtained by Aggarwal and Sirignano [2] for monodisperse sprays with one notable difference that the droplet size distribution now is an additional parameter.

EXPERIMENTAL WORK

The ignition process of liquid fuel consists of complex interacting transport mechanisms of 1) energy transported through conduction, convection, and radiation, 2) mass, transported through diffusion, phase change (evaporation, condensation) and convection, and 3) momentum effected by friction and external forces. In order to investigate the role of each individual transport mechanism and its contribution and importance to the ignition event, controlled experiments together with analytical studies are needed.

A survey of the literature reveals several articles describing the ignition of atomized liquid fuel. Recently the ignition process of bidisperse sprays was modeled and the importance of the mean droplet diameter based on the total surface area of the spray was identified as characteristic diameter. However, the model applied in their computation does not consider radiative energy transfer, thus relies only on conductive and convective transport of the ignition energy to the droplet. Previous work of Aggarwal and Sirignano [2] identified the probabilistic nature of heterogeneous combustible mixtures of monodisperse droplets.

Thus ignition criteria are not precisely determined by the fuel properties, droplet distribution and mixture composition, but also depend on the probabilistic event of a fuel droplet appearing at the right place at the right time under ignition conditions.

Law [17] developed the theory of thermal ignition and characterized the problem by seven non-dimensional parameters. In numerical studies of these parameters and comparison of theoretical results with experiments, Law comes to the conclusion, that two distinctively different thermal ignition characteristics exist. One regime is controlled by droplet heating and ignition occurs for smaller droplets earlier with little sensitivity to the ambient temperature. In the kinetically controlled regime ignition occurs earlier for larger droplets and is very sensitive to the ambient
temperature. Therefore, an ignition criteria based on an effective activation energy is not a meaningful concept to describe the ignition of heterogeneous mixtures.

Peters and Mellor [18] specified a characteristic time of the physical processes which occur during ignition. The ignition limit in their model is reached when the mixing rate of the spark kernel with its environment equals the fuel evaporation rate. An equation is presented which correlates the ignition data over a wide range of fuels, Sauter Mean Diameters, equivalence ratio and pressures. The authors come to the conclusion that in the case of slow kinetics and rapid evaporation chemical kinetics should be included in a heterogeneous ignition model.

The ignition of a single droplet stream injected in a hot gas environment was studied by Sangiovanni and Kesten [19]. Their primary interest focused on investigating the interaction of droplets during ignition of a stream of droplets at different size and spacing. The authors presented the dependency of drop size, gas temperature and fuel volatility as function of drop spacing and discovered an increase of ignition delay times as droplet spacing decreased approaching the limit of a cylindrical filament.

The experiments described by Sangiovanni and Kesten are similar to experiments reported here with the difference that the hot environment is provided by the natural convective boundary layer of a vertical heated flat plate.

The importance of atomization quality, characterized by the Sauter Mean Diameter, on the ignition of kerosene-air mixtures was investigated by Rao and Lefebere [20] and Ballal and Lefebere [21]. In [20] and [21] experiments are conducted to identify the dependency of ignition limits of practical fuels on global, external controllable parameters in a geometry comparable to a turbine combustion chamber.

**Experiment**

The experiment consists of a Berglund-Liu [22] monodisperse aerosol generator, a mechanical syringe pump which monitors the fuel volume flow, a temperature and fuel vapor controlled air supply system and the electrically heated vertical flat plate.

The temperature and fuel vapor concentration of the carrier air stream are maintained constant during experiments. This is accomplished by submerging parts of the air supply system in a constant temperature water bath (20 gal, Blue M Co.) Heating or cooling the air of the carrier stream before it enters the contact towers for fuel vapor mixing provides a means to control the vapor massfraction of the air in the test section. Since the vapor pressure of most hydrocarbon fuels is a sensitive temperature function, submerging parts of the air supply system in water provided the means of controlling this temperature within 0.2 °C. For the reported experiments a background fuel-vapor mass fraction of 0.001 was adjusted to match the conditions of the theoretical modeling.

The diagnostic methods used to investigate the ignition process were all of photographic nature. High speed cinematography (Hycam II) and still frame double flash photography is used to record the ignition event in space and time. The analysis of the photographic records provided the data for the graphs.

Figure 9 illustrates the geometry of the ignition experiment. The carrier air flow conditions were adjusted such that the classic vertical hot flat plate problem of Pohlhausen [23] was reproduced. It was assumed that the convective velocity of 0.50 m/s in the test section can be neglected over the temperature-induced natural convection. The ratio of Grashof number to
the square of the Reynolds number proves to be small. Figure 10 illustrates the similarity solution of [23] and compares this solution with data from Schmidt [24] and data of this work. The measurements were obtained with a micro thermocouple [10μm] which was radiation, conduction and convection corrected.

![Diagram](image)

**Fig.: 9** Geometry of Experiment

**Fig.: 10** Theory and Experiment: Natural Convection of Heated, Vertical Flat Plate Dimensionless Temperature Profile
The good agreement of the temperature measurements justified the use of the similarity solution to describe the thermal and natural convection boundary layers. This solution was used to convert the ignition time-delay information from the theoretical part, into ignition delay lengths using calculated and measured droplet velocities and the velocity and temperature of the surrounding air from the similarity solution.

**Experimental Procedures and Results**

Series of experiments were conducted to investigate the dependency of single droplet stream ignition on the distance from the heat source \( Y \), the heat source temperature \( T_w \), and the droplet diameter \( d \). Decane was used as a test fuel for the experiments presented here. All experiments were conducted in air at room temperature (300K) and atmosphere pressure with an initial decane vapor mass fraction of 0.001.

Together with the liquid decane the overall equivalence ratio of the decane-air mixture in the test section was approximately one with fluctuations of less than 4%. The overall air-fuel mixture composition was obtained measuring the volume flow of the liquid decane at the feed pump to the droplet generator and sampling the air-decane vapor mixture. The samples were analyzed by gas chromatography. The overall equivalence ratio was controlled by drop size and spacing.

The heat source temperature was monitored by five Pt-10%Rh Pt micro thermocouples distributed over the plate. An average plate temperature was obtained from the thermocouple readings and was used as characteristic heat source temperature. During each experiment this averaged flat plate temperature was kept constant by a computer-controlled feedback to the voltage controller regulating the resistive heating of the plate.

**Minimum Surface Temperature for Ignition**

Figure 11 shows the minimum plate temperature \( T_w \) at which ignition occurred when the droplets pass the hot surface at distance \( Y \). Drop sizes in the range 30 \( \mu \)m - 150 \( \mu \)m were investigated. The two curves for 54 \( \mu \)m and 104 \( \mu \)m are representative for these experiments. It was observed that there exists a distance \( Y \) at which the temperature necessary to ignite the droplet stream becomes a minimum. This distance decreased with decreasing drop diameters. Ignition always occurred near the upper end of the plate and sometimes in the buoyant thermal wake of the heat source. Large droplets tend to ignite later (or higher up in the wake) than small droplets. This indicates that the ignition event is evaporation and diffusion controlled and occurs when a preferred mixture composition has developed to establish self-supporting combustion.

These minimum plate temperatures for ignition were obtained by positioning the droplet stream in front of the heat source and increasing the temperature of the surface until ignition occurred. During this procedure, it was observed that the electric power requirement necessary to raise the temperature a specific interval from one value to another value was increasing with decreasing drop size at fixed distance \( Y \). Heat transfer from the plate to the droplets and the higher evaporation rate of smaller droplets at narrower spacing explain this observation.
Fig. 11 Minimum Surface Temperature $T_w$ at which ignition occurred as a function of the distance $Y$ from the Hot Plate

Fig. 12 Ignition Location $X$ as a function of the distance from the Surface at Constant Surface Temperature $T_w$ and four Droplet Diameters $d$
Ignition did not occur for 104 μm droplets when positioned closer than 0.05 mm to the hot surface. 53 μm droplets stopped to ignite at positions closer than 0.03 mm. Very close to the hot surface evaporation occurs at a very high rate such that a fuel vapor cloud around each droplet develops which is of the dimension of the heat source. Diffusion and mixing of air with this vapor occurs in regions of lower temperatures which do not trigger the ignition event. The minimum plate temperature, at which ignition occurred, supplies the heat to a location in the thermal boundary layer at which temperature and composition permit ignition.

Location of Ignition

Ignition was observed at a definite distance X from the leading edge of the flat plate for a stream of droplets, if the surface temperature $T_w$ is higher than the minimum ignition temperature for a specific distance Y from the hot plate. Figure 12 illustrates the dependency of the ignition length X from the distance Y from the flat plate. A minimum length is observed for all drop sizes. This minimum moves away from the heat source with decreasing drop size, as mentioned earlier. Ignition conditions are determined by the heat transfer to the droplets evaporating the liquid decane, the local vapor mass fraction at the ignition location and the temperature of the mixture at this location. These conditions strongly depend on the history of the droplet travelling through the buoyant thermal boundary layer. In order to compare the data obtained in this experiment with the numerical predictions the following assumptions were made: A fuel droplet moving along a vertical heated flat plate experiences a similar temperature and heat transfer history as if it were positioned in front of a surface which temperature suddenly changes. The ignition delay time can be translated into a ignition distance X, providing the droplet velocity is known. The ignition delay time as function of the distance from the heat source was converted into a ignition delay distance.

The equation of motion of a sphere in a laminar viscous medium was solved for a known initial velocity at the droplet generator outlet. The predicted velocity history of a 52.5 μm droplet is in agreement with the photographical data for 53 μm drops. The curve labeled “Theory” of Fig.12 represents transformed ignition delay time predictions of Aggrawal and Sirignano. The experimental data indicate faster ignition than predicted. There are two possible explanations:

a) Due to the motion of the droplet through the thermal boundary layer of the hot plate the heat transfer is enhanced and ignition occurs earlier than predicted with theoretical data for which this effect was not present in the numerical simulation.

b) Since the theoretical model neglected the effect of radiation ignition delay time predictions should result in larger values. Radiation in the infrared part of the spectrum is strongly absorbed by hydrocarbon fuels. The radiation heat transfer mechanism should have a direct effect on the evaporation of the droplet since the droplet surface temperature is directly affected. The heat source of the numerical prediction was 1500 K hot and the droplet ignited at 13mm from the leading edge of the flat plate. A comparable droplet (53 μm) ignited at 7 mm from the leading edge of the plate at a plate temperature of 1100K.

The lack of radiation in the model might be the explanation for this discrepancy.
Fig. 13 Location of Ignition X as Function of Drop Diameter at three Distances Y from the Hot Plate and at Constant Surface Temperature \( T_w \)

**Droplet Size and Ignition Delay**

In Fig. 13 the ignition location of several drop sizes is plotted. The surface temperature is maintained constant at 1150K and experimental data for three distances Y from the flat plate are presented. The agreement seems to be reasonably good for small droplets, however, the predictions have been conducted at 1500K surface temperature. Ignition seems to occur faster than the theory predicts. The discrepancy becomes more obvious for larger droplets, but increasing ignition delay time or distance is also experimentally observed for increasing droplet diameters. The lack of radiation heat transfer and the missing convective heat transfer due to the presence of a buoyant thermal boundary layer in the experiment can explain the disagreement between theory and experimental data.

**Conclusion**

The existence of a minimum ignition delay time or distance as predicted by our theory was experimentally verified. However, the measured values are lower than predicted by the theory. It is speculated that the missing energy transport by radiation and an increased heat flux due to the presence of a thermal free convective boundary layer is responsible for the discrepancies between theory and experiment.
REFERENCES


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LIST OF PUBLICATIONS FROM THIS PROJECT


LIST OF PROFESSIONALS ASSOCIATED WITH THIS PROJECT

W.A. Sigrignano, Dean, University of California Irvine, School of Engineering, Co-principal Investigator

H.T. Sommer, Associate Professor of Mechanical Engineering
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Carl Thalner, Graduate Student, received Master of Engineering 1983

Carol Steen, Research Assistant
Roger Bishop, Graduate Student, received Master of Engineering, 1985
LIST OF PUBLIC LECTURES AND INTERACTION WITH OTHER RESEARCHERS


APPENDIX

Let \( f(r) \) be the size distribution function such that \( f(r)dr \) represents the number of droplets per unit volume in the droplet size range \( r \) to \( r+dr \). The \( i \)th moment of \( r \) can be defined as

\[
[r_{n-m}^m] = \frac{\int_0^\infty f(r)r^{n-m}dr}{\int_0^\infty f(r)r^ndr}
\]  

\[ (A1) \]

\( n=2 \) and \( m=1 \) define the Sauter mean radius,

\[
r_{32} = \frac{\int_0^\infty f(r)r^2dr}{\int_0^\infty f(r)r^2dr}
\]

\[ (A2) \]

whereas \( n=0, m=2 \) give the mean radius, based on the mean surface area of the spray, as

\[
r_{20} = \frac{\int_0^\infty f(r)r^2dr}{\int_0^\infty f(r)dr}
\]

\[ (A3) \]

Since a discrete size distribution is used in this paper, the integrals in Eqs. (A1)-(A3) will be replaced by summations. For example, for bidisperse spray, \( f(r) \) will be non-zero only at two drop sizes which are specified. Note that \( d_{20} \) and \( d_{32} \) used in Section 3 are two times \( r_{20} \) and \( r_{32} \), respectively.
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