

Ignition of Polydisperse Sprays: Importance of D_{20}

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Abstract—Ignition of a polydisperse single-component fuel spray is studied. The physical model consists of a mist of air and fuel droplets contained in a tube. The left end of the tube acts as the ignition source. The polydisperse character of the spray is represented by discrete and finite size distribution. Other notable features of the two-phase ignition model are that the temperature in the droplet interior is resolved spatially as well as temporally, that the inter-phase slip is considered, that a one-step reaction scheme with non-unity exponents of fuel and oxygen concentrations is employed, and that the interesting physical phenomenon is resolved on the scale of the spacing between droplets. An Eulerian-Lagrangian hybrid scheme is used to solve the two-phase equations. The one-dimensional unsteady equations are integrated to obtain the ignition time delays and ignition energies. Influence of initial droplet size, size distribution, overall equivalence ratio, fuel type, and the locations of the nearest droplets to the ignition source is examined. The results clearly demonstrate that the Sauter mean diameter is not capable of representing the ignition characteristics of a polydisperse spray. The polydisperse spray ignition can, however, be well correlated to an equivalent monodisperse spray by using a mean diameter based on the total surface area of the spray. This observation is confirmed over a range of fuel volatility, initial droplet sizes, size distribution, and overall equivalence ratios. For a given size distribution, fuel volatility and overall equivalence ratios, the values of initial droplet sizes for the minimum ignition delays are also obtained. The results also indicate a strong dependence of ignition delays upon the location of the nearest droplets to the ignition source, which underscores the statistical character of the spray ignition process.

1 INTRODUCTION

Ignition studies of combustible fuel-air mixtures are motivated by numerous engineering applications. Fire-safety of aircraft as reported by Campbell (1957), explosions in mines, discussed by Blickensderfer *et al.* (1972), and design of incendiary weapons, discussed by Manheim (1973), 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 (1975, 1976) who used shock tube techniques to study the ignition of a premixed spray column, to Ballal and Lefebvre (1978, 1981) who

to Chan and Polymeropoulos (1981) who also used electric sparks for the ignition of laminar tetrelin-air monodisperse spray. The only theoretical studies reported are by Ballal and Lefebvre (1978, 1981) who used dimensional analysis to express ignition delay time and ignition energy as functions of various parameters, by Peters and Mellor (1980) who also employed dimensional analysis, and by Aggarwal and Sirignano (1985a) who reported a numerical study on the ignition of monodisperse spray by a planar hot wall. In the present paper, the ignition of a polydisperse spray is studied. The physical model and the numerical method are the same as used by Aggarwal and Sirignano (1985b). The major difference is that a polydisperse spray is considered in this paper.

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 (1983). 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.

2 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 and acts as the isothermal ignition source for the mixture. The right end can be either open or 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 (1985) and of Aggarwal *et al.* (1984). The boundary conditions and the initial conditions for the gas phase are the same as those in the study of Aggarwal and Sirignano (1985). The initial conditions for the liquid phase are described in subsection 2a. 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, whereas a Lagrangian approach is followed to integrate the liquid-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.* (1983), Sirignano (1984), and Aggarwal and Sirignano (1985a).

2a Initial Conditions for Spray

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

$$m_f = \frac{0.21 E_r M_f \rho_c L (1 - Y_{fi})}{\psi M_0} - Y_{fi} \rho_c L, \quad (1)$$

where E_r is the overall equivalence ratio based on the total liquid and vapor fuel initially present, ρ_c the initial gas density, L the tube length, ψ the molar stoichiometric ratio of oxygen and fuel, Y_{fi} the initial fuel vapor mass fraction, and M_f and M_0 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

$$m_f = \sum_{k=1}^K m_k \quad (2)$$

and

$$m_k = \frac{4}{3} \pi L \rho_l n_k r_k^3 / d_k. \quad (3)$$

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 (1933), K will be infinite and the summation

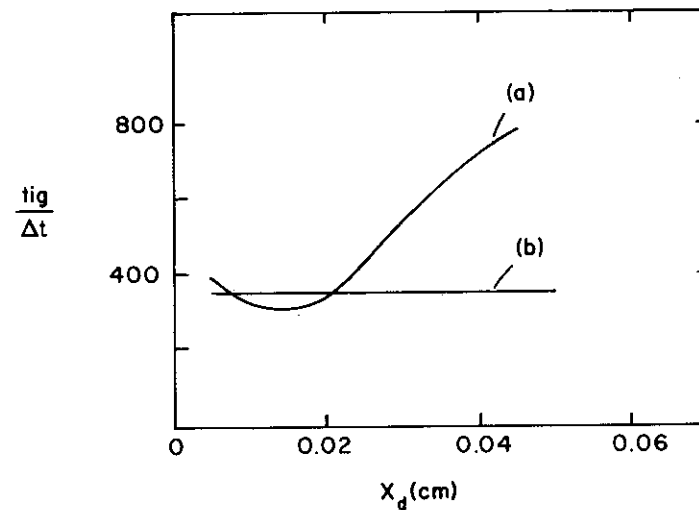


FIGURE 1 Variation of ignition delay time with the location of nearest droplets in each size group for a bidisperse spray. Initial drop diameters $d_0=50$ and 100 microns with equal mass distribution, $E_r=1.0$, decane, (a) location of smaller droplets varied, (b) location of larger droplets varied.

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

$$m_k = \epsilon_k m_f, \quad (4)$$

where ϵ_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 (1985a) 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.

3 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 310 K respectively, initial fuel vapor mass fraction is 0.001 everywhere in the tube, and hot wall temperature is 1500 K. 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 will be consumed without participating in the ignition process, since the heat release from the exothermic reaction is 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.

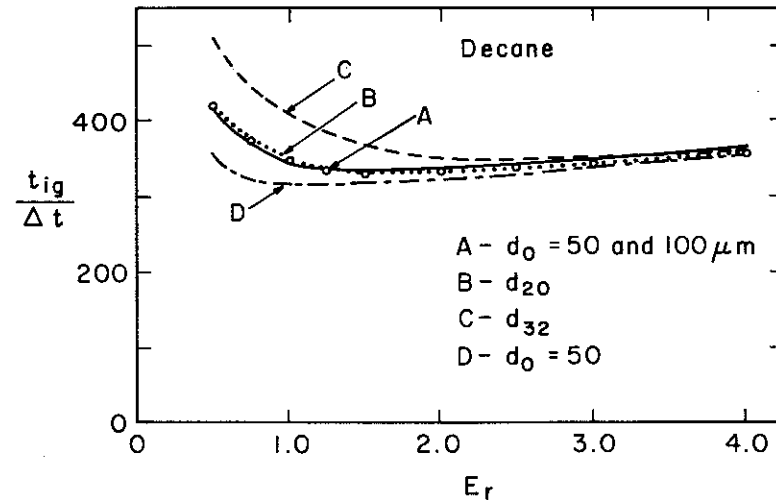


FIGURE 2 Ignition delay time versus overall equivalence ratio for (A) bidisperse spray with mass equally distributed to 50 and 100 micron diameters, (B) monodisperse with d_{20} , (C) monodisperse with d_{32} , and (D) monodisperse with $d_0 = 50$ microns.

In Figure 2, the ignition time delays are plotted versus the overall equivalence ratios for decane fuel.† Four different cases are shown. Curve A is for a bidisperse spray with initial diameters of 50 and 100 microns and 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 bidispersed 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

†Note that in the following results (Figures 2-8) the distance of the nearest droplets from the hot wall is 0.02 cm.

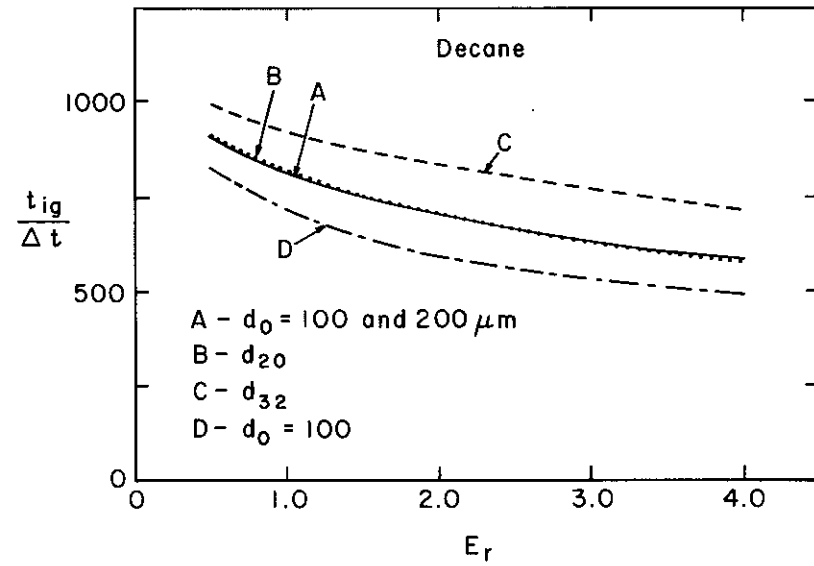


FIGURE 3 Ignition delay time versus overall equivalence ratio for (A) bidisperse spray with initial diameters of 100 and 200 microns, each with equal mass, (B) monodisperse with d_{20} , (C) monodisperse with d_{32} , and (D) monodisperse with $d_0 = 100$ microns.

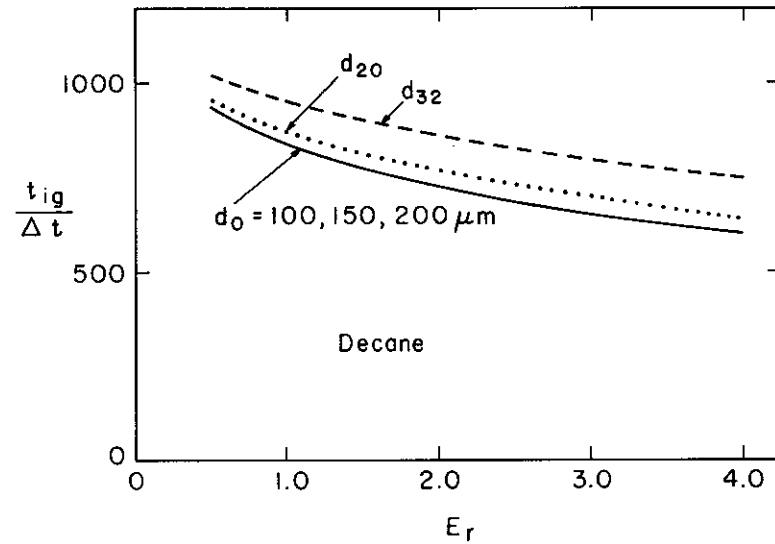


FIGURE 4 Ignition delay time versus overall equivalence ratio for (1) polydisperse spray with three initial drop sizes with equal mass distribution, (2) monodisperse with d_{20} , and (3) mono-

represents the effect 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, of course, requires that the above observation be validated over a wide range of various gas-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_{32} and d_{20} overpredict the ignition time delay by 15 and 4.8 percent, respectively. With non-uniform mass distribution (100, 150 and 200 micron size

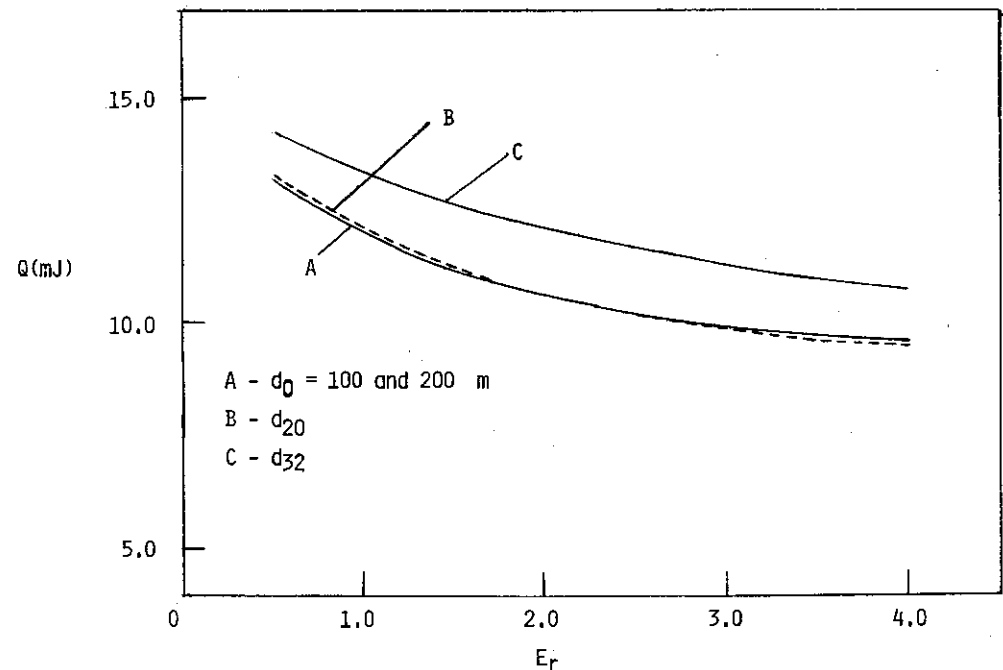


FIGURE 5 Ignition energy versus equivalence ratio for three cases. Curve (A), bidisperse spray with initial diameters of 100 and 200 microns, each with equal mass; curve (B), monodisperse spray with d_{20} ; and curve (C), monodisperse with d_{32} ; decane.

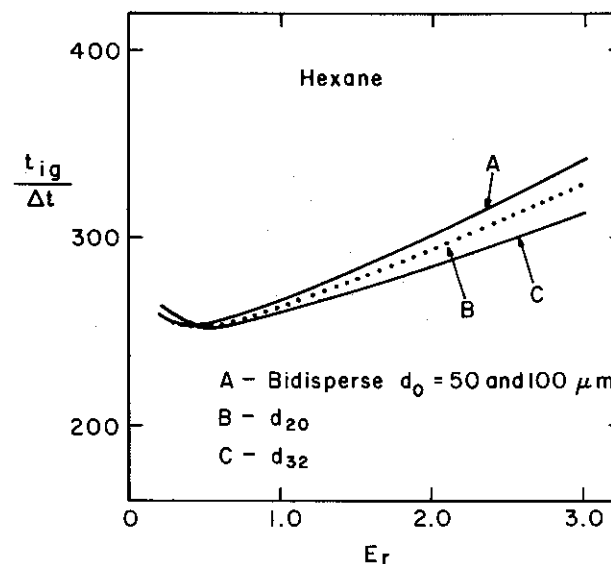


FIGURE 6 Ignition delay time versus overall equivalence ratio for a bidisperse spray with initial droplet diameters of 50 and 100 microns, and two equivalent monodisperse sprays.

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. 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.

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 (1985). The general conclusion there 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

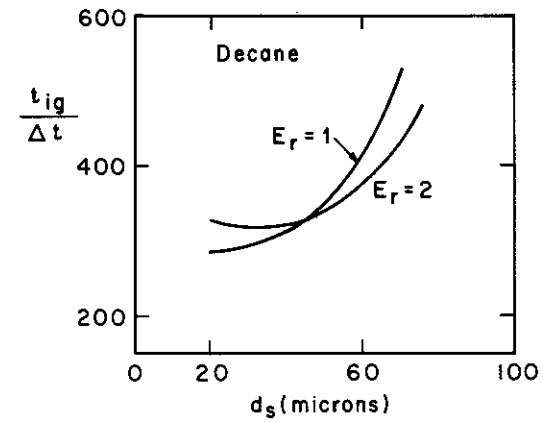


FIGURE 7 Ignition delay time versus the smaller droplet diameter for a bidisperse spray at different overall equivalence ratios: decane.

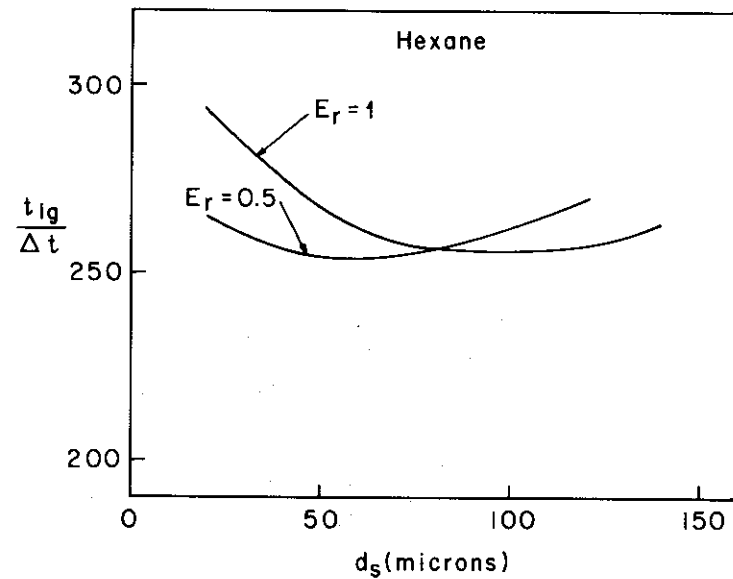


FIGURE 8 Ignition delay time versus the smaller droplet diameter for a bidisperse spray at different overall equivalence ratios: hexane.

versus any one of initial diameters. Here, the results are presented in terms of ignition delay time versus the diameter of the smaller-size droplets (d_s) for a bidisperse spray. The diameter of the larger size spray 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 (1985a); 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 (1985a) 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 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 (1985a). Since it is quite reasonable to expect the same qualitative behavior for polydisperse sprays, these types of calculations are not repeated in this paper.

4 CONCLUSIONS

Following the approach used by Aggarwal and Sirignano (1985a), 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 equivalent 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 diameter. 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 (1985a) for monodisperse sprays with one notable difference that the droplet size distribution now is an additional parameter.

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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 l th moment of r can be defined as

$$[r_{n+l,n}]^l = \frac{\int_0^{\infty} f(r) r^{n+l} dr}{\int_0^{\infty} f(r) r^n dr}, \quad (A1)$$

$n=2$ and $l=1$ define the Sauter mean radius,

$$r_{32} = \frac{\int_0^{\infty} f(r) r^3 dr}{\int_0^{\infty} f(r) r^2 dr}, \quad (\text{A2})$$

whereas $n=0$, $l=2$ give the mean radius, based on the mean surface area of the spray, as

$$r_{20} = \frac{\int_0^{\infty} f(r) r^2 dr}{\int_0^{\infty} f(r) dr}. \quad (\text{A3})$$

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.