Polydisperse spray flame ignition by a pulsed heat flux

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Abstract
A mathematical analysis of the ignition of a polydisperse spray/air mixture by an infinite surface heated in a pulsed manner is presented. In contrast to previous work in the literature, the entire history of the ignition process is accounted for starting from the flame-embryo progenitor stage, through the thermal runaway stage to the final flame propagation stage. For tractability at the current stage, the chemical kinetics is taken to be that of a single global reaction. The spray is modeled using the sectional approach and the influence of fuel spray characteristics on ignition is determined. Good agreement was found between the theoretical predictions and full numerical simulations. Delay in ignition due to the build-up of vapor from the fuel droplets as well as heat loss to the droplets for evaporation are found to play a significant role under certain operating conditions. Comparison between the critical energy flux and the initial spray polydispersity revealed small differences for larger values of the pulse duration but more significant minor differences for smaller pulse durations. Despite these seemingly minor differences, it was shown that the initial spray polydispersity can have a critical influence on whether flame ignition will occur or fail, even for sprays having the same initial SMD.

Keywords
Ignition process, forced ignition, spray combustion, mathematical modeling, polydisperse spray

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I. Introduction
As of now – and for the near future - the world’s increasing energy demands can only be satisfied by the combustion of hydrocarbon fuels. Concerns about efficiency, global warming and the environment continue to motivate much of the research efforts in the area of combustion theory. It is a well-established fact that modern combustors in aircraft need to satisfy a large number of requirements. In particular, under extreme conditions they must reignite without any problems and without any external help following flame extinction. The possibility of extinction also exists in cold and wet conditions (e.g. in a hailstorm) as well as at high altitudes due to oxygen starvation.

Since spark ignition systems are installed in many combustors, it is important to be aware of the amount of spark energy required for successful ignition over a range of operating conditions. In addition, the desire to prevent unwanted explosions in transportation and storage of combustibles motivates exploring the mechanisms at play during the process of ignition. The presence of liquid fuel in the form of a multi-sized spray of droplets that must be ignited only serves to increase the difficulty of ignition. Additional interest stems from the need to determine the effect of fuel property changes, associated with alternative fuels, on ignition characteristics. Fundamental understanding and quantification of ignition energy requirements for fuel sprays are essential for the effective design of injectors and igniters.

Although practical modes of coping with ignition under both normal and extreme conditions are technologically available, the problem is far from being completely understood. Mathematical analyses of the

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The ignition process is generally classified according to two possibilities: (a) auto-ignition caused by chain branching or thermal feedback in homogeneous/heterogeneous mixtures without exposure to an external heat source, or (b) forced ignition which involves an external source of energy, e.g., an electrical spark, a heated surface, a shock wave, a pilot flame, etc. In this work, the focus will be on forced ignition exclusively as it is the most common and popular way of igniting fuel-oxidant mixtures. Although the theory of ignition and thermal explosions of combustible mixtures is one of the fundamental topics in the field of combustion (see, for example, literature and references therein), the theory of forced spray ignition has received hardly any attention.

Experimental research on spray ignition from an external source in both quiescent and flowing mixtures dates back to Lefebvre and co-researchers. The analysis of the experimental data, along with plausible physical arguments, were used to derive rule-of-thumb formulae for calculating the minimum ignition energy and ignition delay time and their dependence on the spray’s characteristics, such as fuel properties, droplet size or Sauter Mean Diameter (SMD) and equivalence ratio. According to these arguments, the ignition event was envisaged in terms of the formation of a so-called ignition kernel (into which energy has been deposited), consisting of a local region of high chemical reactivity and heat release, which is supposed to be the precursor for the establishment of a propagating flame. If the heat loss to the surroundings from the kernel by conduction is less than the heat generated in the kernel, a flame may be established. Otherwise, the initial high temperature in the kernel falls and its size shrinks below the minimum critical size or quenching diameter, leading to extinction. The early work was based on the assumption that successful ignition occurs if the initial energy deposition produces an adequate amount of fuel vapor in the ignition zone and thus ignition is limited by the rate of fuel evaporation. Unlike ignition in homogeneous mixtures, which is dominated by chemical kinetics, the basic argument here was that the chemical reaction time is much shorter than the evaporation time, and thus can be neglected. Similar arguments led Peters and Mellor to arrive at a modified formula for the ignition delay time. A later study extended these phenomenological models to include the effects of finite chemical reaction rates. The underlying assumption in all these works was that the early stages of conception had now occurred, so that an embryonic flame kernel already exists.

Additional effects of spray ignition were investigated experimentally by Danis and Cernansky and co-workers. In these studies, ignition energy data were provided for monodisperse sprays over a range of droplet size and volatility, and equivalence ratios more typical of those found in practical combustors. Compared to homogeneous gaseous mixture ignition, ignition of a spray is significantly more complex as the state of ignition in the latter case may be defined by three distinct ignition modes namely, droplet ignition, droplet cluster ignition, and spray ignition.

Ignition of an individual droplet represents the appearance of a flame surrounding the droplet or in the wake region, with a dimension on the order of the droplet diameter. The cluster or group ignition refers to the ignition around or inside a droplet cloud, while spray ignition implies the appearance of a global flame with a characteristic dimension a few orders of magnitude larger than a droplet. In all these modes, the evaporation of fuel droplets, formation of a combustible gaseous fuel-air mixture, and initiation of chemical reactions producing sufficient radical species precede ignition. Here the focus will be on the third mode of ignition - spray ignition.

In spray-air mixtures, there are additional factors that play a crucial role on ignition; these include droplet heating and vaporization, which in turn depend on droplet size and volatility, and the duration of the energy deposition event, which should be long enough to allow for sufficient fuel vapor build-up. We note that the spray of fuel droplets ostensibly performs a double role. On the one hand, droplet evaporation produces the vapor that will fuel any subsequent combustion. On the other hand, the droplets absorb heat in order to enable evaporation to occur. This dual exothermic/endothermic competitive function lies at the very heart of many spray related combustion phenomena such as laminar spray flame propagation and cellularization.

Aggarwal gave a thorough review of research performed on laminar spray ignition prior to 1998. Turbulent spray ignition is one of the topics of a general review of turbulent combustion ignition by Mastorakos, from experimental and numerical perspectives. More recently, Mastorakos gave an appraisal of research on forced ignition of turbulent spray flames. In addition, the PhD thesis of de Oliveira characterizes statistically details of the part played by uniformly dispersed droplets in the ignition process of a spray flame in well-controlled experiments, and suggests an improved low order ignition model containing a stochastic model based on data from the experimental measurements (see also).
A comprehensive review of previous numerical studies on spray ignition phenomena is given in Aggarwals’ review. Neophytou gave a literature review on ignition and flame propagation in sprays and conducted direct numerical simulations of combustion in laminar and turbulent sprays.

Various researchers performed full three-dimensional DNS (Direct Numerical Simulation) studies of turbulent mono-size spray flame spark ignition (see, for example, literature). These sort of studies enable investigation in detail, over quite a broad spectrum of scales, of various phenomena in turbulent spray combustion such as ignition, flame structure and flow topologies in different regimes etc. However, despite providing much valuable information on the complex interactions in spray ignition/combustion, DNS studies are computationally intensive and, as such, have limitations.

In contrast to the growing abundance of experimental and numerical treatments of spray ignition in the literature, theoretical treatments of ignition considering a two-phase gas-liquid mixture are rather sparse. Some attempts were made in this direction using the method of integral manifolds but they were restricted by considering only an infinite spatially homogeneous case, so that forced ignition was not really accounted for correctly. In spite of this limitation, incorporating this type of methodology locally in detailed modelling of monodisperse and polydisperse spray ignition in diesel engines using a CFD code with the Shell auto-ignition model yielded good agreement with experimental data for a diesel engine.

In a theoretical model of the ignition and propagation of a premixed spherical spray flame, a pre-existing initial flame kernel was assumed. However, the theory makes use of a quasi-steady state model so that the actual evolutionary ignition process is not captured. Although the predictions are insightful, the scope of the model is narrow.

In contrast, unsteady governing equations were solved in the literature to examine the ignition of a polydisperse fuel spray-air mixture in the half-plane, subject to an initial thermal field. The analysis considers fuel build-up due to droplet evaporation but only seeks conditions of thermal runaway, which define when the temperature rises abruptly. Analysis of consequent creation of a propagating flame or a failed extinction event was not pursued. Thus, the complete ignition history from beginning to end was not described.

In view of the dearth of basic theoretical models of forced spray ignition covering the entire life span of the spray flame from its conception through ignition to propagation, the present work attempts to fill this gap. We revisit the problem of laminar spray flame ignition by a heated slab within the framework of a one-dimensional model. A thorough, novel mathematical analysis is required to disentangle the dominant and secondary mechanisms at work when a polydisperse spray of fuel droplets is present in the initial mixture to be ignited by an external heat source. Predictions of the analysis enable evaluation of various effects on the dynamics of the ignition process, such as those relating to the initial mixture composition, droplet size, spray pulse duration, fuel build-up and other spray-related parameters.

2. Mathematical model

We consider a specific configuration that will enable us to investigate the role of a polydisperse fuel spray presence on the ignition process. A planar configuration (Figure 1) is adopted, where a fuel spray-air mixture of temperature $T_0$ exists in the positive half-plane.

At time $t = 0$ the left hand half-plane, $x < 0$, is suddenly exposed to a constant heat energy flux $P$ which is applied for a specified period of time and which brings about the evaporation of small droplets and the build-up of fuel-vapor in a layer adjacent to the boundary $x = 0$. If the temperature remains sufficiently high despite the heat removed by the endothermic vaporization process, an intense chemical reaction starts in this zone. The following sequence of events is envisaged. During an induction phase, an increase in temperature occurs near the boundary, ending up with thermal runaway with which ignition is usually associated. The induction phase is characterized by negligible chemical activity. Once chemical reaction is significantly triggered, thermal runaway occurs. Subsequently, a laminar one-dimensional flame is formed which will eventually propagate into the fresh mixture at a constant speed, or become unstable in some sense (perhaps through cellularization or oscillation) or extinguish if volumetric and liquid fuel heat losses cannot be overcome by the exothermic chemistry. At the current stage, we assume a global, irreversible, one step reaction, described by Arrhenius’s law, can be employed: fuel + oxidant $\rightarrow$ products + heat.

![Figure 1. Ignition of a combustible fuel spray-oxidant mixture by a heated surface.](image-url)
The governing equations for the above configuration are:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0
\]  

(1)

\[
\rho c_p \frac{\partial T}{\partial t} + \rho u \frac{\partial T}{\partial x} = \lambda \frac{\partial^2 T}{\partial x^2} + q_\omega - \ddot{\omega}(T - T_0) - LS_t
\]  

(2)

\[
\rho \left( \frac{\partial Y_O}{\partial t} + u \frac{\partial Y_O}{\partial x} \right) = \rho D_O \frac{\partial^2 Y_O}{\partial x^2} - \omega
\]  

(3)

\[
\rho \left( \frac{\partial Y_F}{\partial t} + u \frac{\partial Y_F}{\partial x} \right) = \rho D_F \frac{\partial^2 Y_F}{\partial x^2} - \omega + S_v
\]  

(4)

\[
\rho \left( \frac{\partial Y_{d_j}}{\partial t} + u_d \frac{\partial Y_{d_j}}{\partial x} \right) = -S_{r_{i,j}}, \quad j = 1, 2, 3, \ldots, N_S
\]  

(5)

\[ S_{r_j} = \rho (\Delta_j Y_{d_j} - \Psi_j Y_{d_{j+1}}) H(T(x^*, t^*) - T_v), \quad j = 1, 2, 3 \ldots N_s \]  

(6a)

\[ S_v = \sum_{j=1}^{N_s} S_{r_{i,j}} \]  

(6b)

\[ (\Delta_j, \Psi_j) = 1.5 \tilde{E}_v \left( \frac{3d_{a,j} - 2d_{i,j}}{d_{a,j}^2 - d_{i,j}^2} \cdot \frac{d_{i,j}}{d_{a,j+1} - d_{i,j+1}} \right) \]  

(6c)

\[ \omega = \rho A Y_O Y_T \exp \left( - \frac{E}{RT} \right) \]  

(7)

Equation (1) is the continuity equation for the mixture. Its form follows from the implicit assumption that the liquid fuel volume fraction is sufficiently small. Therefore, the transport properties will be supposed to be determined primarily by the properties of the gaseous species. It is further assumed that the various transport coefficients such as thermal conductivity, diffusion coefficients, specific heat at constant temperature, etc. and the latent heat of vaporization of the liquid droplets can be satisfactorily specified by representative constant values. It is assumed that the velocity of propagation of the flame is much less than the velocity of sound so that dynamic compressibility effects in the mixture can be neglected. Thus, the density becomes only a function of the temperature through the gas law. Equation (2) is the energy conservation equation written in terms of temperature. Note the source/sink terms on the right hand side corresponding to (a) heat release by chemical reaction (second term), (b) volumetric heat loss (third term), and (c) heat loss due to absorption of heat by droplets for vaporization (fourth term). Equation (3) is the mass fraction conservation equation for the oxidiser. Equation (4) is the mass fraction conservation equation for fuel vapour, with the last term on the right hand side the source term for the production of fuel vapor by evaporating droplets. In order to model the spray of liquid fuel droplets the sectional approach was exploited and details can be found in Greenberg et al.\textsuperscript{40} In this method the “point-wise” size distribution of droplets in the spray is subdivided into a finite number of size sections, \( N_S \) say, each of which contains droplets of diameters that fall within a certain size bracket. By appropriate integration of Williams’ spray equation\textsuperscript{7} sectional mass conservation equations (equation (5)) can be rigorously derived for the droplets in each size section. The source terms on the right hand sides of equations (2), (4) and (5), represent the relevant contributions of the spray. As the droplets are small enough with a low Stokes number we have assumed that they are viewed from a far-field vantage point, i.e. their average velocity is equal to that of their host environment. This implies that, on the average, they adjust instantaneously to the expanding gas velocity. In addition, the temperature of the droplets is taken as equal to that of the surroundings; essentially, the droplets’ heat-up time is small when compared with the characteristic time associated with their motion. Here, use of these latter two assumptions is made mainly for mathematical tractability, but also in order reduce some of the physical clutter to allow us to focus on the main mechanisms at play. The use of the Heaviside function, \( H \), in equation (5) implies that appreciable evaporation of the fuel droplets only commences when the local temperature reaches a prescribed value, \( T_v \), say the liquid fuels boiling temperature. Although any appropriately deemed temperature, such as the wet-bulb temperature, could have been chosen to characterize the onset of evaporation, the liquid fuel’s boiling temperature was taken for convenience. Typically, the effect on the results is quantitative rather than qualitative (see, for example, Greenberg\textsuperscript{41}).

Simplification of the governing equations can be achieved by using the following definitions of a stream function:

\[ \rho = \frac{\partial X}{\partial x}; \quad -\rho u = \frac{\partial X}{\partial t} \]  

(8)

and

\[ x = \int_0^X \left( \frac{\rho_e}{\rho} \right)^{1/2} \, dX \]  

(9)
whence, after normalization (see Appendix 1), the following set of equations results:

\[
\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} + \gamma y_F y_O \exp \left( -\frac{\beta}{\theta} \right) - \alpha(\theta - 1) - \bar{S}_v
\]

(10)

\[
\frac{\partial y_O}{\partial t} = \frac{1}{L_{eO}} \frac{\partial^2 y_O}{\partial x^2} - \frac{\gamma}{\partial O} y_F y_O \exp \left( -\frac{\beta}{\theta} \right)
\]

(11)

\[
\frac{\partial y_F}{\partial t} = \frac{1}{L_{eF}} \frac{\partial^2 y_F}{\partial x^2} - \frac{\gamma}{\partial F} y_O y_F \exp \left( -\frac{\beta}{\theta} \right) + \bar{S}_v
\]

(12)

\[
\frac{\partial y_{d,j}}{\partial t} = -\bar{S}_{v,j}, j = 1, 2, 3 \ldots N_s
\]

(13)

The initial and boundary conditions are:

\[
\frac{\partial \theta}{\partial x} (x = 0, t) = -H(\mu - t), \quad \theta(x \to \infty, t) = 1, \quad \theta(x, t = 0) = 1
\]

(14)

\[
\frac{\partial y_O}{\partial x} (x = 0, t) = 0, \quad y_O(x \to \infty, t) = 1, \quad y_O(x, t = 0) = 1
\]

(15)

\[
\frac{\partial y_F}{\partial x} (x = 0, t) = 0, \quad y_F(x \to \infty, t) = 1 - \delta, \quad y_F(x, t = 0) = 1 - \delta
\]

(16)

\[
y_{d,j}(x, t = 0) = \delta_j, j = 1, 2, 3 \ldots N_s
\]

(17)

The first of the conditions in equation (14) describes the application of the constant energy flux for a period of time \(\mu\). The second condition relates to the value of the normalized temperature far from the left boundary, and the third condition is the initial constant temperature throughout the entire region. The first conditions in equations (15) and (16) define the impermeability of the boundary at \(x = 0\) to mass transfer of oxidizer and fuel vapor, whereas the other conditions represent the normalized mass fractions at infinity and the initial constant values they assume. Finally, equation (17) describes the initial normalized mass fractions of liquid fuel in the different size sections of the droplets, throughout the region. Note that the parameter \(\gamma\) in equations (10) to (12) is known as the Damköhler number for chemical reaction.

\[\gamma = \frac{\gamma_0 e^{-x^2} \exp \left( \frac{\theta}{\theta_c} \right)}{y_F y_O} \]

(19)

where \(\theta_c > 1\) is the critical value of the temperature at which the chemical reactions become sufficiently significant to be non-negligible in equations (10) to (12). Since \(\gamma \to 0\) the Damköhler number can be defined in terms of \(\epsilon\) in the following way:

\[\epsilon = \theta_c^2 / \beta\]

(18)

The former breaks down the entire ignition process evolution into the following stages: (1) inert stage, (2) transition stage, (3) ignition stage, (4) “explosion” stage, and (5) propagation stage.

### Inert stage

We consider the initial scenario in which chemical reaction is completely negligible so that the chemical source/sink terms in equations (10) to (12) can be neglected. This is known as the chemically inert region. The following small parameter can be identified\(^{43}\)

\[\epsilon = \theta_c^2 / \beta\]

(18)

The solution of the governing equations during the chemically inert period is readily derived and, for the liquid fuel’s sectional mass fractions, is found to be:

\[y_{d,j}(x, t) = \sum_{i \neq j} \delta_j \left[ 1 - \exp \left( -\Delta_i \left( t - t_e(x) \right) \right) \right] H \left( t - t_e(x) \right), j = 1, 2, 3 \ldots N_s\]

(20)

with

\[\bar{\Omega}_{j,i} = \begin{cases} \delta_j & j = i \\ \frac{\Omega_{j+1,i}}{\Delta_j - \Delta_i} & j \neq i \end{cases} \]

(21)

where \(t_e(x)\) is the time it takes the temperature at a location \(x\) to reach the liquid fuels boiling temperature \(\theta_c\).

### 3. Solution

In order to solve this problem we extend the single-phase approach of Kapila\(^{42}\) and Olmstead.\(^{43}\)
For the temperature, we obtain:

\[
\theta(x, t) = 1 + \exp[-\alpha(\mu - t)] \left[ 2\sqrt{\frac{\mu - t}{\pi}} \exp \left( -\frac{x^2}{4(\mu - t)} \right) \right] H(\mu - t) + \tilde{L} \left[ \sum_{j=1}^{N} N_j \Omega_{j,j} \exp(-\alpha(t - t_v(x))) \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \exp(-\alpha(t - t_v(x))) \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \exp(-\alpha(t - t_v(x))) \right] - \frac{\Delta_i(t - t_v(x))}{\alpha - \Delta_i}
\]

(22)

The solution for the oxygen mass fraction is:

\[
y_O = 1
\]

(23)

and the solution for the fuel vapor mass fraction is:

\[
y_F(x, t) = 1 - \delta + \left[ \sum_{j=1}^{N} N_j \Omega_{j,j} \frac{1 - \exp(-\Delta_i(t - t_v(x)))}{\alpha - \Delta_i} \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \frac{1 - \exp(-\Delta_i(t - t_v(x)))}{\alpha - \Delta_i} \right]
\]

(24)

Using these solutions at \( x = 0 \) we can estimate the critical values of the variables at which the chemical reaction starts to become significant.

Thus,

\[
\theta_c = \theta_c(0, t_e) = 1 + \exp[-\alpha(\mu - t_e)] \left[ 2\sqrt{\frac{\mu - t_e}{\pi}} \exp \left( -\frac{x^2}{4(\mu - t_e)} \right) \right] H(\mu - t_e) + \tilde{L} \left[ \sum_{j=1}^{N} N_j \Omega_{j,j} \exp(-\alpha(t_e - t_v(0))) \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \exp(-\alpha(t_e - t_v(0))) \right] - \frac{\Delta_i(t_e - t_v(0))}{\alpha - \Delta_i}
\]

(25)

\[
y_{O,c} = 1 - \delta + \left[ \sum_{j=1}^{N} N_j \Omega_{j,j} \frac{1 - \exp(-\Delta_i(t_e - t_v(0)))}{\alpha - \Delta_i} \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \frac{1 - \exp(-\Delta_i(t_e - t_v(0)))}{\alpha - \Delta_i} \right]
\]

(26)

\[
y_{F,c} = y_F(0, t_e) = 1 - \delta + \left[ \sum_{j=1}^{N} N_j \Omega_{j,j} \frac{1 - \exp(-\Delta_i(t_e - t_v(0)))}{\alpha - \Delta_i} \right] - \left[ \sum_{j=1}^{N} \sum_{i=j+1}^{N} \Omega_{j,i} \frac{1 - \exp(-\Delta_i(t_e - t_v(0)))}{\alpha - \Delta_i} \right]
\]

(27)

Further (nonessential) simplification can be achieved by noting that, in general, \( t_v(0) \ll t_e \). Now, the chemical Damköhler number \( \gamma \) is known in terms of given parameters. Hence, by substituting from equations (25) to (27) into equation (19), the critical reference time for cessation of the inert induction stage can be extracted from the implicit equation that is obtained. Once this time is known, it can be resubstituted into equations (25) to (27) to obtain the critical reference temperature and mass fractions of the oxidizer and fuel vapor. It is emphasized that this is only the first stage of the entire ignition history.
Transition stage

The next stage of the solution development involves examining the $O(\varepsilon)$ inner solution in which chemical reaction begins to occur. We make use of the stretched coordinates in the vicinity of $x = 0$, $t = t_c$:

$$x = v\xi, \quad t = t_c + \alpha \tau, \quad \xi > 0, \quad \tau > -\frac{t_c}{\alpha} \rightarrow -\infty$$

(28)

see Figure 2 for a schematic representation.

The usual asymptotic procedure is adopted and use is made of the expansions:

$$\theta = \theta_c + \varepsilon a_0 \tau + b_0 \xi + \varphi_0(\xi, \tau) + \varepsilon^{3/2} \varphi_1(\xi, \tau) + \varepsilon^2 \varphi_2(\xi, \tau) + \ldots$$

$$y_0 = y_{0c} + \varepsilon (a_{00} \tau + b_{00} \xi + r_0(\xi, \tau)) + \varepsilon^{3/2} r_1(\xi, \tau) + \varepsilon^2 r_2(\xi, \tau) + \ldots$$

$$y_F = y_{Fc} + \varepsilon (a_{F0} \tau + b_{F0} \xi + z_0(\xi, \tau)) + \varepsilon^{3/2} z_1(\xi, \tau) + \varepsilon^2 z_2(\xi, \tau) + \ldots$$

(29a,b,c)

Following Kapila,42 by substituting the expansions in the governing equations (and taking the leading order) an (approximate) expression is found for the time associated with this transition stage (for details of the analysis see Appendix 2); that is, the time characterizing the onset of appreciable chemical reaction:

$$t_{transition} = t_c + \alpha \tau = t_c + \frac{\theta^2}{\beta} \tau = t_c + \frac{\theta^2}{\beta} \left[ a_0 - \frac{1}{a_0} \ln \left( \frac{\eta^* m}{-b_0 \sqrt{a_0}} \right) \right]$$

(30)

where parameters featuring on the right hand side are given by

$$m = y_F y_{0c}$$

(31)

$$a_0 = \frac{\partial \theta(0, t_c)}{\partial \tau} = \frac{\exp[-\omega(\mu - t_c)](1 - 2\alpha(\mu - t_c))H((\mu - t_c))}{\sqrt{\pi((\mu - t_c))}} +$$

$$\frac{\sum_{i=1}^N \sum_{j=1}^N \Delta_i \Omega_{ij} \exp(-\omega(\mu - t_c(0))) + \Delta_i \exp(-\Delta_i(\mu - t_c(0)))}{\alpha - \Delta_i}$$

(32)

$$b_0 = \frac{\partial \theta(0, t_c)}{\partial \xi} = -\exp[-\omega(\mu - t_c)] -$$

$$\frac{\sum_{i=1}^N \sum_{j=1}^N \Delta_i \Omega_{ij} \exp(-\omega(\mu - t_c(0))) + \Delta_i \exp(-\Delta_i(\mu - t_c(0)))}{\alpha - \Delta_i}$$

(33)

and $\eta^* \approx -0.431.$42 Thus, during the period $t_c \leq t \leq t_c + \alpha \tau$ the expression for the temperature is given by:

$$\theta(x, t_c + \alpha \tau) = \theta_{mer}(x, t_c) + ef_0(\tau) + O(\varepsilon^{3/2})$$

(34a)

where $f_0(\tau)$ (see Appendix 2, equation (64a)) can be expressed as:

$$f_0(\tau) = -\frac{1}{2} \ln(-\tau) - \left[ \eta^* + \ln \left( \frac{2\sqrt{a_0}}{\pi} \right) \right] + \ldots$$

(34b)

The influence of the spray presence on the ignition time is clearly noticeable via the parameters $a_0, b_0$ as well as implicitly through $\theta_c$ (equation (25)) and $y_F$ (equation (27)). We mention that during the transition stage the temperature is high, but not enough to ignite the mixture.
with

\[
A_0 = \frac{b_0 \exp(\eta^*) \sqrt{a_0}}{m}
\]  

(38b)

By solving equation (36) numerically we can find the time ignition takes place. The numerical solution should provide us with the time where \( U_1(0, t) \) is unbounded. Once again, the spray contribution is readily noted via the parameters \( a_0, b_0 \).

Thus, the expression for time at the end of the ignition stage is:

\[
t_{\text{ignition}} = t_c + \epsilon^2 \hat{T}_\infty
\]  

(39)

where \( \hat{T}_\infty = -7.2198 \) is constant and does not depend on spray-related parameters as the numerical solution was solved at the \( O(\epsilon^2) \) time scale. However, it does depend on the volumetric heat loss parameter. The temperature at the end of this stage is:

\[
\theta(x, t) = \theta(x, t_c + \epsilon^2 \hat{T}_\infty) = \theta_{\text{inert}}(x, t_c + \epsilon^2 \hat{T}_\infty) + \varphi + O(\epsilon^3/2)
\]  

(40)

where \( \varphi \) is expressed in terms of \( U_1 \) from equation (38a). The period for this stage is \( t_c + \epsilon \tau \leq t \leq t_c + \epsilon^2 \hat{T}_\infty \).

**“Explosion” stage**

This stage is characterized by a fast rise in temperature that leads to “explosion” (ignition). Since all the thermal energy is extracted from chemical reaction (minus the heat loss due to droplet evaporation) during this stage the temperature is readily calculated:

\[
\theta_{\text{explosion}} = 1 + \frac{q m_{Q_\alpha}(m_{d_h} + m_{F_\alpha})}{C_p T_0} - \frac{L(m_{d_h} + m_{F_\alpha})}{C_p T_0}
\]  

(41)

This fast increase in temperature takes place on an exponentially short time scale:

\[
\sigma = -\ln(\sqrt{\epsilon} A_0 p)
\]  

(42)

where \( A_0 \) is given in equation (38b), and \( p \to 0 \). Thus, the time period for the “explosion” stage is:

\( t_c + \epsilon^2 \hat{T}_\infty \leq t \leq t_c + \epsilon^2 \hat{T}_\infty + \sigma \).

**Propagation stage**

At this stage, a moderate detachment from the heated wall (at \( x = 0 \)) begins, which leads to eventual steady state flame propagation.
According to Kapila\(^42\) the time until the propagation stage of a single phase gaseous flame is:

\[
l_{\text{propagation}} = t_c + e^2 \bar{T}_\infty + \sigma + \frac{\delta_1}{\bar{c}_0} r, \quad r = O(1) \tag{43}
\]

where

\[
\delta_1 = \sqrt{\frac{\kappa}{A_0}} \exp \left[ \frac{\bar{c}_e}{\bar{e}_0} \left( \frac{1}{1 + \kappa} - 1 \right) \right], \quad \bar{c}_1 = \left( \frac{1 + \kappa}{\bar{c}_0} \right)^\frac{1}{2} \tag{44a,b}
\]

\[
\kappa = \frac{q m_{Ou}(m_{du} + m_{Fu})}{C_p T_0} - \frac{L(m_{du} + m_{Fu})}{C_p T_0} \tag{44c}
\]

In addition,

\[
x_0^2 = \frac{e^{3/2}}{\bar{c}_0} \exp \left[ -\frac{z_0}{\bar{c}_e} \right], \quad 0 < z_0 < \frac{\kappa \theta_c}{\theta_c + \kappa} \tag{45a}
\]

and the flame velocity is determined from:

\[
dx_0/dr = \frac{\bar{c}_1}{\delta_1} U(r), \quad U(r) = \sqrt{2/\kappa} \tag{45c}
\]

Exactly the same analysis is echoed here, but with implicit and explicit terms reflecting the spray’s presence (such as in equation (44a,b) and equation (44c), respectively) leading to appropriate modifications. Moreover, validation of the velocity of propagation for the current case was achieved by setting the volumetric heat loss coefficient to zero and comparing to the expression developed by Weinberg and Greenberg\(^44\) for the laminar spray flame velocity:

\[
S_L = \frac{RT \sqrt{2D TRa}}{E} \exp \left( -\frac{E}{2RT} - \frac{L(m_{du} + m_{Fu})}{qm_{Ou}} \cdot \frac{E}{2RT} \right) \tag{46}
\]

The propagation stage is the last stage in the evolution of the flame that is to be considered here, and, as was observed, the role of the polydisperse spray of droplets in the flame history exhibits itself through apt adjustment of the single gas-phase flame theory.\(^42,43\)

### 4. Results and discussion

In this section, we present results based on the mathematical and numerical analysis. The data used for the calculations was as follows (unless otherwise specified): \(q = 1.279 \times 10^7 \text{ J/kg, } L = 0.04Q, \ A = 10^{10} \text{ S}^{-1}, \ E = 2 \times 10^6 \text{ J/kmol, } c_p = 1255.92 \text{ J/kgK, } T_\infty = 300 \text{ K, } T_0 = 400 \text{ K.} \) The chemical kinetic scheme employed concerns the burning of n-decane. Relevant thermochemical data can be found in literature.\(^45,46\) By specifying the initial fraction of liquid fuel in the total fuel (vapor + liquid) in the fresh mixture, \(\sum_{j=1}^{N_s} \delta_j/(m_{Fu} + m_{du}) = \delta, \) it can be shown that the mass fractions in the fresh mixture are given by the following expressions:

\[
(m_{Ou}, m_{du}, m_{Fu}) = \left( \frac{s - 1 - m_{du} - m_{Fu}}{s \delta}, \delta, \frac{m_{du} (1 - \delta)}{1 + \gamma_{OF}/\Phi} \right) \tag{47}
\]

unless \(\delta = 0, \) for which

\[
m_{Fu} = \frac{s}{(s + \gamma_{OF}/\Phi)} \tag{48}
\]

where \(s \) is the mole fraction of oxygen in the fresh mixture, \(\gamma_{OF} \) is the stoichiometric coefficient and \(\Phi \) is the equivalence ratio. Here, \(\Phi = 1 \) and \(\gamma_{OF} = 3. \) Since this work focuses on the effect of spray polydispersity on the ignition process, the volumetric heat loss coefficient is set equal to zero here.

We consider three initial polydisperse distributions listed in Table 1. The Sauter mean diameter is frequently used in combustion situations. Here we examine this proposition by considering three quite different initial droplet size distributions having a single common SMD. Distribution 1 is initially monosectional. Distribution 2 is initially bi-disperse with smaller droplets occupying size section three and larger droplets size section 9. Finally, distribution 3 has droplets spread out throughout the entire size range. This latter distribution is probably closer to reality. All three initial distributions have a common SMD of 44.8 \(\mu m.\)

Before elaborating on the way in which the initial spray polydispersity influences spray flame ignition it will be informative to follow the evolution of the initial spray distributions of Table 1 at an arbitrary fixed point in space. In Figures 3 to 5 we exhibit the evolution with time of \(y_{ij} \) (see equation (13)) for distributions 1, 2 and 3 respectively.

For all three distributions, the build-up of droplets in adjacent lower sections is readily visible as the droplets in higher sections evaporate and become ineligible for membership in those sections. Hence, for initial distribution 1 (see Figure 3), as droplets become smaller in size section 6, that they initially occupied, there is a...
build-up of the sectional mass fraction in section 5. This process repeats itself as movement to the left of the size distribution occurs due to droplet evaporation over time.

In Figure 4, for the bi-modal distribution 2, the rapid evaporation of the small droplets in the lower sections is clear whilst for the larger droplets, that initially occupied section 9, the evaporation process and subsequent transfer to lower size-sections is slower. Finally, in Figure 5 the gradual evaporation of the droplets in all the size-sections is observed. Of course, accompanying the different internal spray structure evolution plotted in these three figures is the different way in which fuel vapor is released and builds-up, with subsequent impact on the ignition behavior of the resulting spray flames, as we will now discuss.

**Mono-sectional results**

The initially mono-sectional droplet size distribution provides a useful reference, before scrutinizing the more complex influence of initially polydisperse distributions on spray ignition. Hence, the first results we discuss are only for Distribution 1.

We begin by presenting the profiles of temperature – $\theta(x)$, fuel vapor mass fraction – $y_f(x)$, oxygen mass fraction – $y_O(x)$ and reaction rate in Figure 6. Consider first the temperature profiles versus the spatial coordinate for various times. At the initial times, there is a moderate rise in the temperature until $\sim 4$ ms, followed by very fast rise in temperature (thermal runaway) next to the hot wall (at $x = 0$). At $\sim 5$ ms we can notice a propagating flame. Thus, we can deduce that

| Section number | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|----------------|---|---|---|---|---|---|---|---|---|
| Section diameters | 1–5 | 5–10 | 10–20 | 20–30 | 30–40 | 40–50 | 50–70 | 70–90 | 90–110 |
| Distribution 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| Distribution 2 | 0 | 0 | 0.207 | 0 | 0 | 0 | 0 | 0 | 0.793 |
| Distribution 3 | 0.0005 | 0.0005 | 0.0141 | 0.0793 | 0.1662 | 0.2464 | 0.2349 | 0.1547 | 0.1034 |

**Table 1.** The sectional diameters $d_i(\mu m)$ and initial droplet size distributions for examining the influence of different initial droplet size distributions having a common Sauter mean diameter, $D_{32}$, on polydisperse spray flame ignition.
ignition takes place in the range of 4–5 ms. (A more exact ignition time will be found from the detailed profile of temperature versus time at the layer adjacent to the hot wall \((x = 0)\). This scenario is reflected in other profiles. For instance, in the reaction rate profile we can see that till \(~4\) ms there is no appreciable reaction rate, whereas at 5 ms the reaction rate is already non-negligible and the peak of the reaction rate is located inside the domain indicating propagation of the flame from the hot wall inwards.

Additional insight into the picture described before can be deduced from the fuel vapor profile. In the early stages (until \(~4\) ms) there is fuel vapor build-up, due to liquid fuel evaporation, until there is enough fuel vapor to create an appreciable reaction rate. The fuel vapor build-up is high at the layer adjacent to the hot wall \((x = 0)\) and lower as we proceed into the domain. After ignition takes place the fuel vapor is consumed, and the peak of the fuel vapor profile is located within the domain.

Now, after ascertaining that an ignition event indeed takes place, we look at the evolution of the same profiles at \(x = 0\), see Figure 7. These profiles supply additional information to the profiles of Figure 6. For all profiles of Figure 7, we notice that the highest gradient occurs at \(\sim 4.26\) ms. For instance, the temperature profile shows that at earlier times there is a moderate rise. However, when approaching a critical temperature at around \(\theta \approx 5\) an ignition event takes place and thermal runaway happens. This phenomenon is reflected in a fast/sharp temperature rise, fast consumption of fuel vapor and oxygen mass fraction and the appreciable reaction rate clearly seen in Figure 7.

The precise time of the ignition event is obtained by post-processing means and exploits the largest gradient of the reactant mass fraction (in our case fuel vapor mass fraction) integral along \(x = 0\) at all times. In Figure 8, the temperature profile versus time at \(x = 0\) is presented, as in Figure 7. We indicate roughly the various anticipated stages of the development, and have now added a sign indicating the moment of ignition. As can be seen, this moment of ignition occurs just before approaching the complete depletion of the fuel vapor and maximum temperature peak.

It is also instructive to compare the actual times associated with each of the stages considered in the afore-given mathematical analysis. For the case considered here, they are listed in Table 2. Note that the inert stage over-predicts a critical value for \(t_c\). This due to the fact that the equations at this stage completely neglect any chemical activity (hence, the appellation “inert stage”). Essentially, the analysis of this stage

![Figure 5. Internal spray structure evolution close to \(x = 0\) for initial spray size distribution 3.](image)

![Figure 6. Profiles of temperature (top left), fuel vapor mass fraction (top right), oxygen mass fraction (bottom left), reaction rate (bottom right) versus spatial coordinate for various times; initial spray size distribution 1.](image)
provides a very crude approximation for when chemical reaction of any sort is activated. Thus, it becomes patently clear that the value of $\tau$ relevant to the transition stage must be negative, compensating for the overshoot of the “inert stage”. Similarly, for the ignition stage which we have already compared in Figure 8, and the subsequent stages. A comparison between these analytically predicted time values at each stage (other than that of the ignition) and those of the numerical solution of the governing equations is not viable. This is because the numerical solution accounts for all terms in the relevant equations at all times, including the chemical reaction terms. However, these are omitted from the mathematical analysis at the inert stage and

**Table 2.** Actual time values associated with each of the five stages of the mathematical analysis of polydisperse spray flame ignition.

| Stage      | Relevant time | Numerical values of analytical solution at the end of each stage (ms) |
|------------|---------------|-------------------------------------------------------------------|
| Inert      | $t_c$         | 4.7                                                               |
| Transition | $t_c + \kappa T$ | 4.13                                                             |
| Ignition   | $t_c + \kappa^2 T$ | **4.22 (4.26 in numerical solution)** |
| Explosion  | $t_c + \kappa^2 T + \sigma$ | 4.81                                                             |
| Propagation| $t_c + \kappa^2 T + \sigma + \frac{\kappa}{\kappa_1} \tau$ | 4.97                                                             |

**Figure 7.** Profiles of temperature (top left), fuel vapor mass fraction (top right), oxygen mass fraction (bottom left), reaction rate (bottom right) versus time at $x = 0$; initial spray size distribution 1.

**Figure 8.** Temperature profile versus time at $x = 0$. The cross sign indicates the ignition time of the system; initial spray size distribution 1.
partially at the transition stage (see Appendix 2), and are asymptotically estimated at the other stages. Notwithstanding this fact, the analytical and numerical predictions for the entire process provide good agreement, and, in particular, for the moment of ignition.

Use of a full numerical solution enables us to compare with analytical results obtained from the asymptotic analysis described above. The comparison will be performed in terms of the critical heat energy flux needed to be applied at the hot wall layer in order to have a successful ignition event. One of the important parameters in spray combustion is the evaporation coefficient which indicates how fast fuel vapor is produced. Thus, we present critical heat energy flux versus evaporation coefficient for both the numerical and analytical solutions. First of all, it can be clearly seen in Figure 9 that as the evaporation coefficient increases the critical heat energy heat flux for ignition decreases as the evaporation produces sufficient amount of fuel vapor to initiate chemical reaction and subsequently lead to successful ignition event. For a given value of the evaporation coefficient, application of a heat energy flux above the curves will ensure ignition, whereas use of a value below the critical curve will lead to a failed ignition event. Comparing the numerical and analytical solutions it is found that the difference between them is around 5% at most, which validates the asymptotic analysis presented in this work.

Results for initially polydisperse distributions

We now turn to the effect of the initial spray polydispersity on flame ignition. In Figure 10 we present a comparison between the computed and the analytical predictions of the critical heat flux energy for different pulse periods. First, we notice that there is good agreement between the numerical and analytical predictions. The region of operating conditions for which ignition occurs increases as the pulse of heat flux energy increases. This occurs irrespective of the initial spray polydispersity, and is due to the fact that the longer the pulse the more fuel vapor is supplied which mixes with the oxidant and supplies an ignitable combustible mixture. The shorter the pulse the more difficult it becomes to ignite the mixture. It is in this regime that the differences between the initial spray polydispersity come to the fore, although for the conditions used here they are rather minor. For longer pulses, differences induced by the initial spray polydispersity are negligible.

In Figure 11 the temperature evolution at $x = 0$ is drawn, for specific operating conditions for all three initial polydisperse spray distributions. The profiles are more or less the same until about 1.3 ms. At this point it appears that some ignition process is initiated but the temperature increase and subsequent development are noticeably different. The first and third distributions qualitatively follow one another fairly closely for $t > 1.3$, with the highest temperature attained when the first spray distribution is used. A lower temperature is attained when size distribution 2 is utilized, presumably because of the larger droplets in size sections 7, 8 and 9 for which evaporation is slower. The black broken line indicates the flame temperature and it is readily observable that spray distributions 1 and 3 do provide conditions for ignition, in contrast to distribution 2, which fails to do so. We attribute this to the bulk of large droplets in the latter bi-size distribution, which do not evaporate rapidly enough to provide sufficient vapor for ignition to occur. Indeed, Figure 11 strongly indicates how sensitive the successful or failed ignition can be to the initial spray polydispersity.

In Figure 12 the curves in the $x$-$t$ plane are drawn for all three distributions and conditions as per Figure 11. Of course, the flame velocities can be derived

![Figure 9](image-url)

**Figure 9.** Critical heat energy flux ($P_{cr}$) versus evaporation coefficient ($E_v$) for both numerical and analytical solutions.
from these curves. The initial stage until possible thermal runaway shows a zero velocity as conditions of fuel vapor build up and temperature develop. Subsequently, the usual nonlinear flame velocity behavior can be seen, as the flame is in its initial embryonic stage. Subsequently, both spray distributions 1 and 3 enable ignition and flame propagation to occur so that the gradients of the two relevant curves become constant, indicating a constant burning velocity. The burning velocity of the flame from distribution 1 is greater than that from distribution 3, due to the higher mass fraction of fuel vapor available at ignition in the former case (not shown here), making the reaction more energetic. On the other hand, the curve for initial spray distribution 2 indicates a slight early attempted embryonic stage, which aborts as ignition cannot be attained, with the “flame” velocity dropping accordingly to zero. Once again, this illustrates how delicately the success or failure of ignition depends on the initial spray polydispersity.

Finally, in Figure 13 we show the critical heat energy flux ($P_{\text{crit}}$) as a function of the initial equivalence ratio. The similarities between results for distributions 1 and 3 echo that previously observed in Figures 11 and 12. Also, generally speaking, the higher critical ratio required for ignition by distribution 2 reflects the difficulty attaining ignition due to insufficient fuel vapor being available because of the presence of almost 80%...
of the liquid fuel in larger droplets (see Table 1). This effect is reduced as the initial mixture becomes richer, so that more fuel vapor becomes available for ignition and any heat loss effect due to droplet evaporation is less focused (see also Kats and Greenberg36). In any event, the qualitative shape of the curves and the existence of minimum ignition energy (MIE) type of behavior (see literature5,6) bear some resemblance to independent experimental evidence,11 albeit for monodisperse sprays, thereby providing some encouragement for the correctness of the theory, within the limits of its basic assumptions.

5. Conclusions

A new mathematical analysis of the thermal ignition of a polydisperse spray/air mixture by an infinite heated surface having a pulsed heat energy flux was presented. The primary aim was to track the entire history of the ignition process, starting from the flame embryo progenitor stage, through the thermal runaway stage to the final flame propagation stage. The polydisperse spray was modeled using the sectional approach. Good agreement was found between the theoretical predictions and full numerical simulations for all cases studied. The critical heat energy flux for ignition was determined as a function of the liquid fuel’s evaporation coefficient. Comparison between the critical energy flux and the initial spray polydispersity revealed small differences for larger values of the pulse duration but more significant minor differences for smaller pulse durations. Despite these seemingly minor differences, it was shown that the initial spray polydispersity can have a critical influence on whether flame ignition will occur or fail, even for sprays having the same initial SMD. In addition, good quantitative agreement was found...
between the theoretical predictions and independent experimental evidence of a minimum ignition energy.

It is acknowledged that the actual nature of spray ignition in realistic combustion systems is stochastic (see, for example, literature\textsuperscript{10,21}) and not deterministic. Nevertheless, it seems that the current theory, within the bounds implied by its underlying assumptions such that inter-droplet inhomogeneities are not resolved, can shed light on certain processes occurring during spray flame ignition if the appropriate spatial scale is considered. Although our formulation does account for the realistic possibility of volumetric heating, its’ effect was neglected in the Results section since our main emphasis was to examine the effect of spray polydispersity on the ignition process. We hope to dedicate a future study to this issue. Finally, we note that only a single pulse of ignition process. We hope to dedicate a future study to this issue. Finally, we note that only a single pulse of heat flux was considered in the current work. Multiple pulses are often applied in practical combustion engines and a parametric detailed study of the sensitivity of polydisperse spray ignition to a series of thermal pulses is ongoing.

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References
1. Neophytou A. Spark ignition and flame propagation in sprays. PhD thesis, Cambridge University, 2011.
2. Williams FA. Combustion theory: the fundamental theory of chemically reacting flow systems. 2nd ed. Menlo Park, CA: Benjamin/Cummings Publishing Company, Inc., 1985.
3. Glassman I, Yetter RA and Glumac NG. Combustion. Cambridge, MA: Academic Press, 2014.
4. Zeldovich IA, Barenblatt GI, Librovich VB, et al. Mathematical theory of combustion and explosions. New York, NY: Consultants Bureau, 1985.
5. Subba Rao HN and Lefebvre AH. Ignition of kerosene fuel sprays in a flowing air stream. Combust Sci Technol 1973; 8: 95–100.
6. Rao KVL and Lefebvre AH. Minimum ignition energies in flowing kerosine-air mixtures. Combust Flame 1976; 27: 1–20.
7. Ballal DR and Lefebvre AH. Ignition and flame quenching of quiescent fuel mists. Proc Roy Soc Lond A 1978; 364: 277–294.
8. Ballal DR and Lefebvre AH. Ignition and flame quenching of flowing heterogeneous fuel-air mixtures. Combust Flame 1979; 35: 155–168.
9. Peters JE and Mellor AM. An ignition model for quiescent fuel sprays. Combust Flame 1980; 38: 65–74.
10. Ballal DR and Lefebvre AH. A general model of spark ignition for gaseous and liquid fuel-air mixtures. Proc Comb Symp 1981; 18: 1737–1746.
11. Danis AM. Spark ignition of monodisperse fuel sprays. PhD thesis, Drexel University, Philadelphia, PA, 1987.
12. Danis AM, Namer I and Cernansky NP. Droplet size and equivalence ratio effects on spark ignition of monodisperse n-heptane and methanol sprays. Combust Flame 1988; 74: 285–294.
13. Danis AM, Namer I and Cernansky NP. Fuel pre-vaporization effects on the minimum ignition energy of n-heptane spray/vapor mixtures, Technical Report, American Society of Mechanical Engineers, New York, NY, 1987.
14. Dietrich DL, Cernansky NP, Danis AM, et al. Model for the ignition of a monodisperse fuel spray. Combust Sci Technol 1991; 79: 325–339.
15. Aggarwal SK. Single droplet ignition: theoretical analyses and experimental findings. Prog Energy Combust Sci 2014; 45: 79–107.
16. Greenberg JB. Propagation and extinction of an unsteady spherical spray flame front. Combust Theory Model 2003; 7: 163–174.
17. Greenberg JB, McIntosh AC and Brindley J. Linear stability analysis of laminar premixed spray flames. Proc R Soc Lond A 2001; 457: 1–31.
18. Aggarwal SK. A review of spray ignition phenomena: present status and future research. Prog Energy Combust Sci 1998; 24: 565–600.
19. Mastorakos E. Ignition of turbulent non-premixed flames. Prog Energy Combust Sci 2009; 35: 57–97.
20. Mastorakos E. Forced ignition of turbulent spray flames. Proc Combust Inst 2017; 36: 2367–2383.
21. de Oliveira PM. Ignition and propagation mechanism of spray flames. PhD thesis, Cambridge University, 2019.
22. de Oliveira PM, Allison PM and Mastorakos E. Ignition of uniform droplet-laden weakly turbulent flows following a laser spark. Combust Flame 2019; 199: 387–400.
23. de Oliveira PM and Mastorakos E. Mechanisms of flame propagation in jet fuel sprays as revealed by OH/fuel planar laser-induced fluorescence and OH* chemiluminescence. Combust Flame 2019; 206: 308–321.
24. de Oliveira PM, Sitte MP and Mastorakos E. Polydispersity effects in low-order ignition modeling of jet fuel sprays. Combust Sci Technol 2019. https://doi.org/10.1080/00102202.2019.1678918
25. Neophytou A and Mastorakos E. Simulations of laminar flame propagation in droplet mists. Combust Flame 2009; 156: 1627–1640.
26. Neophytou A, Mastorakos E and Cant RS. Complex chemistry simulations of spark ignition in turbulent sprays. Proc Combust Inst 2011; 33: 2135–2142.
27. Wacks DH and Chakraborty N. Flame structure and propagation in turbulent flame-droplet interaction: a direct numerical simulation analysis. Flow Turbul Combust 2016; 96: 1053–1081.
28. Wacks DH and Chakraborty N. Flow topology and alignments of scalar gradients and vorticity in turbulent spray flames: a direct numerical simulation analysis. Fuel 2016; 184: 922–1081.

29. Wacks DH, Malkes SP and Chakraborty N. Statistical behavior of fuel mass fraction variance transport in turbulent flame-droplet interaction: a direct numerical simulation analysis. Numer Heat Trans Part A Appl 2016; 70: 1087–1110.

30. Goldfarb I, Goldshtein V, Kuzmenko G, et al. On thermal explosion of a cool spray in a hot gas. Proc Combust Inst 1998; 27: 2367–2374.

31. Goldfarb I, Gol’dshtein V, Greenberg JB, et al. Thermal explosion in a droplet-gas cloud. Combust Theory Model 2000; 4: 289–316.

32. Bykov V, Goldfarb I, Gol’dshtein V, et al. Thermal explosion in a hot gas mixture with fuel droplets: a two reactant model. Combust Theory Model 2002; 6: 339–359.

33. Bykov V, Goldfarb I, Gol’dshtein V, et al. Auto-ignition of a polydisperse fuel spray. Proc Combust Inst 2007; 31: 2257–2264.

34. Sazhina EM, Sazhin SS, Heikal MR, et al. A detailed modelling of the spray ignition process in diesel engines. Combust Sci Technol 2000; 160: 317–344.

35. Han W and Chen Z. Effects of finite-rate droplet evaporation on the ignition and propagation of premixed spherical spray flame. Combust Flame 2015; 162: 2128–2139.

36. Kats G and Greenberg JB. Forced thermal ignition of a polydisperse fuel spray. Combust Sci Technol 2018; 190: 849–877.

37. Kats G and Greenberg JB. An improved model for investigating the effect of spray polydispersity on laminar premixed spray flame ignition. Atomic Spr 2020; 30: 895–911.

38. Aggarwal SK and Sirignano WA. Ignition of fuel sprays: deterministic calculations for idealized droplet arrays. Proc Combust Inst 1985; 20: 1773–1780.

39. Kats G and Greenberg JB. Analysis of the ignition of a combustible fuel spray-oxidant mixture. In: AIAA Science and Technology Forum and Exposition, 7-11 January, San Diego, USA, 2016, AIAA Paper 2016-1209.

40. Greenberg JB, Silverman I and Tambour Y. On the origins of spray sectional conservation equations. Combust Flame 1993; 93: 90–96.

41. Greenberg JB. Finite rate evaporation and droplet drag effects in spherical flame front propagation through a liquid fuel mist. Combust Flame 2007; 148: 187–197.

42. Kapila AK. Evolution of deflagration in a cold combustible subjected to a uniform energy flux. Int J Eng Sci 1981; 19: 495–509.

43. Olmstead WE. Ignition of a combustible half space. SIAM Appl Math 1983; 43: 1–15.

44. Weinberg N and Greenberg JB. Linear stability analysis of laminar premixed fuel-rich double-spray flames. Int J Spray Combust Dyn 2014; 6: 87–112.

45. Stull DR and Prophet H. JANAF thermochemical tables. 2nd ed. NSRDS-NBS 37. Washington, DC: U.S. Department of Commerce, National Bureau of Standards, 1971.

46. Vargaftik NB. Tables on the thermophysical properties of liquids and gases. 2nd ed. Hoboken: John Wiley and Sons, 1975.

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### Appendix

#### Notation

- $a_0, b_0$ constants $[-]$  
- $A$ pre-exponential constant $[s^{-1}]$  
- $c_p$ specific heat $[J/kg K^{-1}]$  
- $D_T$ thermal diffusion coefficient $[m^2 s^{-1}]$  
- $D_O$ oxygen mass diffusion coefficient $[m^2 s^{-1}]$  
- $E$ activation energy $[Joules mol^{-1}]$  
- $f_0, f_1, f_2, \varphi_0, \varphi_1, \Psi_0$ related functions to inner zone temperature $[-]$  
- $g_0, g_1, g_2, r_0, r_1, R_0$ related functions to inner zone oxygen mass fraction $[-]$  
- $H$ Heaviside function  
- $L, L$ dimensional and non-dimensional latent heat of vaporization $[Joules kg^{-1}]; [-]$  
- $\text{Le}$ Lewis number $[-]$  
- $m_{Fu}$ initial mass fraction of gaseous fuel $[-]$  
- $m_{Ou}$ initial mass fraction of gaseous oxygen $[-]$  
- $m_{lu}$ initial mass fraction of liquid fuel $[-]$  
- $P$ heat energy flux $[Joules s^{-1} m^{-2}]$  
- $q$ heat of reaction $[Joules kg^{-1}]$  
- $R$ universal gas constant $[Joules K^{-1} mol^{-1}]$  
- $S$ related functions to inner zone gaseous fuel mass fraction $[-]$  
- $S_r$ mole fraction of oxygen in the fresh mixture $[-]$  
- $s_0, s_1, s_2, z_0, z_1, Z_0$ total rate of droplet evaporation $[s^{-1}]$  
- $S_r$ dimensional and non-dimensional time $[s]; [-]$  
- $T, \theta$ dimensional and non-dimensional temperature $[K]; [-]$  
- $x, x'$, $X$ dimensional and non-dimensional spatial coordinate $[m]; [-]; [-]$  
- $Y, y$ dimensional and non-dimensional mass fraction  
- $\hat{x}, x$ radiative heat loss coefficients $[m^3 K Joules^{-1} s^{-1}], [s^{-1}]$  
- $\alpha_{OF}$ stoichiometric coefficient $[-]$  
- $\beta = E/RT_0$ constant $[-]$  
- $\delta$ initial ratio of mass fraction of liquid fuel to total fuel $[-]$  
- $\Delta_j, \Psi_j, \hat{\Delta}_j, \Psi_j$ dimensional and non-dimensional vaporization Damkohler numbers  
- $\epsilon$ small parameter $[-]$
\[ \Phi \text{ equivalence ratio } [-] \]
\[ \gamma \text{ non-dimensional Damköhler number } [-] \]
\[ \eta^* = -0.434 \text{ constant} \]
\[ \lambda \text{ thermal conductivity } [\text{J K}^{-1} \text{m}^{-1} \text{s}^{-1}] \]
\[ \mu \text{ pulse duration } [\text{s}] \]
\[ \rho \text{ density } [\text{kg m}^{-3}] \]
\[ \tau \text{ non-dimensional temporal coordinate stretching variable } [-] \]
\[ \xi \text{ non-dimensional spatial coordinate stretching variable } [-] \]
\[ \vartheta \text{ heat release parameter } [-] \]
\[ \omega \text{ reaction rate } [\text{s}^{-1}] \]

**Appendix 1**

In this appendix we give details of the analysis of the transition stage that makes use of substituting the expansions in equation (29a,b,c) in the governing equations and taking the leading order. We obtain

\[ \frac{\partial^2 \varphi_0(\xi, \tau)}{\partial \xi^2} = 0 \quad \xi > 0, \quad \tau > -\infty \quad (49) \]

subject to:

\[ \frac{\partial \varphi_0}{\partial \xi} (\xi = 0, \tau) = 0, \quad \varphi_0(\xi, \tau \rightarrow -\infty) = 0 \quad (52) \]

\[ \frac{\partial \xi}{\partial \xi} (\xi = 0, \tau) = 0, \quad \xi_0(\xi, \tau \rightarrow -\infty) = 0 \quad (53) \]

\[ \frac{\partial}{\partial \xi} (\xi = 0, \tau) = 0, \quad \xi_0(\xi, \tau \rightarrow -\infty) = 0 \quad (54) \]

It is not hard to show that the solutions of equations (49) to (51) are:

\[ \begin{cases} 
\varphi_0(\xi, \tau) = f_0(\tau), & f_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = g_0(\tau), & g_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = s_0(\tau), & s_0(\tau \rightarrow -\infty) = 0 
\end{cases} \quad (55a,b,c) \]

where the functions \( f_0, g_0 \) and \( s_0 \) will be found later.

In order to continue it is necessary to consider the governing equations to \( O(\varepsilon^{3/2}) \). They are found to be:

\[ \frac{\partial^2 \Psi_1(\xi, \tau)}{\partial \xi^2} = -\gamma_0 \exp[a_0 \tau + b_0 \xi + \varphi_0] \quad \xi > 0, \quad \tau > -\infty \quad (56a) \]

subject to

\[ \begin{cases} 
\varphi_0(\xi, \tau) = f_0(\tau), & f_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = g_0(\tau), & g_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = s_0(\tau), & s_0(\tau \rightarrow -\infty) = 0 
\end{cases} \quad (55a,b,c) \]

\[ \frac{\partial^2 \xi_1(\xi, \tau)}{\partial \xi^2} = \frac{Le_0 \gamma_0}{\partial \xi} \exp[a_0 \tau + b_0 \xi + \varphi_0] \quad \xi > 0, \quad \tau > -\infty \quad (56b) \]

subject to

\[ \begin{cases} 
\varphi_0(\xi, \tau) = f_0(\tau), & f_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = g_0(\tau), & g_0(\tau \rightarrow -\infty) = 0 \\
\xi_0(\xi, \tau) = s_0(\tau), & s_0(\tau \rightarrow -\infty) = 0 
\end{cases} \quad (55a,b,c) \]
\[ \frac{\partial \sigma_1}{\partial \xi} (\xi = 0, \tau) = 0, \quad \varphi_1(\xi, \tau \to -\infty) = 0 \] (57a)

\[ \frac{\partial z_1}{\partial \xi} (\xi = 0, \tau) = 0, \quad z_1(\xi, \tau \to -\infty) = 0 \] (57b)

\[ \frac{\partial r_1}{\partial \xi} (\xi = 0, \tau) = 0, \quad r_1(\xi, \tau \to -\infty) = 0 \] (57c)

Note that the exponential in equations (56a) to (56c) is rooted in the Arrhenius term for the global chemical reaction we have assumed. The solution of these equations is given by:

\[ \varphi_1(\xi, \tau) = \frac{\gamma_0}{b_0} \exp[a_0 \tau + f_0(\tau)] \left[ -\xi + \frac{\exp(b_0 \xi)}{b_0} \right] + f_2(\tau), \quad f_2(-\infty) = 0 \] (58a)

\[ z_1(\xi, \tau) = \frac{LeF\gamma_0}{b_0} \exp[a_0 \tau + f_0(\tau)] \left[ -\xi + \frac{\exp(b_0 \xi)}{b_0} \right] + g_2(\tau), \quad g_2(\tau \to -\infty) = 0 \] (58b)

\[ r_1(\xi, \tau) = \frac{LeF\gamma_0}{b_0} \exp[a_0 \tau + f_0(\tau)] \left[ -\xi + \frac{\exp(b_0 \xi)}{b_0} \right] + s_2(\tau), \quad s_2(\tau \to -\infty) = 0 \] (58c)

These solutions are not sufficient to close the problem completely. For closure additional terms of \( O(e^{1/2}) \), such that \( O(1) \gg O(e^{1/2}) \gg O(e) \) applies, are required. To achieve this, further coordinate stretching is necessary via:

\[ x = e^{1/2}X, \quad X > 0 \quad (\xi = e^{-1/2}X \Rightarrow \xi \equiv e^{1/2}X) \] (59)

The time coordinate remains unchanged. In terms of the new coordinate the expansions for the dependent variables assume the form:

\[ \theta = \theta_c + b_0 e^{1/2}X + \alpha \psi_0(X, \tau) + \ldots \] (60a)

\[ y_F = y_F + b_0 e^{1/2}X + e Z_0(X, \tau) + \ldots \] (60b)

\[ y_o = y_o + b_0 e^{1/2}X + e R_0(X, \tau) + \ldots \] (60c)

Substituting them into the governing equations one finds that the leading \( O(e) \) they become:

\[ \frac{\partial \psi_0(X, \tau)}{\partial \tau} = \frac{1}{LeF} \frac{\partial^2 \psi_0(X, \tau)}{\partial X^2} \] (61a)

\[ \frac{\partial Z_0(X, \tau)}{\partial \tau} = 1 \frac{\partial^2 Z_0(X, \tau)}{LeF \partial X^2} \] (61b)

subject to

\[ \psi_0(X \to \infty, \tau) = 0; \quad \psi_0(X, \tau \to -\infty) = 0 \quad X > 0, \quad \tau \to -\infty \] (62a)

\[ Z_0(X \to \infty, \tau) = 0; \quad Z_0(X, \tau \to -\infty) = 0 \] (62b)

\[ R_0(X \to \infty, \tau) = 0; \quad R_0(X, \tau \to -\infty) = 0 \] (62c)

The missing condition for closure at this order is found by matching at \( X = 0 \) between the two regions of \( O(e), O(e^{1/2}) \). After much tedious algebra the solutions are extracted

\[ \psi_0(X, \tau) = -\frac{\gamma_0}{b_0} \int_{-\infty}^\tau \frac{\exp\left(-\frac{X^2}{4(\tau - \sigma)} + a_0 \sigma + f_0(\sigma)\right)}{\sqrt{\pi}(\tau - \sigma)} \, d\sigma \] (63a)

\[ Z_0(X, \tau) = \sqrt{LeF} \frac{\gamma_0}{b_0} \int_{-\infty}^\tau \frac{\exp\left(-\frac{X^2}{4(\tau - \sigma)} + a_0 \sigma + f_0(\sigma)\right)}{\sqrt{\pi}(\tau - \sigma)} \, d\sigma \] (63b)

\[ R_0(X, \tau) = \sqrt{LeF} \frac{\gamma_0}{b_0} \int_{-\infty}^\tau \frac{\exp\left(-\frac{X^2}{4(\tau - \sigma)} + a_0 \sigma + f_0(\sigma)\right)}{\sqrt{\pi}(\tau - \sigma)} \, d\sigma \] (63c)

where

\[ f_0(\tau) = -\frac{\gamma_0}{b_0} \int_{-\infty}^\tau \frac{\exp(a_0 \sigma + f_0(\sigma))}{\sqrt{\pi}(\tau - \sigma)} \, d\sigma \] (64a)

\[ g_0(\tau) = -\sqrt{LeF} \frac{\partial}{\partial F} f_0(\tau) \] (64b)

\[ s_0(\tau) = -\sqrt{LeF} \frac{\partial}{\partial \sigma} f_0(\tau) \] (64c)

\( f_0(\tau) \) is determined via numerical solution of equation (64a). Following [41,42] this is done by recasting the integral into a canonical form. The numerical evaluation leads to a value of \( \tau \) for which the integral becomes unbounded, thereby signifying the end of the transition stage. This, in turn, supplies the value of \( \eta^* \approx 0.431 \) mentioned in the text and the expressions in equations (30) and (34b).