

MODELING OF DIESEL SPRAY IGNITION

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Introduction

Understanding of preignition processes in mixing layers of fuel sprays is one of the prerequisites of further improvements in the combustion performance of diesel engines [1, 2]. The aim of the paper is to estimate the ignition location in the vicinity of fuel spray based on the approximate self-similar theory of the isothermal mixing layer, perturbation analysis, empirical data on ignition delay, and tracking trajectories of notional particles.

Modeling of Spray Mixing with Air

Consider a planar fuel spray injected at velocity u_1 into the combustion chamber filled with air of density ρ_2 , pressure p , and temperature T (Fig. 1). Considering the flow at section AB, adopt the following simplifying assumptions: (i) the duration of liquid disintegration is very short; (ii) the spray consists of fine fuel drops and its behavior is similar to the behavior of dense gas with the equivalent density $\rho_1 = \alpha_0 \rho_f + (1 - \alpha_0) \rho_2$, where α_0 is the fuel volume fraction at the spray symmetry plane and ρ_f is the fuel density; and (iii) turbulent mixing of the spray with air is isothermal. The set of equations governing fuel–air mixing then takes the form [3]:

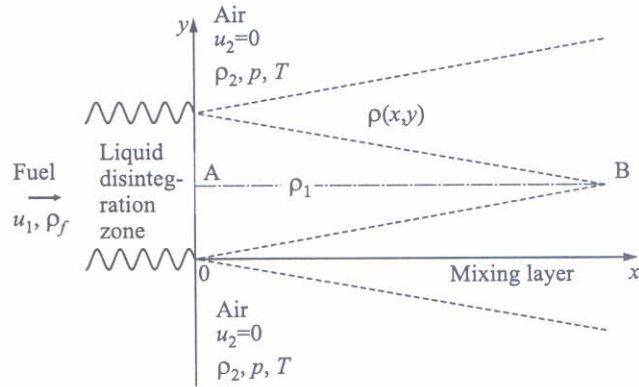


Figure 1 Schematic of the spray mixing layer

$$\begin{aligned}
 \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} &= 0 \\
 \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} &= l^2 \frac{\partial u}{\partial y} \frac{\partial}{\partial y} \left[\rho \frac{\partial u}{\partial y} \right] \\
 u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} &= l^2 \frac{\partial u}{\partial y} \frac{\partial^2 \rho}{\partial y^2}
 \end{aligned} \tag{1}$$

where x and y are the Cartesian coordinates (Fig. 1), u and v are the components of the velocity vector, ρ is the mixture density, $l = \sqrt{2}cx$ is the Tollmin's mixing length [4], and c is constant. Boundary conditions for Eqs. (1) are:

$$\begin{aligned}
 y = \infty : \quad \frac{\partial \rho u}{\partial y} &= 0, \quad \rho u = \rho_1 u_1, \quad \rho v = 0 \\
 y = -\infty : \quad \frac{\partial \rho u}{\partial y} &= 0, \quad \rho u = \rho_2 u_2
 \end{aligned}$$

The fact that variables ρu and ρv are constant at the edges of the mixing layer implies that the problem can have a self-similar solution. Introducing a dimensionless independent variable, $\varphi = y/(ax)$, dimensionless density $\chi(\varphi)$, and stream function $F(\varphi)$, such that

$$\rho = \rho_1 \chi(\varphi), \quad \rho u = \rho_1 u_1 F', \quad \rho v = \rho_1 u_1 a(\varphi F' - F)$$

where a is constant and prime denotes differentiation with respect to φ , one can arrive at the following ordinary differential equation for χ [3]:

$$\chi''' + \chi \ln \chi - \chi \ln(\chi_2) = 0 \quad (2)$$

with five boundary conditions:

$$\begin{aligned} \varphi = \varphi_1 : \quad \chi &= 1, & \chi' &= 0, & \chi'' &= \varphi_1 \ln \chi_2 \\ \varphi = \varphi_2 : \quad \chi &= \chi_2, & \chi' &= 0 \end{aligned}$$

Knowing χ , velocity components u and v can be determined as:

$$\begin{aligned} \frac{u}{u_1} &= \frac{F'}{\chi} = 1 - \frac{\ln \chi}{\ln \chi_2} \\ \frac{v}{u_1} &= \frac{\varphi F' - F}{\chi} = -\frac{\varphi \ln(\chi/\chi_2) + \chi''/\chi}{\ln \chi_2} \end{aligned} \quad (3)$$

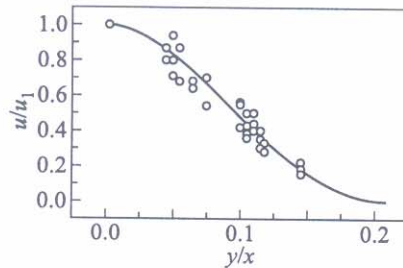


Figure 2 Comparison of predicted (curve) and measured (symbols, [5]) velocity profile in the diesel spray at distance $x = 20$ mm from the nozzle ($\varphi_1 = 0.95546$ and $\varphi_2 = -2.0235$)

the spray axis. The following values of air and fuel densities were used: $\rho_2 = 30 \text{ kg/m}^3$ and $\rho_f = 845 \text{ kg/m}^3$. Self-similar variable φ in Fig. 3 was determined based on the value $a = 0.07$ obtained from Fig. 2. In spite of the fact that experiments [5] dealt with cylindrical rather than planar sprays, the agreement of the results is encouraging. Clearly, at a

Equation (2) can be integrated numerically by the shooting technique. To determine the value of constant a entering the definition of φ , experimental data of [5] were used. Figure 2 shows the fit of the numerical solution of Eq. (2) with experimental data [5] obtained at $a = 0.07$.

Figure 3 shows the comparison of predicted (curves) and measured (symbols, [5]) profiles of fuel volume fraction $\alpha(\varphi) = (\chi - \chi_2)/(\rho_f/\rho_1 - \chi_2)$ in a diesel spray at 10, 20, and 30 mm from the nozzle along

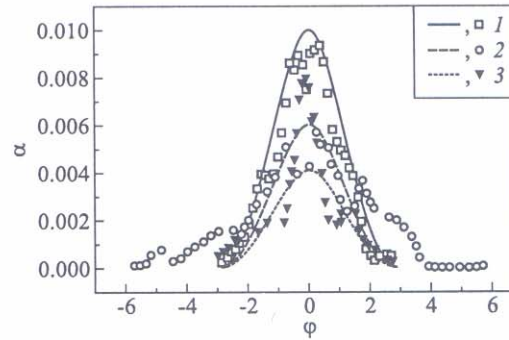


Figure 3 Comparison of predicted (curves) and measured (symbols, [5]) radial profiles of fuel volume fraction in a diesel spray at different distances from the nozzle: 1 — $x = 10$ mm, 2 — 20, and 3 — $x = 30$ mm

distance of 10 mm, the fuel volume fraction is only 0.01, indicating the validity of simplifying assumption (*i*). Moreover, partial fuel density, $\alpha\rho_f$, is much less than partial air density, $(1 - \alpha)\rho_2$, i.e.,

$$(1 - \alpha)\rho_2 \gg \alpha\rho_f \quad (4)$$

Ignition Location

In a diesel spray, fuel (or air) concentration varies due to both transport (convection and diffusion) processes and chemical transformation. Because Eqs. (1) do not take into account fuel evaporation, the diffusion equation for air density, $(1 - \alpha)\rho_2$, with an additional source term describing air consumption in chemical reactions should be used. In view of condition (4), this equation can be approximately replaced with the equation for the mixture density, ρ . Thus, instead of Eqs. (1), one has to solve the following set of equations:

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

$$\begin{aligned} \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} &= l^2 \frac{\partial u}{\partial y} \frac{\partial}{\partial y} \left[\rho \frac{\partial u}{\partial y} \right] \\ u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} &= l^2 \frac{\partial u}{\partial y} \frac{\partial^2 \rho}{\partial y^2} + S \end{aligned} \quad (5)$$

which differs from Eqs. (1) only by the nonzero source term, S . For simplicity, the chemical reaction in the mixing layer is taken of the zero order with $S = -k \exp(-E/(RT))$, where E is the activation energy, R is the gas constant, T is the temperature, and k is the preexponential function. Equations (5) are aimed at describing mixture evolution before ignition, therefore it is reasonable to assume that the preignition chemical processes develop at constant pressure.

To determine the ignition location, the solution of Eqs. (5) was compared with the solution of Eqs. (1). A certain normalized difference between the corresponding local densities was taken as the ignition criterion: Ignition was assumed to occur if the difference attained a predefined value, ε_0 . The natural definition of ε_0 follows from the definition of the preexplosion heating $\Delta T = RT^2/E$ [6], i.e., $\varepsilon_0 = \Delta T/T = RT/E$.

With the introduction of source term S , the problem loses self-similarity. Because ε_0 is usually quite small, assume that the fuel volume fraction in the reactive case, α' , can be expressed in terms of α and small parameter, $\varepsilon \leq \varepsilon_0$:

$$\alpha'(x, y) \approx \alpha(x, y)[1 - \varepsilon(x, y)] \quad (6)$$

Substituting Eq. (6) in Eqs. (5), one arrives at the following equation for ε :

$$\begin{aligned} u\alpha \frac{\partial \varepsilon}{\partial x} + v\alpha \frac{\partial \varepsilon}{\partial y} - l^2 \alpha \frac{\partial u}{\partial y} \frac{\partial^2 \varepsilon}{\partial y^2} \\ = 2l^2 \frac{\partial u}{\partial y} \left[\frac{\partial \alpha}{\partial y} \frac{\partial \varepsilon}{\partial y} \right] + \frac{S}{\rho_1 (\rho_f/\rho_1 - \chi_2)} \end{aligned} \quad (7)$$

As $\varepsilon \ll \alpha' \approx \alpha$, the left-hand side of Eq. (7) is negligibly small compared to the right-hand side (RHS), and one finally obtains the equation:

$$\frac{\partial \varepsilon}{\partial y} \approx \frac{S}{2l^2 \rho_1 (\rho_f/\rho_1 - \chi_2) (\partial u/\partial y \cdot \partial \alpha/\partial y)} \quad (8)$$

with the boundary condition: $\varepsilon = 0$ at $y = y_-$, where y_- is the lower boundary of the mixing layer (see Fig. 1). Note that RHS of Eq. (8) is the known function of x and y . Equation (8) can be integrated numerically:

$$\varepsilon = \frac{1}{2l^2\rho_1(\rho_f/\rho_1 - \chi_2)} \int_{y_-}^y \frac{S dy}{\partial u/\partial y \cdot \partial \alpha/\partial y} \quad (9)$$

and, due to the boundary condition, an arbitrary function of x arising in the course of the integration is zero.

Based on the solution of Eq. (9), one can plot the isoline, $\varepsilon = \varepsilon_0$, which will reflect possible ignition sites in the mixing layer. To specify ε_0 , the following procedure was used. On the one side, according to [6], ignition delay of the adiabatic thermal explosion governed by the zero-order reaction is given by:

$$\tau_i = \frac{c_p RT^2 \rho}{kQE} \exp\left(\frac{E}{RT}\right) \quad (10)$$

where c_p is the specific heat at constant pressure, Q is the heat effect of chemical reaction. On the other side, one can apply empirical relationships for the ignition delay like [2]:

$$\tau = Ap^{-n} \exp\left(\frac{E}{RT}\right) \quad (11)$$

where A is constant, p is pressure, and n is the constant exponent. Comparing Eqs. (10) and (11), one obtains

$$k = \frac{c_p RT^2 \rho}{AQE} p^n$$

For specific calculations, the empirical relationship obtained by one of the authors (R. Z. Kavtaradze) was used:

$$\tau = 0.55 \cdot 10^{-3} p^{-1.3} \exp\left(\frac{4400}{T}\right)$$

where τ is expressed in s, p in atm, and T in K. In the calculations, the following values of governing parameters were used: $\rho_2 = 30 \text{ kg/m}^3$,

$\rho_f = 845 \text{ kg/m}^3$, $E = 8800 \text{ cal/mol}$, $T = 900 \text{ K}$, $p = 40 \text{ atm}$, $u_1 = 100 \text{ m/s}$, $A = 0.55 \cdot 10^{-3}$, $n = -1.3$, $c_p = 1183 \text{ J/(kg}\cdot\text{K)}$, $Q = 2.65 \text{ MJ/kg}$, and $\varepsilon_0 = 0.05$. Note that the characteristic preexplosion heating at these values of the parameters is $\Delta T/T = RT/E \approx 0.05$ and corresponds with the ignition criterion $\varepsilon_0 = 0.05$.

The result of numerical integration of Eq. (9) is shown in Fig. 4 as a thick solid curve. The most prominent effect of chemical activity on the density field occurs at the boundaries of the mixing layer. This

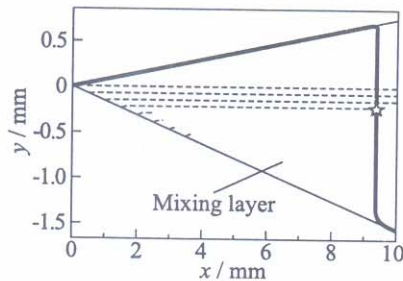


Figure 4 Predicted ignition location in a mixing layer of diesel spray. Thick solid curve corresponds to the isoline $\varepsilon = \varepsilon_0$. Thin solid lines show the predicted boundaries of the mixing layer. Thin dashed curves show the predicted trajectories of notional particles. Star denotes ignition location, where $t = \tau_i$ and $\varepsilon = \varepsilon_0$

is caused by the fact that derivatives $\partial u/\partial y$ and $\partial \alpha/\partial y$, tend to zero at the boundaries and the relative effect of the chemical source term is higher than the diffusion term in Eqs. (5). At cross-section $x \approx 9.3 \text{ mm}$, condition $\varepsilon = \varepsilon_0$ holds across the mixing layer. Ignition likely occurs in this cross-section, whereas it is hardly possible at the edges of the mixing layer due to excessively fuel-lean (low boundary in Fig. 4) or fuel-rich (upper boundary in Fig. 4) mixture.

Now, by tracing various particles entering the mixing layer, one can determine the ignition location. As a matter of fact, particle trajectories

can be readily plotted based on the known velocity field (see Eqs. (3)). For illustration purposes, Fig. 4 shows several such trajectories (dashed curves). There exists a trajectory that crosses curve $\varepsilon = \varepsilon_0$ at time $t = \tau_i = 0.638 \text{ ms}$ after entering the mixing layer. The point of intersection (denoted by a star) is the predicted ignition location. Clearly, ignition occurs in the depth of the mixing layer at a distance of about 9 mm from the nozzle. Such distances are usually observed in experiments [1, 2]. Predicted fuel volume fraction at the ignition location is 0.00204. As fuel evaporation is not taken into account explicitly, it is

impossible to indicate the gas-phase equivalence ratio at the ignition point.

Concluding Remarks

The mathematical model for the isothermal mixing layer of a diesel spray with air has been suggested. The model provides a satisfactory agreement with available experimental data in terms of the profiles of velocity and fuel volume fraction in the mixing layer. Supplementing the model with the chemical source term allows determining the ignition location in the mixing layer.

Acknowledgments

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