

Phenomenological Autoignition Model for Diesel Sprays Using Reduced Chemical Kinetics and a Characteristic Scalar Dissipation Rate

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ABSTRACT

This study focuses on the development of an autoignition model for diesel sprays that is applicable to phenomenological multi-zone combustion models. These models typically use a single-step Arrhenius expression to represent the low-temperature chemistry leading up to autoignition. There has been a substantial amount of work done in the area of n-heptane autoignition in homogeneous mixtures. Reduced kinetic mechanisms with ten reactions or less have been proposed in the literature to represent the complex low-temperature oxidation of n-heptane. These kinetic models are attractive for multi-zone simulations because of the low number of reactions involved. However, these kinetic mechanisms and the multi-zone treatment of the fuel spray do not account for the effect of turbulence/chemistry interactions on the chemical reaction rate. In this work a correlation has been developed for the total ignition delay time that is a combination of the homogenous ignition delay and dissipation effects. The homogeneous ignition delay is predicted from a chemical reaction mechanism for n-heptane, and the dissipation effects are captured through a phenomenological expression for a characteristic scalar dissipation rate. The characteristic scalar dissipation rate includes effects of injection pressure, ambient density, and injector hole size. The characteristic scalar dissipation rate is compared to a critical scalar dissipation rate to assess the additional delay due to turbulence/chemistry interactions. The autoignition model was implemented into a multi-zone spray model and validated against constant volume ignition delay measurements of diesel sprays.

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INTRODUCTION

The combustion process in a modern direct injection (DI) diesel engine is very complicated. It consists of fuel injection, break-up, mixing, vaporization, ignition, fuel oxidation, and pollutant formation/destruction. When attempting to simulate this process, which many engine manufacturers are doing today to develop their diesel engines in a timely, cost effective manner, the predictive capability of the models over a wide range of operating conditions is of critical importance.

There are wide range of phenomenological diesel combustion models that are used to predict the in-cylinder processes and ultimately the engine performance and emissions of DI diesel engines. There are zero-dimensional or single-zone models, such as the one proposed by Rezaei et al. [1], which uses empirical correlations for the spray penetration, fuel/air mixing, and premixed and diffusion controlled burn rates to predict the engine performance of a DI diesel engine. There are other zero-dimensional models that use stochastic reactors to estimate the fuel distribution in-cylinder using probability density functions. An example of this type of modeling approach is presented by Franken and Mauss [2]. Finally, there are multi-zone spray models which also use empirical formulations to describe the evolution of the

fuel spray, mixing, and combustion processes, but discretize the fuel spray into many zones, on the order of 10 to several hundred zones. In this study a multi-zone spray and combustion model was used as a framework to develop the proposed autoignition model. The important aspects of the multi-zone spray model will be reviewed in a subsequent section as it pertains to the proposed autoignition model.

Accurately predicting ignition delay of the diesel spray is of interest in all the aforementioned modeling approaches because of its direct impact on the intensity of the heat release immediately following autoignition, as well as its indirect effect on engine noise and pollutant emissions [3]. Autoignition in DI diesel engines occurs under essentially non-premixed conditions and is a considerably different phenomenon than homogeneous (premixed) autoignition, such as knock in a spark ignition engine [4]. During a diesel injection event, fuel and air mix rapidly, forming a wide range of local temperatures and equivalence ratios. Reflecting this variety of temperatures and concentrations, the chemical reaction rate is different in each local mixture. The ignition of a spray therefore emerges as an ensemble of ignition in these packets of the

heterogeneous mixture. To describe these phenomena, spray ignition models should account for the fact that mixing and chemical reactions progress simultaneously [5].

Multi-zone spray and combustion models, like the one used in this study, discretize the fuel spray into zones that are treated as well stirred reactors. Multi-zone models are typically developed to run on the order of minutes, for use in steady-state or transient cycle simulations. Subsequently, the transport of species between zones is not calculated considering the computational cost that would incur. Mixing between fuel zones is not considered, and the only constituent crossing the fuel zone's boundary is air from the surroundings. Therefore the chemistry taking place in the zones is entirely kinetically controlled, which typically results in very fast reaction rates. There are obviously inhomogeneities in the spray, and the fuel and oxidizer do not have enough time to mix down to the molecular level during the ignition delay period. Therefore, reaction rates could partially be controlled by mixing [6]. The objective of this work was to develop an autoignition model for diesel sprays that is tailored for multi-zone spray models that use phenomenological models to describe very simply the evolution of the fuel zones. The proposed autoignition model accounts for low-temperature chemical kinetics and the effect of mixing and turbulent dissipation on the chemical reaction rate.

MULTI-ZONE DIESEL SPRAY & COMBUSTION MODELING FRAMEWORK

Multi-zone diesel combustion models are designed to be a middle ground between the simplest zero-dimensional codes and the more complex multi-dimensional, Computational Fluid Dynamics (CFD) models. However, multi-zone models, while trying to save on computational time, can be lacking in their ability to capture the important physics taking place in the combustion chamber. A multi-zone diesel combustion model developed at Caterpillar Inc. will be the framework for developing the proposed autoignition model.

In multi-zone diesel combustion models, the fuel spray is discretized into zones (i.e. fuel zones) that are treated as open thermodynamic systems and the rest of the cylinder is a single zone, the air zone. There have been several multi-zone diesel models proposed over the years: Hiroyasu and Kodota's model was one of the earliest [7], the National Technical University of Athens has proposed a two-dimensional and three-dimensional model [8,9], and the University of Michigan has proposed a multi-zone model to be used in transient diesel engine cycle simulations [10].

Multi-zone models account for the spray evolution, air entrainment into the fuel zones, ignition, combustion, pollutant formation, and wall heat transfer. This is accomplished by applying the conservation of mass and energy to each zone and empirical sub-models to capture the complex physical and chemical processes taking place in each zone. Figure 2 illustrates the evolution of the fuel zones generated by the code and the assumed physical and chemical processes that they undergo.

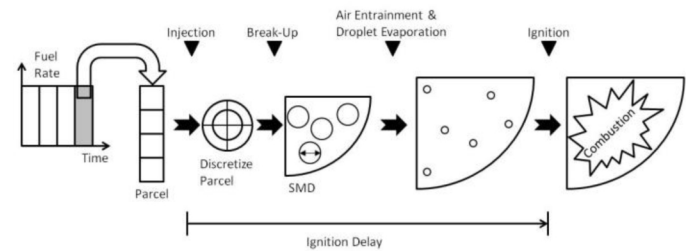


Figure 1. Evolution of fuel zones as modeled in the multi-zone framework.

Fuel is injected into the combustion chamber according to the fuel injection schedule, forming a parcel every crank angle that then moves in the spray axial direction (i.e. x-direction). As a fuel parcel is injected into the cylinder, it is subdivided into several zones in both the circumferential and radial direction as shown in Figure 1. As the injection proceeds, more zones are added in the axial direction (i.e. x-direction).

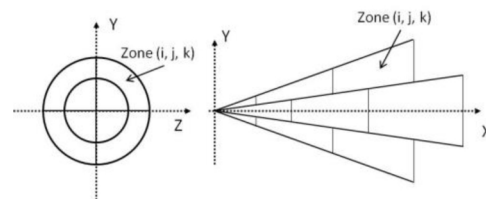


Figure 2. Illustration of fuel zone initialization, development and resulting penetration and dispersion.

The zones in each parcel are assumed to contain the same mass of fuel; however the amount of fuel in the zones within different parcels may vary according to the fuel injection schedule. Then, it is assumed that the fuel spray atomizes to fine droplets that nominally have a diameter equal to the Sauter Mean Diameter (SMD), which is empirically calculated. However, droplet sizes in different parcels may vary according to the cylinder conditions at the moment of injection. At the computed break-up time, the zones begin to entrain air according to a simplified conservation of momentum equation. Simultaneously the fuel droplets in the zone begin to evaporate and produce fuel vapor. The zones continue to evolve concurrently entraining air and evaporating fuel creating a wide range of equivalence ratios across all the zones. Once a zone's age has reached the empirically determined ignition time, all the premixed fuel in that zone is burned at an empirically calculated rate based on an Arrhenius form expression. Then, the mixing-controlled combustion takes over. All the while every zone is still entraining air, evaporating fuel, and creating pollutant emissions based on their respective empirical sub-models.

A few of the relevant sub-models in the currently used multi-zone framework will be discussed in the subsequent sections as they pertain to the proposed autoignition model. These sub-models will not be discussed in their entirety because they are not the focus of the current work and available in the literature. However, they will be introduced to provide an overview of their fidelity, as they make predictions that cascade as inputs to the proposed autoignition model.

Spray Penetration, Dispersion, and Breakup

Multi-zone models depend on empirical correlations to describe spray penetration and air entrainment into fuel zones over time. Therefore the fidelity of the spray penetration model is crucial for accuracy. The multi-zone model used in this work follows the work of Assanis and Jung [10], for which the spray penetration expressions were extended from Hiroyasu and Arai [11] for a general discharge coefficient. Before the liquid sheet breaks up, when $t < t_{break}$, the liquid penetration is linear with time.

$$S_{axial} = C_d \left(\frac{2\Delta P}{\rho_f} \right)^{0.5} t \quad (1)$$

where C_d is the discharge coefficient of the injector nozzle, ΔP is the pressure difference across the injector nozzle, ρ_f is the liquid fuel density, and t is time. After breakup, when $t > t_{break}$, the penetration rate of the spray has a square root dependence with time.

$$S_{axial} = 2.95 \left(\frac{\Delta P}{\rho_a} \right)^{0.25} (d_n t)^{0.5} \quad (2)$$

In the above correlations, S_{axial} is the spray penetration down the axis of the jet (x-direction), t is the current simulation time, d_n is the diameter of the fuel injector nozzle, and ρ_a is the density of the medium into which the fuel jet is being sprayed, in this case the air zone. To account for the increased drag at the periphery of the spray and its effect on spray penetration, an empirical correlation factor was applied.

$$S_r(r_i) = z S_r(r_i) \quad (3)$$

$$z = e^{-v_{min} * \left(\frac{\alpha * \pi * r}{360 * r_{inj}} \right)^{v_{max}}} \quad (4)$$

Here, α is a function of the nozzle discharge coefficient, r is the radial location of the fuel zone in the spray, r_{inj} is the radius of the injector nozzle, and v is the array of fuel zone velocities.

Other aspects of the fuel spray model such as spray spreading angle, droplet breakup time, and initial droplet size follow the work of Assanis and Jung [10], which is all built on previous literature of empirical relationships for diesel spray evolution. For the sake of brevity, these relationships will not be reviewed here because they are not the main focus of the current work.

Air Entrainment into Fuel Zones

The air entrainment rate into a given zone is controlled by the conservation of momentum applied to that zone. The initial momentum of a fuel zone upon nozzle exit is equal to the momentum of the zone at any subsequent distance traveled. Assuming that the zone jet momentum is conserved (i.e. globally steady) the momentum at any point in time can be set equivalent to the initial fuel jet momentum.

$$m_f u_i = (m_f + m_a) \frac{ds}{dt} \quad (5)$$

where m_f is the mass of fuel in a given zone at the time of injection, u_i is the zone injection velocity, m_a is the mass of air in the zone at a given point in time, and ds/dt is the rate of change of the zone's penetration with respect to time (i.e., the zone's instantaneous velocity), which is determined from empirical correlations for spray penetration, s , shown earlier. Solving equation (5) for m_a and differentiating with respect to time yields

$$\frac{dm_a}{dt} = - \frac{m_f u_i \frac{d^2 s}{dt^2}}{\left(\frac{ds}{dt} \right)^2} \quad (6)$$

which can be solved numerically to give the transient evolution of the mass of air in each fuel zone.

Fuel Droplet Evaporation

Once the breakup time criteria has been satisfied, a distribution of droplet sizes exists in each fuel zone. The process of droplet vaporization involves a combination of mass and heat transfer, as illustrated in Figure 3 for a given droplet of fuel.

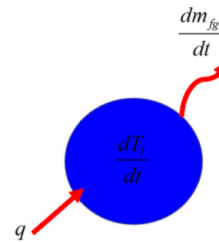


Figure 3. Liquid fuel droplet evaporation parameters.

In the current multi-zone model, the droplet evaporation process is modeled following the work of Borman and Johnson [12] and Gosman and Johns [13]. The rate of diffusion of fuel vapor away from the droplet is given as

$$\frac{dm_{fg}}{dt} = - \frac{dm_l}{dt} = \pi d_l N D_v Sh \frac{P}{R_u T_m} \ln \left(\frac{P}{P - P_{vs}} \right) \quad (7)$$

where m_{fg} is the mass of fuel vapour, m_l is the mass of liquid fuel in the droplet, d_l is the instantaneous droplet diameter, N is the number of droplets in a bin of the droplet size distribution predicted by the breakup model, D_v is the mass diffusivity, which is a property of the mixture, in this case fuel and air, Sh is the Sherwood number, P is the total pressure of the surrounding air, R_u is the universal gas constant, T_m is the mean temperature between the ambient and the droplet, and P_{vs} is the saturation pressure corresponding to the temperature of the droplet. Convective heat transfer from the hot gas to the liquid fuel droplets in a given zone is modelled following the methodology of Gosman and Johns [13]

$$q = \pi d_l N k_m (T_a - T_l) Nu \left(\frac{z}{e^z - 1} \right) \quad (8)$$

where k_m is the mean thermal conductivity, N_u is the Nusselt number, and z is a factor to correct for the effects of boundary layer thickening around the droplet due to mass transfer. Lastly, the resulting rate of liquid fuel temperature rise is given by the an energy balance as

$$\frac{dT_l}{dt} = \frac{1}{m_l C_{pl}} \left(q - \lambda \frac{dm_{fg}}{dt} \right) \quad (9)$$

where λ is the latent heat of vaporization of the liquid fuel, C_{pl} is the specific heat at constant pressure of the liquid fuel, and q is the convective heat transferred to the droplet, given by [equation \(8\)](#).

Fuel Zone Ignition Delay

The ignition delay is defined as the time interval between the start of injection of a fuel zone and its ignition, the point of significant chemical heat release. In single-zone and multi-zone models, the ignition delay is typically calculated with a single step Arrhenius expression. In some models, multi-step Arrhenius expressions have been used to capture the negative temperature coefficient regime of two-stage ignition fuels [14]. In the multi-zone model used in this work, the original ignition delay model was a single step model written as

$$ID = A \cdot P^{-n} \cdot \exp\left(\frac{E}{RT}\right) \quad (10)$$

where ID is ignition delay [ms], E/R is apparent activation temperature [K], P is the gas pressure [atm], T is gas temperature [K], and A and n are constants. The empirical constants of Watson et al. [15] are used, which are $A = 3.45$, $n = 1.02$, and $E/R = 2,100$ [K]. The multi-zone model evaluates the ignition delay in each of the fuel zones. In an engine the pressure and temperature change during the ignition delay period due to the compression resulting from piston motion. To account for the effect of changing conditions, the following empirical integral relation, known as the Livengood-Wu integral, is typically used to calculate the ignition delay time, t_{ign} [16].

$$\int_{t_{inj}}^{t_{ign}} \frac{dt}{ID(t)} \approx 1 \quad (11)$$

This empirical model for calculating the ignition delay of a spray has been shown to be successful, but only over a limited range of operating conditions and requires tuning. As stated earlier, the objective of this work was to develop a phenomenological autoignition model for diesel sprays that that can be used in a multi-zone framework, but captures to characteristics of the low temperature chemistry of the fuel and the effects of mixing and dissipation on the reaction rate (i.e., turbulence chemistry/interactions).

This completes the review of the multi-zone spray and combustion modeling framework used in the current work. There are additional sub-models, with varying levels of empiricism for the premixed combustion rate, the diffusion combustion rate, NOx formation, soot formation and oxidation, heat transfer, fuel zone/wall interactions, and zone thermodynamic coupling. However, due to the fact that these sub-models do not directly impact the proposed autoignition model they will not be discussed here. For a detailed overview of these models, refer to Dempsey [17].

FLAMELET COMBUSTION MODELING & SCALAR DISSIPATION RATE

The flamelet modeling approach is not simply an autoignition model, but instead is a concept for modeling the overall combustion process of non-premixed reacting flows. However, it is presented here briefly because some of the basic concepts and assumptions are used in the proposed autoignition model. The inherent concept behind flamelet modeling is that in non-premixed turbulent diffusion flames, like that of a DI diesel spray, a substantial fraction of the chemical reactions take place in thin layers that may locally be treated as laminar reaction sheets. It is assumed that the turbulent time and length scales are large compared to the chemical ones, so that the chemical reaction zone cannot be intruded by turbulent eddies. The diffusion flamelet can only be stretched by the turbulent movement and thus the chemical structure of the flame remains [18]. Essentially, the turbulent diffusion flame is being treated as an ensemble of one-dimensional laminar diffusion flamelets, with the spatial dimension being the mixture fraction Z , which is defined as

$$Z = \frac{m_{fuel}}{m_{fuel} + m_{oxidizer}} \quad (12)$$

It can be seen that the mixture fraction has limiting values of unity in the pure fuel stream and zero in the pure oxidizer stream. It should also be noted that Z is proportional to the mass fractions of the elements, and therefore is not affected by combustion but only by mixing. The mass and energy equations for the one-dimensional laminar flamelets are shown in [equations \(13\) and \(14\)](#), respectively.

$$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{w}_i \quad (13)$$

$$\rho \frac{\partial T}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} + \frac{1}{c_p} \frac{\partial P}{\partial t} - \sum_{i=1}^n \frac{h_i}{c_p} \dot{w}_i \quad (14)$$

In these equations Y_i is the mass fraction of species i , $\dot{w}_i$ is the production rate of species i determined from the chemical mechanism being used, and χ is scalar dissipation rate, which can be thought of as the rate of molecular mixing between the fuel and oxidizer. The chemical mechanism can be very simple or fully detailed chemistry of the fuel being used. The instantaneous scalar dissipation rate is defined as

$$\chi \equiv 2D \left(\frac{\partial Z}{\partial x} \right)^2 \quad (15)$$

where D is the diffusion coefficient of the mixture fraction and x is the one-dimensional spatial coordinate with its origin at the stoichiometric mixture fraction.

The scalar dissipation rate can be interpreted as the inverse of a characteristic diffusion time. It is the only direct coupling between the turbulent flow field and the chemistry in CFD based flamelet combustion models. It accounts for strain effects, flame stretch, and curvature induced by the turbulent fluctuations in the flow field and is therefore a critical parameter in flamelet modeling [18]. The local scalar dissipation rate is commonly modeled in CFD based flamelet codes following the work of Jones and Whitelaw [19].

$$\chi = C_\chi \frac{\varepsilon}{k} Z''^2 \quad (16)$$

where C_χ is an empirical constant with a value of 2.0, ε is the mean turbulent kinetic energy dissipation rate, k is the mean turbulent kinetic energy, and Z'' is the mean mixture fraction variance, all of which are calculated in the CFD model. This brief introduction to flamelet combustion modeling will be referenced as the framework for the proposed autoignition model is laid out.

PROPOSED AUTOIGNITION MODEL

In diesel engines, the autoignition process takes place on a time scale that is relatively long compared to the relevant fluid dynamic time scales. Therefore, the effects of convective and diffusive species and energy transport during the ignition delay period cannot be ignored [20]. These effects are not ignored in CFD simulations of reacting flows due to the convective, diffusive, and turbulent transport between computational cells. However, in the current multi-zone spray modelling framework, there is no transport between fuel zones, and thus the mixing impacts on the chemistry are ignored in each fuel zone.

The objective of this work was to develop an accurate and computationally efficient autoignition model for diesel sprays to be used in multi-zone engine simulations that captures the effects of mixing and dissipation on the ignition delay. The proposed model calculates the ignition delay as a coupling of the delay due to low-temperature chemical reactions and a characteristic scalar dissipation rate.

At the most fundamental level, ignition occurs when the rates of heat release due to low-temperature reactions are fast relative to the various loss mechanisms. The loss mechanisms are transport of thermal energy and reaction intermediates away from the reaction zone [21]. The influence of the scalar dissipation rate on a steady state diffusion flamelet is best illustrated by the well-known S-shaped curve, which is shown in Figure 4 [18]. Here the maximum temperature, T_{max} , is plotted against the inverse of the scalar dissipation rate at the stoichiometric mixture, χ_{st}^{-1} .

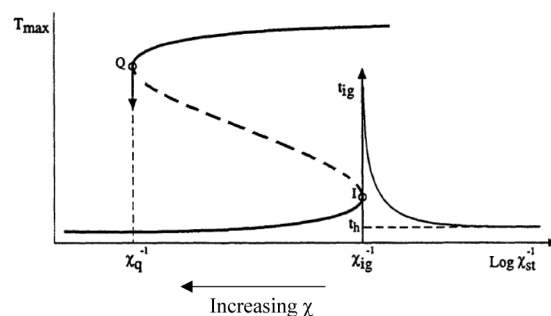


Figure 4. Maximum flamelet temperature as a function of the scalar dissipation rate at stoichiometric mixture fraction [18].

The upper branch of the curve represents burning flamelets. As the scalar dissipation rate is increased, the maximum flame temperature decreases due to diffusive heat losses. It continues to decrease until the heat release due to combustion cannot compensate for the diffusive heat losses, and the flamelet extinguishes at χ_q . The maximum temperature at point Q is that of the surrounding oxidizer.

The lower branch represents the unburnt, or not yet ignited state. Considering the temperature is relatively low here, and thereby the chemical reactions are slower, diffusive losses dominate over the production of radicals (i.e. intermediate species) and heat. If the scalar dissipation rate is decreased (moving to the right), the chemical production rate and diffusive losses balance at a higher temperature. At point I the chemical production rate can no longer be balanced by diffusive losses, and the flamelet ignites, jumping up on the upper portion of the curve. (Note, the dotted section of the curve represents an imaginary region where the flamelet never resides). Thus, the flamelet can only ignite if $\chi < \chi_{ig}$. The value of χ_{ig} depends only on the chemistry, or in other words is a function of the fuel, temperature, pressure, and mixture composition. It can be thought of as, how much strain can the unburnt fuel/air mixing layer withstand and still ignite.

Also illustrated in the inset of Figure 4 is how the ignition delay time is affected by the scalar dissipation rate. To illustrate, start at a point on the inset curve, as the scalar dissipation rate increases towards point I , the ignition delay asymptotes to infinity. On the other hand, if the scalar dissipation rate decreases away from point I , the ignition delay asymptotes to the homogenous ignition delay (i.e. a stagnant fully premixed mixture), denoted by the horizontal line, t_h [18]. This discussion shows that the autoignition in non-premixed systems is inhibited by the scalar dissipation rate (i.e. strain rate) in the mixing layer between fuel and oxidizer.

Thus, ignition in non-premixed systems cannot occur until the scalar dissipation rate is smaller than χ_{ig} . In DI diesel engines the scalar dissipation rate at the start of injection is typically significantly higher than χ_{ig} [4]. However, as the spray penetrates the combustion chamber, spreading axially and radially, the local scalar dissipation rate decreases due to lower local velocity gradients, eventually dropping below the critical scalar dissipation rate for autoignition, χ_{ig} .

To further illustrate the impact of dissipation on the ignition of non-premixed systems such as a diesel engine spray, Pitsch and Peters [4] used one-dimensional flamelets as outlined in the previous section. By solving equations (15) and (14) simultaneously, plots of

mixture temperature vs. mixture fraction can be generated at various instances in time. They did this at fixed thermodynamic conditions with a pressure of 40 bar, fuel temperature of 400 K, and an oxidizer temperature of 800 K. The results from their simulations are shown in Figure 5 [4].

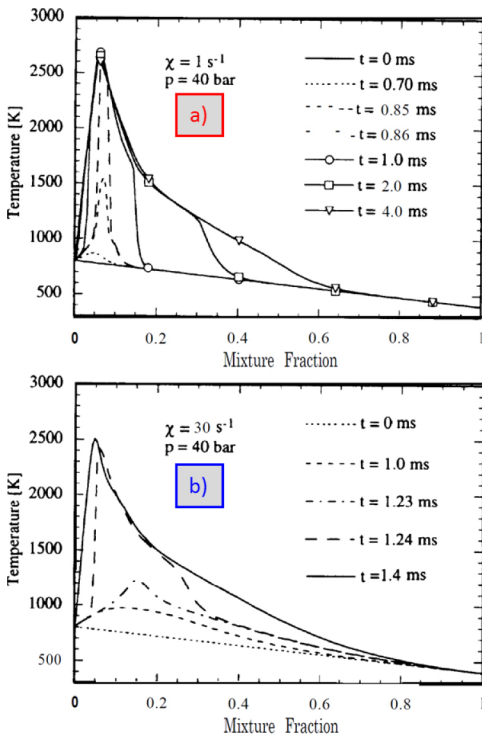


Figure 5. Temperature distributions across the mixture fraction space during the ignition process with fixed thermodynamic conditions, but for varying scalar dissipation rates of a) 1 s^{-1} and b) 30 s^{-1} [4].

As shown in Figure 5a, for a low scalar dissipation rate of 1 s^{-1} the temperature rise due to exothermic chemical reactions is limited to a thin region near the stoichiometric mixture fraction ($Z_{st} \approx 0.062$). The maximum temperature in this region is reached rapidly with ignition occurring at 0.86 ms. Then heat diffuses to the rich and lean sides igniting those mixtures. Steady state is not reached before 4 ms.

On the contrary, Figure 5b shows a very different picture at the same thermodynamic conditions and with the same fuel chemistry, but with a much higher scalar dissipation rate of 30 s^{-1} . In this case, heat is still generated at near the stoichiometric mixture fraction, but it is quickly carried away by diffusive transport to the rich and lean regions. Ignition does not occur until 1.23 ms, which is significantly later than the previous case due to high rates of dissipation despite being at the same thermodynamic conditions. Additionally, at the higher dissipation rate, ignition occurs on the rich side of stoichiometric. Steady state for this case is reached much faster at around 1.4 ms, also due to the high rate of diffusive transport.

Understanding that the total ignition delay tends to infinity for χ approaching χ_{ig} and it also tends to the homogeneous ignition delay for χ approaching zero, Pitsch and Peters [4] suggested an approximation formula for the ignition delay of non-premixed systems of the form

$$t_{ig}^t = t_{ig}^h + \frac{K}{\log\left(\frac{\chi_{ig}}{\chi_{st}}\right)} \quad (17)$$

where t_{ig}^t is the total ignition delay, t_{ig}^h is the homogeneous ignition delay due to low-temperature chemistry, χ_{st} is the scalar dissipation rate at stoichiometric mixture fraction, χ_{ig} is the critical or maximum scalar dissipation that is allowable for autoignition of the mixture at the current conditions, and K is a constant. The constant K is assumed to be a function of the fuel and independent of the oxidizer temperature and pressure. Pitsch and Peters recommend $K = 0.054 \text{ ms}$, recognizing however that studies at 40 and 50 bar do show a slight pressure dependence of K [4].

Equation (16), which is how the local value of the scalar dissipation rate is calculated in CFD based flamelet combustion models, shows that the scalar dissipation rate is determined by the turbulence levels and the mixture gradients. In multi-zone spray models, neither the instantaneous nor ensemble averaged turbulent flow field is resolved, and thus calculating the scalar dissipation rate in this same manner is not feasible.

Instead, in this work it is proposed that a characteristic (i.e. global) scalar dissipation rate be calculated to capture the effects of delaying ignition due to dissipative losses. In DI diesel engines, turbulence is essentially generated by the liquid injection and depends mainly on the injection velocity. Therefore, the scalar dissipation rate in a diesel spray can be interpreted as a measure of the injection velocity or injection pressure. In other words, a given spray jet has a single characteristic scalar dissipation rate associated with it. There are a large number of parameters that define an engine fuel spray, ranging from swirl ratio to length of the injector nozzle passage way. In order to derive an equation for a characteristic scalar dissipation rate, a dimensional analysis was done to create dimensional homogeneity with the scalar dissipation rate used in CFD flamelet models.

Experimental studies have shown that the time scale in a diesel spray upstream of the lift-off length is proportional to the square root of the ratio of fuel density to ambient density as shown by Naber and Siebers [22]

$$t^+ [s] = \frac{d_f \sqrt{\frac{\rho_f}{\rho_a}}}{a \tan\left(\frac{\Theta}{2}\right) U_f} \quad (18)$$

where a is a constant of 0.66 developed by Naber and Seibers [22], 9 is the spreading angle of the spray, ρ_f is the liquid fuel density, ρ_a is the ambient density, d_f is the effective area of the injector orifice, and U_f is the injection velocity at the exit of the injector orifice. Following the empirical correlation from Naber and Siebers, it was assumed in this work that the major parameters that define a unique diesel spray in terms of mixing and dissipative losses are: ambient density, fuel density, injection velocity, and injector nozzle (orifice) diameter. Thus, the characteristic scalar dissipation rate can be calculated as